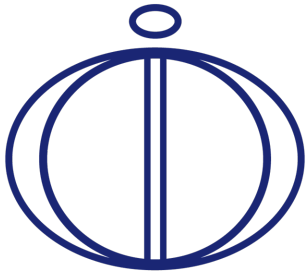
Diffusion Module (DICTRA) Documentation Set

Thermo-Calc Version 2021b



Thermo-Calc Software

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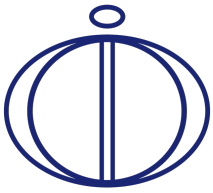
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The Diffusion Module (DICTRA) User Guide

Thermo-Calc Version 2021b



Thermo-Calc Software

Introduction to the Diffusion Module (DICTRA)

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About This Guide

This guide includes an overview of the program and describes in generic terms how you can define a system, set up and perform simulations, and then visualize the results. There is also a section to help you troubleshoot your simulation.

The guide is primarily for users already familiar with Thermo-Calc and for those who intend to use Console Mode. The Graphical Mode version is integrated into the Thermo-Calc desktop and its functionality is primarily described in the Thermo-Calc documentation.

Which Mode Should I Use?

The Diffusion Module (DICTRA) is available in both Graphical Mode and Console Mode, although Console Mode has a couple of more advanced features.

Before you start using this guide, it is recommended that you review the Thermo-Calc documentation and become familiar with using both modes. Also see Graphical Mode vs Console Mode to give you an overview of the differences. Understanding the capabilities of each mode will help you during the design of a simulation.



The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. This can be important to remember if you create a simulation in one mode and then decide to switch to the other mode.

What Do I Do Next?

How you proceed depends on your experience with the software as well as your level of expertise with diffusion simulations. In addition to this guide the following supplemental documentation and training resources can help you learn how to use the Diffusion Module (DICTRA).

Documentation Resources

You can search or browse all the documentation available either from within Thermo-Calc (press F1 or go to **Help → Online Help**) or browse the PDFs included with your installation by going to **Help → Manuals Folder**).



You can also download *The Role of Diffusion in Materials - a Tutorial*available from our website.

Training and Video Tutorials

Some of the Graphical Mode examples have video tutorials available both on our website or our YouTube channel. Watching those videos may help you with your simulation in Console Mode. You may also decide to enroll in a training course or if you have several people interested in on-site training.



Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.

About the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to Thermo-Calc. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulation calculations are both time- and space-dependent. The Diffusion Module (DICTRA) is available in both Graphical Mode (as the *Diffusion Calculator*) and Console Mode (as the *DICTRA module*).

The Diffusion Module (DICTRA), which is often just referred to as DICTRA, is ideally suited to solve diffusion simulations that include a moving boundary (*Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. Simulations are one-dimensional and three different geometries can be performed: planar, cylindrical, and spherical.

Examples of cases that have been simulated using the Diffusion Module (DICTRA) include:

- Microsegregation during solidification
- Homogenization of alloys
- Growth/dissolution of carbides, nitrides and intermetallic phases
- Coarsening of precipitate phases
- Interdiffusion in compounds, e.g. coating systems
- Austenite to ferrite transformations in steel
- Carburization, nitriding and carbonitriding of high-temperature alloys and steels
- Post weld heat treatment
- Sintering of cemented-carbides

In order to perform a simulation in the Diffusion Module, both a thermodynamic database and a kinetic database is needed. The thermodynamic database is a normal Thermo-Calc database, whereas the kinetic database contains information about the atomic mobility of individual elements in various phases.

Using the Diffusion Module (DICTRA) you can solve a variety of problems, some of which are described in Types of Diffusion Simulations.

An Important Note About Terminology

DICTRA is an acronym for *DIffusion-Controlled TRAnsformations*. The software of the same name has been included in the suite of Thermo-Calc products for many years. When you are working on Console Mode the terminology reflects this historical connection as do all the literature that cites the use of DICTRA.

With the introduction of the Graphical Mode version of DICTRA, and to better describe what the Add-on Module does, the product name is now the *Diffusion Module (DICTRA)*. However, this means some of the terminology between the modes cannot be consistent even though the theory and concept behind the software is fundamentally the same. For example, in Graphical Mode the term "DICTRA" is not used when describing the Diffusion Calculator node.

In Console Mode there is also some terminology to be aware of as there are two submodules within the program: the DICTRA_MONITOR: For running simulations of diffusion controlled transformations module and DIC_PARROT: Assesses experimental data and uses this data to optimize mobilities module.



In the documentation for Console Mode, *DICTRA* and *DICTRA module* are used interchangeably to refer to the DICTRA_MONITOR module.

Graphical Mode vs Console Mode

There are two interfaces available in Thermo-Calc: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface. Thermo-Calc and the Diffusion Module (DICTRA) are available in both modes, and the Precipitation Module (TC-PRISMA) and Process Metallurgy Module are only available in Graphical Mode.

If you are a new user, Graphical Mode is a good way to learn how to work with Thermo-Calc. Depending on what you want to simulate, Console Mode can have more functionality but until you are comfortable with the concepts, it is recommended you start in Graphical Mode.



In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a Wizard available to guide you through the process of defining the project.

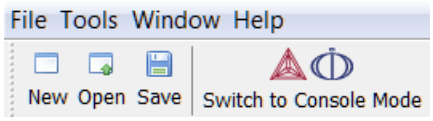


In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, ask you a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations and plotting the results.

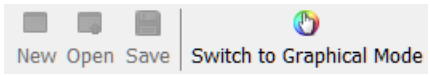
How to Switch Between Modes

The first time you open Thermo-Calc, it defaults to Graphical Mode. For any future instance it defaults to the last mode used.

Along the top of the GUI is the **GRAPHICAL MODE TOOLBAR** where you switch between modes.



In Console Mode, except for the **SWITCH TO GRAPHICAL MODE** button, the toolbar is not used.





See Menu, Toolbar and Keyboard Shortcuts for information about the **Tools**, **Window** and **Help** menus, which are available in both modes.

File Extensions

The file extensions are different based on the mode you are in (Graphical vs. Console). In Console Mode the extensions are also based on whether you are working with Thermo-Calc or the Diffusion Module (DICTRA).



In Graphical Mode, the Thermo-Calc project files have the extension *.`tcu`. This includes the examples for the add-on Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA).



In Console Mode, Thermo-Calc macro files have a *.`TCM` extension and the Diffusion Module (DICTRA) file extension is *.`DCM`. In addition to macro files in Console Mode the are also *Log* files and *Workspace* files, which also differ.

Modes Run Simultaneously

The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings. See Global Settings: Graphical and Console Mode Plotting.

Data Optimization and Thermodynamic / Kinetic Assessments



Although many calculations can be done in either mode, data optimization and thermodynamic or kinetic assessments are only available in Console Mode.

Key Differences Between Modes

Below are some of the main differences between the available features or simulation types in Graphical Mode (GM) and Console Mode (CM). There are also other differences not listed in the table such as slight differences between terminology and the file formats, for example.

Comparing Graphical Mode and Console Mode Features



For the Graphical Mode version of the Diffusion Module, additional functionality is scheduled for future versions of Thermo-Calc.

Feature or type of simulation	GM	CM	Comment
FEATURES			
Plots	x	x	
Planar, cylindrical and spherical geometries	x	x	
Homogenization	x	x	
Homogenization functions	x	x	The varieties with excluded phases are only available in Console Mode.
Tables	x	x	
Setting boundary conditions	x	x	For Graphical Mode, the Mixed activity and Zero Flux and Composition boundary conditions are available. Additional boundary conditions are planned.
Importing Scheil segregation profiles		x	
Data optimization (PARROT)		x	
SIMULATION TYPES			
Isothermal and Non-Isothermal simulations	x	x	
Growth of intermediate phases in compounds	x	x	

Feature or type of simulation	GM	CM	Comment
Growth or dissolution of precipitates	x	x	
Microsegregation during solidification	x	x	
Austenite to ferrite transformations	x	x	
Interdiffusion in compounds	x	x	
Coarsening		x	
Carburizing, and Nitriding and nitrocarburization	x	x	
Paraequilibrium		x	
Thermomigration		x	
Grain boundary models		x	
Pearlite models		x	
Interpolation scheme		x	
Cell calculations		x	

Diffusion Module (DICTRA) Licenses

You can start (and install) the Thermo-Calc software without a valid license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.

Network License Restrictions

The Diffusion Module (DICTRA) requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use the Diffusion Module (DICTRA) even if you have access to a license server with a valid network license file. This is because other clients who are part of your network installation may have checked out all instances of the network license allowed to run simultaneously.

Graphical Mode and Entering Demo Mode



In Graphical Mode only, and for users with a network license, you must exit Thermo-Calc to release the license for use. The license is checked out as soon as you add a Diffusion Calculator and remains unavailable to others until you exit the program.



With a network license, and if as per above you temporarily do not have access to a license, you are automatically put into *Demo Mode*. Then the Diffusion Calculator is available with three elements. See Diffusion Module Options in Graphical Mode for more information.

Console Mode



In Console Mode, a license is checked out when you enter the DICTRA module and it is checked back in when you leave the module. You do not need to exit the program.



If you are working in Console Mode and try to enter DIC_PARROT after having been in the PARROT module earlier in the session, a message displays: `DICTRA PARROT disabled after using PARROT`. To enter DIC_PARROT relaunch Thermo-Calc and enter these commands starting in the SYS module: GOTO_MODULE DIC_PAR.



Search the online help or see the *Thermo-Calc Installation Guide* for more about network licenses.

Diffusivity Theory and Diffusion Types

In this section:

Types of Diffusion Simulations 14
Diffusion in a Single-Phase System 15
Moving Boundary Muftiphase System 16
Diffusion in Disperse Systems 17
Diffusivity Theory 18

Types of Diffusion Simulations

The Diffusion Module (DICTRA) is used to simulate diffusion-controlled transformations in multicomponent alloys. A short summary of the types of simulations it can handle are listed below and whether it is available in Graphical (GM) or Console (CM) Mode.

The three main simulation types that are available for both modes are briefly discussed in this section.



For Graphical Mode, see the *Quick Start Guide* for examples of single phase, moving boundary phase and multiphase simulations.



For Console Mode, also see Models in the Diffusion Module and the *Quick Start Guide*.

Simulation type	Examples	Graphical Mode	Console Mode
One-phase simulations	Homogenization of alloys	x	x
	Carburizing and decarburizing of e.g. steel in austenitic state		x
Moving boundary simulations	Growth or dissolution of precipitates	x	x
	Microsegregation during solidification	x	x
	Austenite to ferrite transformations	x	x
	Growth of intermediate phases in compounds	x	x
	Coarsening of precipitates		x
Long-range diffusion in multiphase systems	Interdiffusion in compounds, e.g. coating systems	x	x
	Nitriding and nitrocarburization		x
	Carburizing of high-temperature alloys	x	x
Cooperative growth	Growth of pearlite in alloyed steels		x
Deviation from local equilibrium	Calculations under paraequilibrium conditions		x

Diffusion in a Single-Phase System

This type of simulation is available for both Graphical and Console Mode.

The simplest simulation is one where certain elements in one phase diffuse over time in that single phase. To simulate this, you create one region and enter one phase into that region. You can set up the system under various conditions by defining profiles for how temperature and pressure change over time.

In Console Mode you can also simulate how the boundary conditions of the region change over time.

Simulate diffusion in a single-phase system



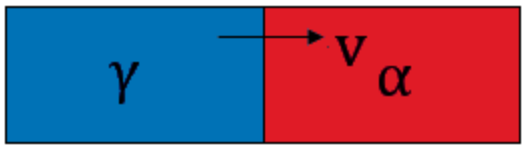
Moving Boundary Muftiphase System

This type of simulation is available for both Graphical and Console Mode.

With two regions in a single cell you can simulate how diffusion causes phase transformations. For example, you can simulate how an individual particle grows or dissolves as a function of time. The result is a simulation of how the boundary between the regions migrate over time. As in the case of a one-phase simulation, you can set up the system under various conditions by defining profiles for how temperature changes over time.

In Console Mode you can also set up the system to see how the boundary conditions of the region change over time.

Simulate a moving boundary multiphase system



Normally, simulations are performed under the assumption that thermodynamic equilibrium holds locally at all phase interfaces.

In Console Mode it is also possible to simulate a moving phase boundary problem while assuming that para-equilibrium conditions apply at the phase boundary.

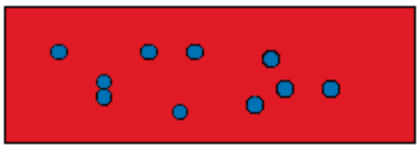
Diffusion in Disperse Systems

This type of simulation is available for both Graphical and Console Mode.

You can perform simulations where one or more dispersed phases are present in a matrix phase. For example, you can simulate how carburization causes precipitation of carbides in an austenitic matrix phase. In both Graphical Mode and Console Mode, problems involving diffusion in disperse systems are handled with homogenization model.

In Console Mode and if you are using the disperse model instead of the recommended homogenization model, the dispersed phases act as point sinks or sources of solute atoms in the simulation and the fraction and composition is calculated from the average composition in each node, assuming that equilibrium holds locally in each volume element.

Simulate diffusion in a disperse system



The homogenization model allows you to take into account diffusion in all phases for which you have kinetic data; the homogenization model treats all phases in the same way regardless of which phase is entered as type matrix and which phases are entered as type spheroid.

In Graphical Mode, the *Homogenization* model is automatically selected as the default solver when multiple phases are selected in a region.

In Console Mode, there are two ways in which you can simulate diffusion in a system that contains a dispersed phase, but it is strongly recommended that you use the *homogenization model*. See About the Homogenization Model.

Simulate diffusion with the homogenization model



Diffusivity Theory

In order to perform simulations using the Diffusion Module (DICTRA), both thermodynamic and kinetic descriptions are needed. Moreover, the results and the accuracy of the simulations critically depend on the quality of these descriptions. So far there is much less kinetic data which has been systematically assessed in the same way as thermodynamic data.

In the theoretical treatment of diffusive reactions one usually works with diffusion coefficients which are evaluated from experimental measurements. In a multicomponent system a large number of diffusion coefficients have to be evaluated, and moreover, they are generally functions of alloy composition and are interrelated. A database would thus be very complex. A superior alternative is to store atomic mobilities in the database, rather than diffusion coefficients. The number of parameters which need to be stored in a multicomponent system are then substantially reduced and the parameters are independent. The diffusion coefficients, which are used in the simulations, can then be obtained as a product of a thermodynamic and a kinetic factor.

The thermodynamic factor is essentially the second derivatives of the molar Gibbs energy with respect to the concentrations, and is known if the system has been assessed thermodynamically. The kinetic factor contains the atomic mobilities, which are stored in the kinetic database. The purpose of this topic is to describe how concentration, temperature and pressure dependence of the atomic mobility can be modeled, as well as to describe relations between the different diffusion coefficients and the atomic mobility.

Modeling of the Atomic Mobility

From absolute-reaction rate theory arguments the mobility coefficient for an element B, $\mathrm{M_B}$ may be divided into a frequency factor M_B^0 and an activation enthalpy, $\mathrm{Q_B}$, i.e.

[*Eq. 1*] $$M_B = M_B^0 \exp\left(-\frac{Q_B}{RT}\right)\frac{1}{RT}{}^{mg}\Gamma$$

${}^{mg}\Gamma$ is a factor taking into account the effect of the ferromagnetic transition [Jönsson, 1994a]. ${}^{mg}\Gamma$ is a function of the alloy composition. It has been suggested by Jönsson, 1994b that one should expand the logarithm of the frequency factor, $\ln M_B^0$, rather than the value itself, thus the mobility, $\mathrm{M_B}$, is expressed as:

[*Eq. 2*] $$M_B = \exp\left(\frac{RT\ln M_B^0}{RT}\right)\exp\left(-\frac{Q_B}{RT}\right)\frac{1}{RT}{}^{mg}\Gamma$$

Both $\mathrm{RT}\ln M_B^0$ and $\mathrm{Q_B}$ generally depend upon the composition, temperature, and pressure. In the spirit of the CALPHAD approach [Ågren, 1996], the composition dependency of these two factors, is represented with a linear combination of the values at each endpoint of the composition space, and a Redlich-Kister expansion, viz.

$$\Phi_B = \sum_i x_i \Phi_B^i + \sum_i \sum_{J>i} x_i x_j \left[\sum_{r=0}^{m} {}^r\Phi_B^{i,j} (x_i - x_j)^r \right] \quad \text{[Eq. 3]}$$

where Φ_B represents $\mathrm{RT}\ln \mathrm{M_B}$ or $\mathrm{-Q_B}$. Φ_B^i is the value of Φ_B for pure *i* and thus represents one of the endpoint values in the composition space. ${}^r\Phi_B^{i,j}$ are binary interaction parameters. The commas separate different species interacting with each other. $\mathrm{x_i}$ and $\mathrm{x_j}$ are mole fractions of elements *i* and *j* respectively. Each individual Φ parameter, i.e. Φ_B^i and ${}^r\Phi_B^{i,j}$ is stored in the database and may be expressed as a polynomial in temperature and pressure, if necessary. The Φ_B^i and ${}^r\Phi_B^{i,j}$ are referred to in the database as MF and MQ parameters, e.g.

$$\mathrm{MF(BCC_A2\&CR,NI:VA;0) = R*T*LN(+8.50E\text{-}05)}$$

is used to represent the frequency factor to the mobility of Cr in pure Ni, i.e. $\mathrm{RT}\ln M_{Cr}^{Ni0}$, whereas:

$$\mathrm{MQ(BCC_A2\&CR,NI:VA;0) = \text{-}2.18E{+}05}$$

represents $-Q_{Cr}^{Ni}$. The magnetic effect is represented by Jönsson's model [1994a].

$${}^{mg}\Gamma = \exp(6\alpha\xi)\exp\left(\frac{-\alpha\xi Q_B}{RT}\right) \quad \text{[Eq. 4]}$$

where ξ represents the state of the magnetic order ($0 < \xi < 1$) at the temperature under consideration and α is treated as a constant, approximately equal to 0.3 in bcc alloys. For fcc alloys the ferromagnetic effect on diffusion is usually neglectable, i.e. $\alpha \approx 0$. When there is magnetic ordering it is thus necessary to make the division into MF and MQ because ${}^{mg}\Gamma$ depends on $\mathrm{Q_B}$, i.e. MQ. The full expression then becomes:

$$RT\ln[RTM_B] = RT\ln M_B^0 - Q_B + RT\ln {}^{mg}\Gamma = \sum MF + \sum MQ + RT\ln {}^{mg}\Gamma$$

Both MF and MQ may be arbitrary polynomials in temperature and if there is no magnetic effect, i.e. $\mathrm{RT}ln^{mg}\Gamma = 0$, it is sufficient to enter either one of them. For example, the mobility of Cr in pure Ni may as well be stored as:

$$\mathrm{MF(FCC_A1\&CR,\,NI:VA;0)} = 0$$

and

$$\mathrm{MQ(FCC_A1\&CR,NI:VA;0)} = -Q_{Cr}^{Ni} + \mathrm{RT}\ln M_{Cr}^{Ni0}$$

In order to build a database it is necessary to find values on MF and MQ (or when no magnetic effect is considered MQ alone). In many cases such data can be found in the literature. The tracer diffusivity D_B^* is directly related to the mobility M_B by means of the Einstein relation

[*Eq. 5*] $$D_B^* = RTM_B$$

and when there is no magnetic effect on the mobility, e.g. ${}^{mg}\Gamma = 1$, then from Equation 2 and Equation 5 it is found that:

[*Eq. 6*] $$\mathrm{MQ} = RT\ln M_B^0 - Q_B = RT\ln D_B^*$$

In a more complex database the model parameters are determined from an optimization procedure, where all experimental information is taken into account, see for example Jönsson, 1995 and Engström and Ågren, 1996.

Relationship Between Diffusion Coefficients and Atomic Mobilities

Phenomenological Coefficients

For crystalline phases the vacancy-exchange mechanism of diffusion is predominant, i.e. diffusion occurs by atoms jumping into neighboring vacant lattice sites. From the absolute reaction rate theory, and by assuming that the vacancy concentration is governed by thermodynamic equilibrium, the diffusional flux of a component *k* in the lattice fixed frame of reference can be expressed as [Andersson and Ågren, 1992]:

[*Eq. 7*] $$\tilde{J}_k = -c_k y_{Va}\Omega_{kVa}\frac{\partial \mu_k}{\partial z}$$

Here $\mathrm{c_k}$ is the amount of *k* per unit volume, $\mathrm{y_{Va}}$ is the fraction of vacant lattice sites on the sublattice where *k* is dissolved, Ω_{kVa} is a kinetic parameter which gives the rate of exchange if there is a vacancy adjacent to a *k*-atom,

and μ_k is the chemical potential of component *k*. The mobility $\mathrm{M_k}$ is here defined as:

[*Eq. 8*] $\mathrm{M_k} = \mathrm{y_{Va}}\Omega_{\mathrm{kVa}}$ when *k* is substitutional

[*Eq. 9*] $\mathrm{M_k} = \Omega_{\mathrm{kVa}}$ when *k* is interstitial

From Equation 7, Equation 8 and Equation 9 it is possible to identify the so called phenomenological parameters that relate the flux of *k* to all the driving forces, i.e. $\mathrm{L_{kk}} = \mathrm{c_k M_k}$ when *k* is substitutional, $\mathrm{L_{kk}} = \mathrm{c_k y_{Va} M_k}$ when *k* is interstitial, and $\mathrm{L_{ki}} = 0$ when $\mathrm{k} \neq \mathrm{i}$. The fluxes in the lattice-fixed frame of reference may now be expressed as:

[*Eq. 10*] $$\tilde{J}_k = -\sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z} = -L_{kk} \frac{\partial \mu_k}{\partial z}$$

Transformation to the volume-fixed frame of reference, or the number-fixed frame of reference with respect to the substitutional elements, which may be regarded as the same, if as assumed in the Diffusion Module (DICTRA), the partial molar volumes are independent of concentration, and the partial molar volumes of the interstitials are neglected, yields

[*Eq. 11*] $$J_k = -\sum_{i=1}^{n} L'_{ki} \frac{\partial \mu_i}{\partial z}$$

where

[*Eq. 12*] $$L'_{ki} = \sum_{j=1}^{n} (\delta_{jk} - c_k V_j) L_{ji}$$

where δ_{jk} is the Kronecker delta, i.e.,=1 when j=k and 0 otherwise. $\mathrm{V_j}$ is the partial molar volume of element *j*.

Interdiffusion Coefficients

Generally, it is much more convenient to express the fluxes as functions of concentration gradients, rather than gradients in chemical potential. This is accomplished by rewriting Equation 11 using the chain rule of derivation, i.e.

[*Eq. 13*] $$J_k = -\sum_{i=1}^{n} L'_{ki} \sum_{j=1}^{n} \frac{\partial \mu_i}{\partial c_j} \frac{\partial c_j}{\partial \mathrm{z}}$$

or equally if the unreduced diffusivities, D_{kj} are introduced,

[*Eq. 14*] $$J_k = -\sum_{j=1}^{n} D_{kj} \frac{\partial c_j}{\partial \mathrm{z}}$$

The D_{kj} matrix introduced in Equation 14 may be identified by comparing with Equation 13,

[*Eq. 15*] $$D_{kj} = \sum_{i=1}^{n} L'_{ki} \frac{\partial \mu_i}{\partial c_j}$$

The $\frac{\partial \mu_i}{\partial c_j}$ are purely thermodynamic quantities, sometimes they are referred to as thermodynamic factors. It is now evident that the diffusivities may be looked upon as consisting of two separate parts, one purely thermodynamic and one kinetic.

There is a relation between the n concentration gradients in Equation 14 and for practical calculations one usually chooses to eliminate one of them. The reduced diffusivities in a volume-fixed frame of reference, where it is assumed that all the substitutional species have the same partial molar volumes, and furthermore, only the substitutional species contribute to the volume, i.e. the Diffusion Module (DICTRA) frame of reference, is expressed as,

[*Eq. 16*] $D^n_{kj} = D_{kj} - D_{kn}$ when *j* is substitutional

[*Eq. 17*] $D^n_{kj} = D_{kj}$ when *j* is interstitial

where *n* is taken as the dependent species. Using these diffusivities Equation 14 now becomes,

[*Eq. 18*] $$J_k = -\sum_{j=1}^{n-1} D^n_{kj} \frac{\partial c_j}{\partial z}$$

Equation 18 contains the so-called interdiffusion coefficients, sometimes referred to as chemical diffusivities. These diffusivities may be evaluated experimentally from e.g. diffusion couple experiments.

Intrinsic Diffusion Coefficients

The individual or intrinsic diffusion coefficients, that are defined in the lattice-fixed frame of reference by:

[*Eq. 19*] $$\tilde{J}_k = -\sum_{j=1}^{n-1} {}^{i}D^n_{kj} \frac{\partial c_j}{\partial z}$$

can also be evaluated from diffusion couple experiments, if in addition to concentration profiles the Kirkendall velocity can be estimated from the movement of inert markers. As the interdiffusion coefficients, the intrinsic diffusion coefficients can also be calculated from the mobilities. However, this time by applying the chain rule of derivation on Equation 10 and remembering that $L_{ki} = 0$ when $k \neq i$, i.e.

[*Eq. 20*] $$\tilde{J}_k = -\sum_{j=1}^{n} L_{kk} \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z}$$

The intrinsic diffusion coefficients may be identified in Equation 20 as:

[*Eq. 21*] $$^{i}D_{kj} = L_{kk} \frac{\partial \mu_k}{\partial c_j}$$

Also here there is a relation between the *n* concentration gradients. If one of the concentrations are chosen as dependent, and if the same approximation as previously used for the partial molar volumes of the different elements is applied, then the intrinsic diffusion coefficients defined in Equation 19 are finally found.

[*Eq. 22*] $$^{i}D^{n}_{kj} = {}^{i}D_{kj} - {}^{i}D_{kn}$$ when *j* is substitutional

[*Eq. 23*] $$^{i}D^{n}_{kj} = {}^{i}D_{kj}$$ When *j* is interstitial

Self-diffusion Coefficient

The self-diffusion coefficient of A is the diffusivity of A in the limit of pure A. Studies of self-diffusion usually utilize radioactive tracer atoms A* of the same element.

Impurity Diffusion Coefficient

When the diffusion of a solute B in a solvent A is studied at an extremely small concentration of B, which e.g. radio tracers permit, then the impurity diffusion coefficient of B in A is observed.

References

1. Jönsson, Björn. 1994a. “Ferromagnetic Ordering and Diffusion of Carbon and Nitrogen in Bcc Cr-Fe-Ni Alloys.” Zeitschrift Fur Metallkunde 85 (7): 498–501.
2. Jönsson, Björn. 1994b. “Assessment of the mobility of carbon in C-Cr-Fe-Ni FCC alloys.” Zeitschrift Fur Metallkunde 85 (7): 502–9.
3. Ågren, John. 1996. “Calculation of Phase Diagrams: Calphad.” Current Opinion in Solid State and Materials Science 1 (3): 355–60.
4. Jönsson, Björn. 1995. “Assessment of the Mobilities of Cr, Fe and Ni in Bcc Cr-Fe-Ni Alloys.” ISIJ International 35 (11): 1415–21.
5. Engström, Anders, and John Ågren. 1996. “Assessment of Diffusional Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys.” Zeitschrift Fur Metallkunde 87 (2): 92–97.

6. Andersson, Jan-Olof, and John Ågren. 1992. “Models for Numerical Treatment of Multicomponent Diffusion in Simple Phases.” Journal of Applied Physics 72 (4): 1350–55.

Working in Graphical Mode

Working with the Diffusion Module (DICTRA) in Graphical Mode is directly related to working with Thermo-Calc through the use of the Diffusion Calculator. See the Thermo-Calc documentation for more details about working in Graphical Mode.

In this section:

Diffusion Module Options in Graphical Mode 26

Basic Terminology in Graphical Mode 30

Setting up a Diffusion Simulation in Graphical Mode 32

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Diffusion Module Options in Graphical Mode

The Diffusion Module is an Add-on Module to the core Thermo-Calc software.



A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*. This is not available in Console Mode. See Demonstration (Demo) Mode to learn more.

Diffusion Simulation Template

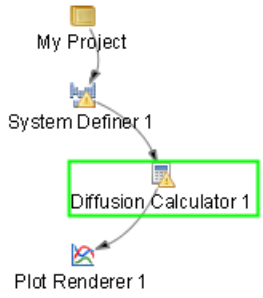
A **Diffusion Simulation** template is available to all Thermo-Calc users when in Graphical Mode.

If you are using the Diffusion Module in Demo Mode, see Demonstration (Demo) Mode for what is available to you. Even if you have a license, you may find yourself in Demo Mode if you have a network license and all the licenses are checked out.

Using the Template

When you first open Thermo-Calc in Graphical Mode, on the **My Project** window, click the **Diffusion Simulation** button to add a *System Definer*, *Diffusion Calculator* and *Plot Renderer* to the **Project** tree.

Click the **Diffusion Simulation** icon in the Templates window to add **THESE NODES** to the Project.



- Creating a Project from a Template.

Diffusion Calculator

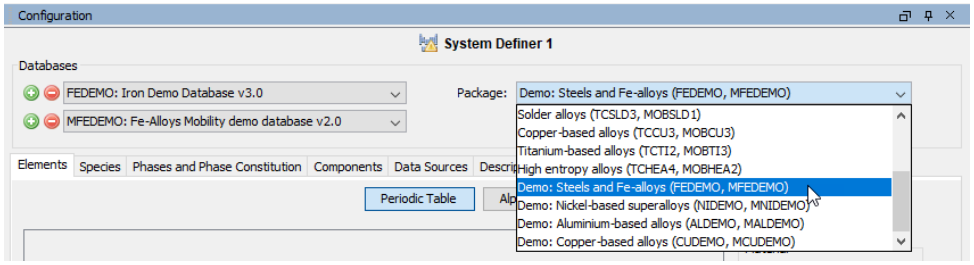
A Diffusion Calculator allows you to set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles and the thermal profile, plus additional options. Many of the settings are automatically set as you define your system. Details about this activity are described in Diffusion Calculator.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Diffusion Module simulation. If you have a Diffusion Module (DICTRA) license you can run all the examples because the demonstration database packages are included with your installation.

Select the database packages from the **System Definer Configuration** window to run a simulation.

If you are in Demo Mode, see Demonstration (Demo) Mode to learn more.



Demonstration (Demo) Mode

The Diffusion Module and some examples are available to all Thermo-Calc users but only for simulations with three elements. If you do not have a license for then you are in *Demo Mode* when using the Diffusion Calculator or Diffusion Simulation template.

Diffusion Simulation Template

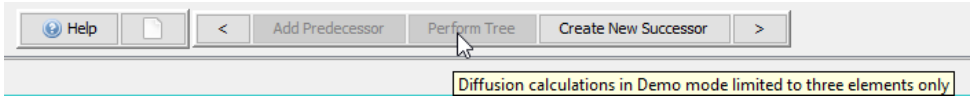
When you are in DEMO mode, in the **Templates** area this is indicated by the text under the logo.



Diffusion Calculator

If you are experimenting with the Diffusion Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Diffusion Calculator, the **Perform** button is unavailable and the tooltip explains why.



Even if you have more than three elements, the Plot Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Basic Terminology in Graphical Mode

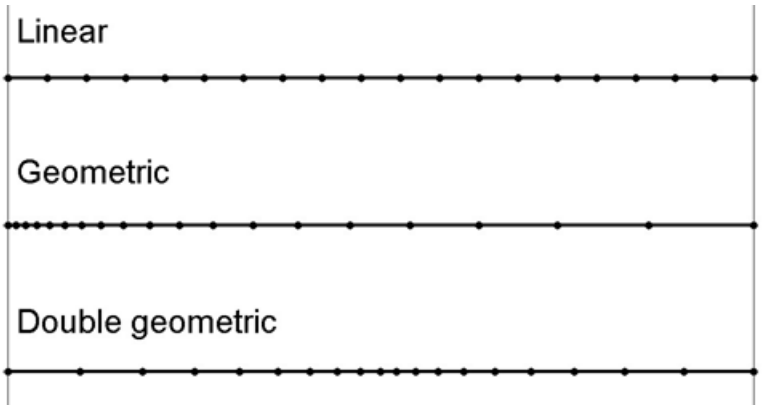
These terms are specific to working in Graphical Mode. The overall simulation in Console Mode is comparable but there are some differences in terminology and functionality.

Region

In Graphical Mode, a system consists of one *cell* with one or multiple *regions* in which the diffusion problem is to be solved.

Grid Types

These grid types are used in diffusion simulations: linear, geometric and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region must contain at least one *phase*. The so-called *homogenization model* is used if multiple phases are added inside a region, then the average properties of the local phase mixture is used. Phase(s) can also be added to interphases of region(s) and then only participate in the simulation if the driving force for precipitation of the phase exceeds a predefined value. A new region is then created where the name of the region is set to the name of the phase but with `R_` added as a prefix.

Composition

These types of composition variables are used in the configuration of the Diffusion Calculator: *mass (weight) fraction*, *mass (weight) percent*, *mole fraction*, or *mole percent*.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$\mu_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume. Weight fraction, mole fraction or u-fraction can be used when plotting the results from a simulation.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where compositions vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical* or *spherical*.

The *planar* geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

- See Setting up a Diffusion Simulation in Graphical Mode then go to Working in Graphical Mode for links to the other relevant content.

Setting up a Diffusion Simulation in Graphical Mode

When you are using the Graphical Mode version of the Diffusion Module (DICTRA), the steps to set up a simulation are a combination of adding *Activity* nodes (the System Definer, Diffusion Calculator and Plot Renderer) and then defining the applicable settings for each of these nodes in a Configuration window.

The following is a general overview of the steps to set up the simulation.

1. Use the **Diffusion Simulation** template to add the System Definer, Diffusion Calculator and Plot Renderer activity nodes.
2. On the **System Definer**, you select the thermodynamic and kinetic databases, add elements and phases, and generally define the system.
3. On the **Diffusion Calculator**, you set the geometry (by default the geometry is planar), add region(s) and enter grid(s) and phase(s) in the region(s). You then enter composition(s) of phase(s).
4. On the **Plot Renderer** or **Table Renderer**, you choose how to visualize your diagrams, and then run the simulation, i.e. you **Perform** the sequence of nodes you have defined in the tree to produce the output simulation.



Go to Working in Graphical Mode for links to the relevant content to continue.

Graphical Mode Diffusion Calculator Examples

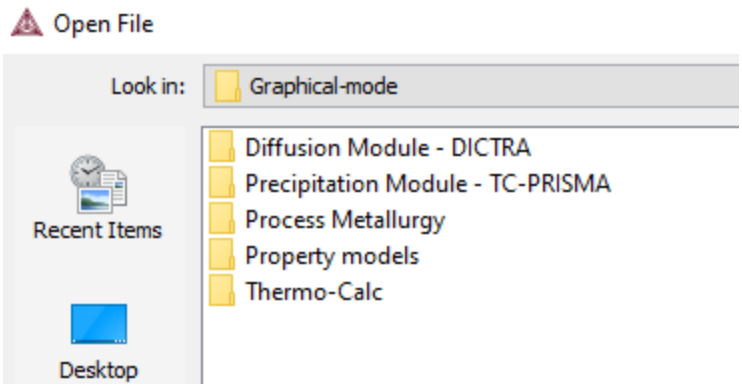
- About the Examples
- See Diffusion Module (DICTRA) Graphical Mode Examples for links to the examples.

Opening the Diffusion Calculator Examples

Graphical Mode examples are available for Thermo-Calc and the Add-on Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), and Process Metallurgy Module. There are also examples for the Property Models, including the Steel Model Library and more. These are in the format of project files (*.tcu).

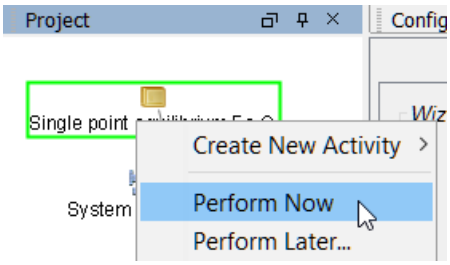
To open an example project file for Thermo-Calc and the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Process Metallurgy Modules:

1. Open Thermo-Calc.
2. Confirm you are in Graphical Mode. If not, click the **Switch to Graphical Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**.
4. The examples are divided into folders. Navigate to the folder and project file you want and double-click to open.



5. The Graphical Mode examples are stored without calculated results so you will want to run the example calculation and generate a plot or table. To do this, click the first node in the tree at the top of the **Project** window. Then right-click and select

Perform now.


Project
Config
Single point
Create New Activity
System
Perform Now
Perform Later...

Working in Console Mode

In this section:

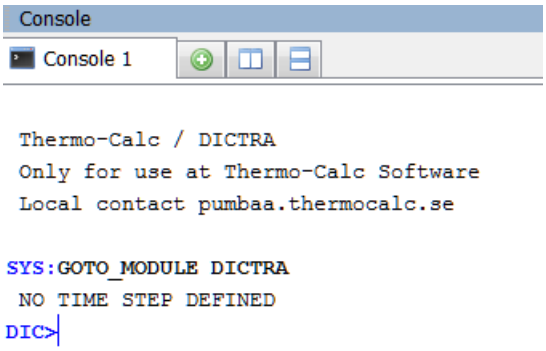
Opening DICTRA in Console Mode 36
Opening a Macro File (Console Mode) 37
About the Console Mode File Formats 39

Opening DICTRA in Console Mode

1. Open Thermo-Calc in Console Mode.

   By default, Thermo-Calc opens in the most recently used state. If it opens in Graphical Mode, on the toolbar, click **Switch to Console Mode**.

2. In the `SYS` module, type `GOTO_MODULE DICTRA`. For a list of all the available commands in the current module, at the prompt type a question mark (?) and press <Enter>. For a description of a specific command, type `Help` followed by the name of the command.



Opening a Macro File (Console Mode)

You can open the macro files (*.TCM or *.DCM files) in different ways.

- From the main menu,
- Using a command, or
- By dragging and dropping the file into the Console window.

How to Open an Example Macro

To open a specific macro file from the Examples folders included with your installation:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Double-click the **Diffusion Module - DICTRA** folder to view the subfolders.



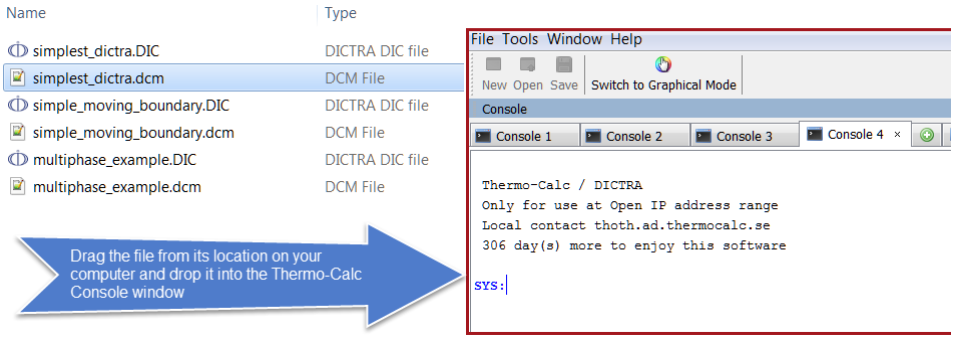
The three Quick Start example macros and the PDF guide are in the first folder called **Beginner Guide**.

How to Open a Macro with a Command

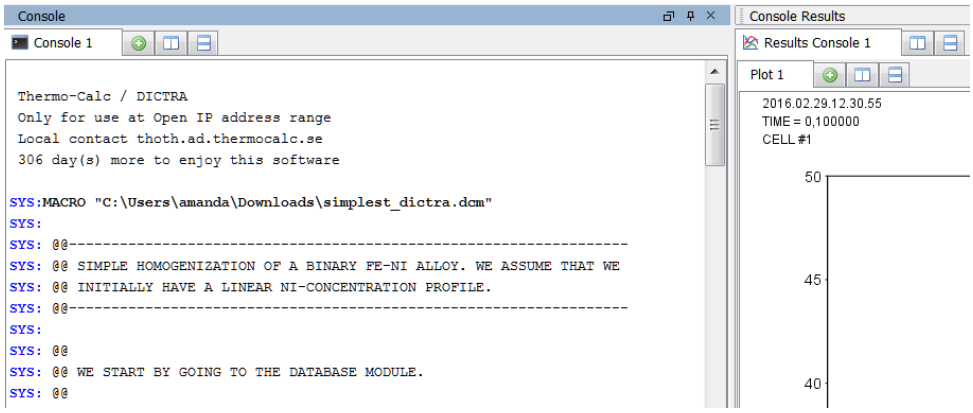
At the `SYS` prompt, type `MACRO_FILE_OPEN` and press <Enter>. In the file dialogue window that opens, locate and select the macro file on your computer.

How to Open a Macro File by Dragging and Dropping it into Console Mode

For example, navigate to the **Beginner Guide** folder and then drag the file from its location into Thermo-Calc Console window.



The macro automatically runs after you drop it into the Console window.



Double-click to Open a File

Navigate to the macro file location, for example where each set of file examples is in its own folder. When you double-click, it opens the file in a new instance of Thermo-Calc.

About the Console Mode File Formats

The Diffusion Module (DICTRA) in Console Mode uses different file formats: *log* files (*.TCM), *macro* files (*.DCM) and *workspace* files (*.DIC).



Also see Graphical Mode vs Console Mode. If you are working with Thermo-Calc in Console Mode, see Working with the Console Mode File Types.

Log Files

Log files (*.TCM) are plain text files and are just macro files used to save a sequence of commands. These files can be edited in a text editor.

- To start saving your input into a file, in the SYS module type `SET_LOG_FILE`, followed by the name of the file that you want to save your command sequence to.
- When creating a command sequence, and if you want to save the output in the log file, type `SET_ECHO` before SET_LOG_FILE. This is useful if you later want to use the log file as a macro file because the macro file lists the full commands instead of only the short names.

Macro Files

Macro files (*.DCM) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

- To run a macro file, in the SYS or DICTRA module type `MACRO_FILE_OPEN`, followed by the name of the macro file. DICTRA runs the MACRO_FILE_OPEN sequence that the file contains.
- To remain in the console and keep working in the DICTRA module, in the SYS, DICTRA, POLY, or POST module add the command SET_INTERACTIVE at the end of the macro file. Alternatively, use `EXIT` as the final command.

Workspace Files

Workspaces files for the Diffusion Module (DICTRA) have the file extension *.DIC, which allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations.

- At the `DIC` prompt use SAVE_WORKSPACES.
- To load the data and calculation results of a workspace file, at the `DIC` prompt use READ_WORKSPACES.

Overview of a System

In this section:

Typical Console Mode Workflow 42
About Regions and Grids 42
About System, Cells and Regions 43
About Phases 43
About Composition Variables 44
About Global Conditions 45
About Boundary Conditions in Console Mode 45
About Geometry and Coordinates 46
About Operators and Functions 47

Typical Console Mode Workflow

The basic work flow in Console Mode is as follows.

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module you define the system. Before performing a calculation, you must define your system and retrieve thermodynamic and kinetic data. The data is retrieved from the database files.
3. The data needed to describe a system is sent to the **GIBBS** module. When the data is in GIBBS, the software can access the retrieved data. The retrieved data is accessible to the **POLY** module, which is involved in simulations that require that equilibrium calculations are performed.
4. In the **DICTRA_MONITOR** you:
    a. Set the initial state of the system and define its geometry and boundary conditions. The simplest system has one cell that contains one region, but you may put additional regions in a cell and put additional cells in your system.
    b. Define the phases each region contains.
    c. Set various parameters for the numerical calculations.
    d. Run the simulation from within the DICTRA_MONITOR.
5. In the **POST** module you plot and visualize your data.
    a. Choose the data to plot
    b. Change the appearance of the diagram
    c. Save the diagram as an image file (available in several formats).

About Regions and Grids



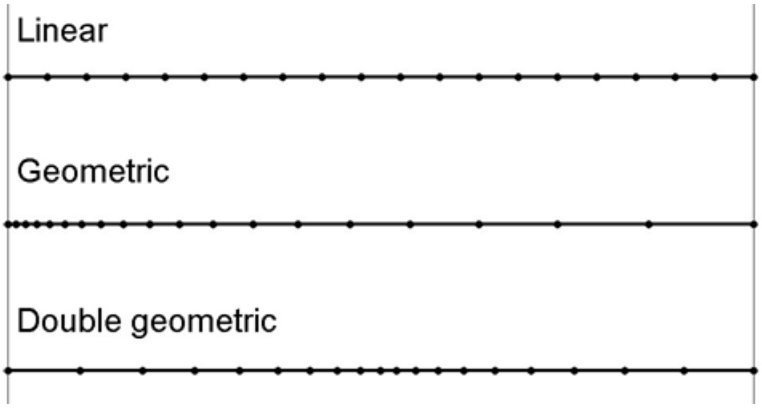
For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Also see Creating Regions and Gridpoints.

A *region* contains one or more phases. If a region contains several phases one of those must be entered as a *matrix phase* whereas the others are entered as *spheroid*.

A region must also contain a number of *grid points*. The composition is only known at these grid points and the software assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

These grid types are used in diffusion simulations: linear, geometric and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



About System, Cells and Regions

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

A system normally consists of one *cell*. This cell contains one or several *regions* in which the diffusion problem is to be solved. A system of diffusion equations is solved for each region. The size of the system is the sum of sizes of all the regions in all the system's cells.

The interface between two regions typically moves as the result of a simulation, that is, the regions grow or shrink. Such an interface is called an *inner interface*. The boundary of a cell is called an *outer interface* and the condition of this type of interface may be affected by the choice of boundary conditions.

For some simulations it is useful to have several cells in a system. Matter can move between cells. However, it is assumed that there is diffusional equilibrium between all cells (this means that there are no differences in diffusion potentials between cells). In other words, the size of a cell is fixed during the simulation.

By default this is a *closed system*, which means that matter cannot move across its boundaries. However, you can change this setting for both the *lower boundary* (left side/centre) and the *upper boundary* (right side/surface) of the system. You can also set these boundary conditions to vary as a function of time, temperature and/or pressure.

About Phases

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Entering Phases in Regions and Specifying Phase Compositions in a Region.

Each region contains one or more *phases*. A phase can be of the *matrix*, *spheroid* or *lamellar* type. A phase can be introduced with the status *active* (the default) or *inactive*.

An inactive phase is a phase which does not participate in the calculations until it is stable. If a phase is inactive, then the driving force for precipitation of the phase is continuously monitored. When the driving force exceeds a predefined positive value, the phase take parts in the simulation and the phase automatically becomes active. A new region is then created and the formerly inactive phase is entered as the matrix phase of the new region. The name of the region is set to the name of the phase that just became active but with `R_` added as a prefix.

Region Phase Types

Phase type	Description
Matrix	The region's primary phase. If there is only one phase in a region, then that phase is automatically a matrix.
Spheroid	Used to treat one or several dispersed phases in a matrix. Unless the homogenization model is invoked, which happens automatically when a spheroid phase is entered, then diffusion is only considered in the matrix phase; the spheroid phases then only act as sources and sinks of the diffusing elements.
Lamellar	Used to simulate the growth of a eutectic or eutectoid region. The software only treats the growth, not the dissolution, of such a region. The *pearlite calculation model* is used for a phase that is lamellar.

About Composition Variables



For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Two types of composition variables are used within the program: site-fractions and u-fractions, although you can also use weight fraction or mole fraction, for example.

The *site-fractions* are used to set up the problem and interface with POLY-3 (in Console Mode). The site fraction of a species *k*, y_k, is the fraction of equivalent lattice sites occupied by species k. It is the only concentration variable that uniquely defines the composition and the constitution of a phase and it is necessary to use the site fraction in the storage of the data during a simulation.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$u_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume.

About Global Conditions

There are several global parameters that influence the diffusion rate in simulations: temperature, pressure and heat content removal. These parameters are defined as functions of time. The temperature can also be a function of the spatial position, and heat content removal can be a function of temperature or pressure.

For heat content removal, the amount of extracted heat per time unit is normalized and the size of the system is normalized to one mole of atoms.

- Setting Global Conditions in the *Thermo-Calc User Guide*

About Boundary Conditions in Console Mode

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

- SET_CONDITION

Boundary Condition Descriptions

Boundary condition	Description
FIX_FLUX_VALUE	Enter functions that yield the flux times the molar volume for the independent components. Can be a function of time, temperature and pressure. Use this boundary condition with caution as it may cause unrealistic compositions.
STATE_VARIABLE_VALUE	A legal equilibrium condition expression in POLY-3 syntax that reduces the degrees of freedom. This type should be used with care as no checks are done in advance to determine if it is a legal expression. Do not specify the conditions for temperature and pressure here as these are taken from the global conditions.
POTENTIAL_FLUX_FUNCTION	Use to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $$J_k = f_k(T,P,TIME)^*\left[POTENTIAL_k^N - g_k(T,P,TIME)\right]$$

Boundary condition	Description
	The functions f and g may have time (TIME), temperature (T), and/or pressure (P) as arguments. N is an integer. The potentials are those with user defined reference states.
ACTIVITY_FLUX_FUNCTION	Use to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $$J_k = f_k(T,P,TIME)^* \left[ACTIVITY_k^N - g_k(T,P,TIME) \right]$$ The functions f and g may have time (TIME), temperature (T), and/or pressure (P) as arguments. N is an integer. The activities are those with user-defined reference states.
ITERATIVE_ACTIVITY_FLUX_ FUNCTION	Same as ACTIVITY_FLUX_FUNCTION but an iterative scheme is used to determine the flux. Use this if the other command encounters problems.
CLOSED_SYSTEM	Corresponds to a fix flux value, which is set to zero at all times. This is the default boundary condition.
MIXED_ZERO_FLUX_AND_ ACTIVITY	The flux of selected components is set to zero and the activity of others may be set to a prescribed value.
GAS	This option can cause a change in system volume. The flux of selected components is set to zero and the activity of others can be set to a prescribed value. Use this to treat an expanding system, e.g. the growth of an external oxide scale.

About Geometry and Coordinates

Specifying the Geometry

The Diffusion Module (DICTRA) can only handle diffusion problems where composition vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical* or *spherical*.

Planar Geometry

This geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Cylindrical and Spherical Geometries

- Cylindrical geometry corresponds to an infinitely long cylinder of a certain radius.
- Sypherical geometry corresponds to a sphere with a certain radius.

By default for both geometries, the lower boundary (the zero coordinate) is at the centre of the cylinder/sphere. The upper boundary (the coordinate with the highest value) is at the *surface* of the cylinder/sphere. You can enter a left most coordinate that is larger than zero to allow for tube and hollow sphere geometries.

About Operators and Functions

Sometimes you need to specify functions when setting up a system. For example, to make global and boundary conditions vary as a function of time.

The following operators can be used in writing functions. Use a semi-colon (;) to mark the end of a function.

Available Operators for Writing Functions

Operator	Description
+, -, *, /	Addition, subtraction, multiplication, division
**	Exponentiation, raising one quantity to the power of another, e.g. x^2.
ABS()	Absolute value
ERF(X)	Error function
EXP(X)	Exponential
LOG(X)	Natural logarithm
LOG10(X)	Base 10 logarithm
SIGN(X)	Sign function SIGN(X) is -1 when X<0, is 0 when X=0 and is 1 when X>0.
SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)	• Trigonometric functions: sine, cosine, tangent • Inverse trigonometric functions: arcsine, arccosine, arctangent
SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH (X)	• Hyperbolic trigonometric functions • Inverse hyperbolic functions
SQRT(X)	Square root

Creating a DICTRA Simulation



These topics describe in general terms what options you have when setting up your diffusion simulation in Console Mode.

In this section:

Defining a System in Console Mode 49

Setting Up and Running a Simulation 50

Setting Global Conditions 50

Specifying Time-Dependent Profiles 51

Creating Regions and Gridpoints 52

Entering Phases in Regions 53

Specifying Phase Compositions in a Region 54

Specifying the Geometry 55

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Defining a System in Console Mode



Define your system with as few elements (components) and phases as possible; keep the simulation as simple as possible to avoid making the simulation unsolvable.

In order to perform a simulation in the Diffusion Module, both a thermodynamic database and a kinetic database is needed. The thermodynamic database is a normal Thermo-Calc database, whereas the kinetic database contains information about the atomic mobility of individual elements in various phases.

Database (TDB) Module Commands

1. Open Thermo-Calc in Console Mode. At the `SYS` prompt, type `GOTO_MODULE DATA`.
2. Use SWITCH_DATABASE to select databases. Unless you directly specify the name of the database as a parameter to the command, the available databases are listed. Specify the one to use.
3. Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements available in the current database, type `LIST_DATABASE Elements`.)
4. Use REJECT with the keyword, `Phases` to make sure that unnecessary phases are not retrieved from the database.
5. Use RESTORE with the keyword, `Phases` to restore any phases that have been excluded.
6. Use GET_DATA to read from the database and send the thermodynamic data about your system to the GIBBS and DICTRA workspace.
7. Use APPEND_DATABASE to select the database from which you want to retrieve kinetic data.
8. Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way as you would for the thermodynamics data (see steps 2, 3 and 4).
9. Use GET_DATA to read from the database and add the kinetic data to the thermodynamic data that already exists in the GIBBS and DICTRA module workspace.
10. Use APPEND_DATABASE again to add thermodynamic or kinetic data from another database. When all the data needed is retrieved, you can start using the DICTRA module.

Setting Up and Running a Simulation

1. Before you can set up and start a simulation, you must have retrieved thermodynamic and kinetic data and defined your system. See Defining a System in Console Mode.
2. Set conditions that hold globally in the system using SET_CONDITION `Global`. Normally, this is the temperature condition.
3. Enter a region into the current cell using ENTER_REGION. Give the region an arbitrary name. If the region that you create is not the cell's first region, then by default it is attached to the right side of the last region created in the cell.
4. For each region, use ENTER_GRID_COORDINATES to specify the region's size (width) as well as the type of grid and the number of grid points to be used in the region. The size is specified in meters.
5. Use ENTER_PHASE_IN_REGION to enter a phase into a region. Specify whether the phase is active/inactive, which type of phase it is, and what the name of the phase is.
6. Use ENTER_COMPOSITIONS to specify the initial composition of a phase that you have entered in a region. You can specify the composition in terms of site fraction, mole fraction, mole percent, weight fraction, weight percent or u-fraction. The composition profile may be entered by a user or be read from a file.
7. Use SET_CONDITION `Boundary` to set non-default boundary conditions.
8. Use ENTER_GEOMETRICAL_EXPONENT to enter the geometrical exponent that defines the geometry of the system. If you do not specify the geometrical exponent, then it is assumed that the system has a planar geometry.
9. Use SET_SIMULATION_TIME to set the simulation time.
10. If you want to use a specific model for the simulation calculations, then set the DICTRA module to use a COARSENING_MODEL, PARA_EQUILIBRIUM_MODEL, HOMOGENIZATION_MODEL or GB_MODEL. Also see About the Pearlite Model .
11. You are now ready to run the simulation. However, it is recommended that you use SAVE_WORKSPACES to save the setup before running the simulation.
12. Use SIMULATE_REACTION to start the simulation. To ensure that the simulation is run with default settings (answer `Y`), otherwise you may be prompted to specify certain values during the running of the simulations (if phases appear or disappear in the simulation).

Setting Global Conditions

Use SET_CONDITION and choose `Global`. Global conditions include temperature (T), heat content removal (Q) and pressure (P), and these reduce the degrees of freedom for equilibrium calculations.

About Global Conditions

If the heat content removal is specified then only the initial temperature should be entered with the SET_INITIAL_TEMPERATURE command.

- In practice, the pressure is rarely specified. By default the pressure is assumed to be constant and equal to 1 bar.
- For each condition, you can define a profile over time that consists of several intervals of time, or *ranges*, with each range having its own function to define the value of the condition.
- Temperature can be entered as a function of time (TIME) and/or spatial coordinate (X). The pressure condition can be defined as a function of time (TIME). The heat content removal can be defined as a function of temperature (T), pressure (P) and/or time (TIME).

  For example, the following function could specify a cooling rate if it is used to specify how the global condition temperature (T) changes with time (TIME) during a certain range: `1900-1*TIME;`

- Temperature can also be entered as time/temperature pair values.

Specifying Time-Dependent Profiles

In the DICTRA module you are often prompted to specify a time-dependent profile for a condition.

To define the profiles or intervals, enter information as follows:

LOW TIME LIMIT

To determine the time when the function starts to apply.

HIGH TIME LIMIT

To determine the time when the function stops applying. Use an asterisk (*) to set the high limit to the time when the simulation ends.

ANY MORE RANGES

Enter `Y` to specify an additional range with a time-dependent function, which starts to apply at the time step after the high time limit of the previous range is reached.

Creating Regions and Gridpoints

Enter a new region by specifying its name and, unless it is the first region, how it should be located with respect to one already existing region. The size of a region is determined when a grid is entered into the region.

About System, Cells and Regions and About Regions and Grids

How to Create a Region

1. Complete Defining a System in Console Mode.
2. Use ENTER_REGION to enter a region into the system.
3. Enter an arbitrary name for the region at the `Region name` prompt.
4. If this is the first region you create in your system, then you are finished. Otherwise, continue to the next step.
5. Enter the name of an already existing region to which the new region is attached.
6. Specify whether the new region should be `Attached to the right of` the existing region. Enter `Y` to attach to the existing region's right side or `N` to attach it to its left side.
7. If the system has a cylindrical or spherical geometry, then this is a question of whether to put the new region outside the existing region, so that the new region surrounds the existing one, or to put it at the existing region's centre, so that the existing region surrounds the new region.

How to Add Gridpoints to a Region

This topic describes how you specify the size and grid point distribution to use in a region.

1. Complete Defining a System in Console Mode and Creating a region.
2. Use ENTER_GRID_COORDINATES followed by the name of the region.
3. Specify the width of the region in meters.
4. At the `Number of points` prompt enter the number of grid points for the region.
5. Specify the type of grid point distribution to have in the region.
   - `Linear` for an equally spaced grid.
   - `Read_Point_by_Point` to read a number of specific grid points from a data file.

- `Geometric` for a grid that yields a varying density of grid points in the region. Enter the `Value of R in the geometrical series`, which determines the distribution. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.
- `Double_Geometric` to have a high number of grid points in the middle or at both ends of a region. Specify two geometrical factors. `Value of R in the geometrical series for lower part of region` for the distribution in the lower (left) part of a region, and `Value of R in the geometrical series for upper part of subregion` for the distribution in the upper (right) part of a region.

Entering Phases in Regions



There is no supersaturation locally within a given region.

When defining a region you need to enter one or more phases into the region. The number and type of phases depends on the simulation you want to run.

- To simulate diffusion of components within one phase, enter one matrix phase into the region.
- To simulate how an interface between regions moves, enter two regions with at least one phase in each.
- To simulate growth of one or more dispersed phases in a matrix phase, enter one matrix phase and one or more spheroid phases.

▶ About Phases

Entering Phases in a Region

1. Complete Defining a System in Console Mode and Creating Regions and Gridpoints.
2. Use ENTER_PHASE_IN_REGION. Specify whether the phase is to be `Active` or `Inactive`.
3. For an inactive phase, specify the following:
   - Enter the name of the region and the side of that region which the phase is attached to.
   - Enter the required driving force (evaluated as DGM[1], and it is dimensionless (phase) in POLY-3) to be used for determining whether an inactive phase is stable.
   - Enter the `CONDITION TYPE` that the phase boundary condition should be set to if the inactive phase becomes stable. (Inactive phases are only considered in the simulation calculations once it is stable.)
4. For an active phase specify the following:
   - `REGION NAME` for the region in which the phase is to be entered.
   - `PHASE TYPE`: `Matrix`, `Lamellar` or `Spheroid`. `SPHEROID` is only available if a `MATRIX` phase is created first. You can only enter one matrix phase in each region.
   - Enter the `PHASE NAME`. You can append a hash sign (`#`) and a digit at the end of the phase name to designate the composition set number (e.g. `FCC#2`). If you do not append this and the phase has more than one composition set, then you are prompted to specify a composition set number.

Specifying Phase Compositions in a Region

When you specify the composition of a phase, you do this by specifying the composition of the phase within its region—a composition profile.

About Phases and DICTRA Commands

How to Specify Phase Compositions in a Region

1. Complete Defining a System in Console Mode, Creating Regions and Gridpoints and Entering Phases in Regions.
2. Use ENTER_COMPOSITIONS to enter a composition of a phase in a certain region.
3. Enter the `Region name` of the region in which the phase has previously been entered.

---

1. DGM is the POLY variable for the driving force that is already divided by RT.

4. Enter the `Phase name` of the phase whose composition you want to specify.
5. If the phase is spheroid, then for `Use equilibrium value` enter `Y` to automatically calculate the equilibrium fractions of the phase and its constitution at the start of the simulation. Specify the initial `Volume fraction of` the spheroid phase.
6. Enter the `Dependent component`. Sometimes the dependent component is automatically set and there is no prompt.
7. Enter a `Composition type` for the constitution of the phase. The options are: SITE_FRACTION, MOLE_FRACTION, MOLE_PERCENT, WEIGHT_FRACTION, WEIGHT_PERCENT, and U_FRACTION.
8. Enter the `Type` of composition profile (that is, the type of composition profile). The options are:

- `Linear` to have an equally spaced composition distribution. Specify the composition at the first (leftmost) grid point (`Value of first point`) and at the last (rightmost) grid point (`Value of last point`).
- `Read_point_by_point` to read the composition at each grid point. The specification of these can either be read from a DATA-file that you are prompted to select or entered directly at the terminal. If you want to enter them at the terminal, then enter `READ_POINT_BY_POINT` and press <Enter>.
- `Geometric` for a distribution that yields a higher concentration of the component at the lower end of the region if a geometrical factor larger than one is given and a higher concentration at the upper end of the region if the factor is smaller than one. You are prompted to specify the `Value of R in the geometrical series` which determines the distribution.
- `Function` for the global distance denoted 'gd'. Useful functions include the error function (`erf(gd)`) and the heavy-side step function (`hs(gd)`). For example, the function `3+2hs(x-1e-4)` specifies a concentration of 3 at the region's left side and 5 at the region's right side, with a sharp step in the concentration profile at 1e-4m=100µm.

Specifying the Geometry

By default a DICTRA module system has a planar geometry. To change the geometry of the system, use ENTER_GEOMETRICAL_EXPONENT followed by a number `0` (planar), `1` (cylindrical) or `2` (spherical).

▶ About Geometry and Coordinates

With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere. The highest coordinate (right boundary) is defined by

the cylinder or sphere radius. If you want a geometry corresponding to a tube or a hollow sphere, then use SET_FIRST_INTERFACE to locate the system's left boundary at a coordinate that is greater than zero.

Setting Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

How to Set Boundary Conditions

1. Complete Defining a System in Console Mode and Creating Regions and Gridpoints.
2. Use SET_CONDITION and choose `Boundary`. Then specify whether you want to set the LOWER or the UPPER boundary.
3. Specify which condition type you want to set the boundary to.
4. Enter any parameter values that are necessary for the condition type you have chosen.
5. Specify the `LOW TIME LIMIT`, when the function you define starts to apply.
6. If required, enter the function that is applied during the time interval. For most condition types, the function may have time, temperature and pressure as arguments.
7. Enter the `HIGH TIME LIMIT` for the interval.
8. If you want to define a different function for another time interval, then enter `Y` when prompted with `ANY MORE RANGES`. Then enter another function for the next range.
9. When you have defined functions for all the ranges you want, enter `N` at the `ANY MORE RANGES` prompt.

Adding (Creating) Cells

If you add cells to a system, then each new cell is always placed next to the system's right outer boundary. Use the command CREATE_NEW_CELL.

Importing a Scheil Segregation Profile

You can import a previously calculated Scheil segregation profile into the Diffusion Module (DICTRA). A Scheil calculation is a conservative estimate of the segregation that occurs during solidification and is useful when estimating the necessary time/temperature for a homogenizing heat treatment.

From a practical point of view it is also a simple and fast calculation compared to a more accurate, but computationally more difficult, diffusion simulation.



In order to limit the computational effort, this feature cannot be combined with the fast diffusers option in the Scheil module.

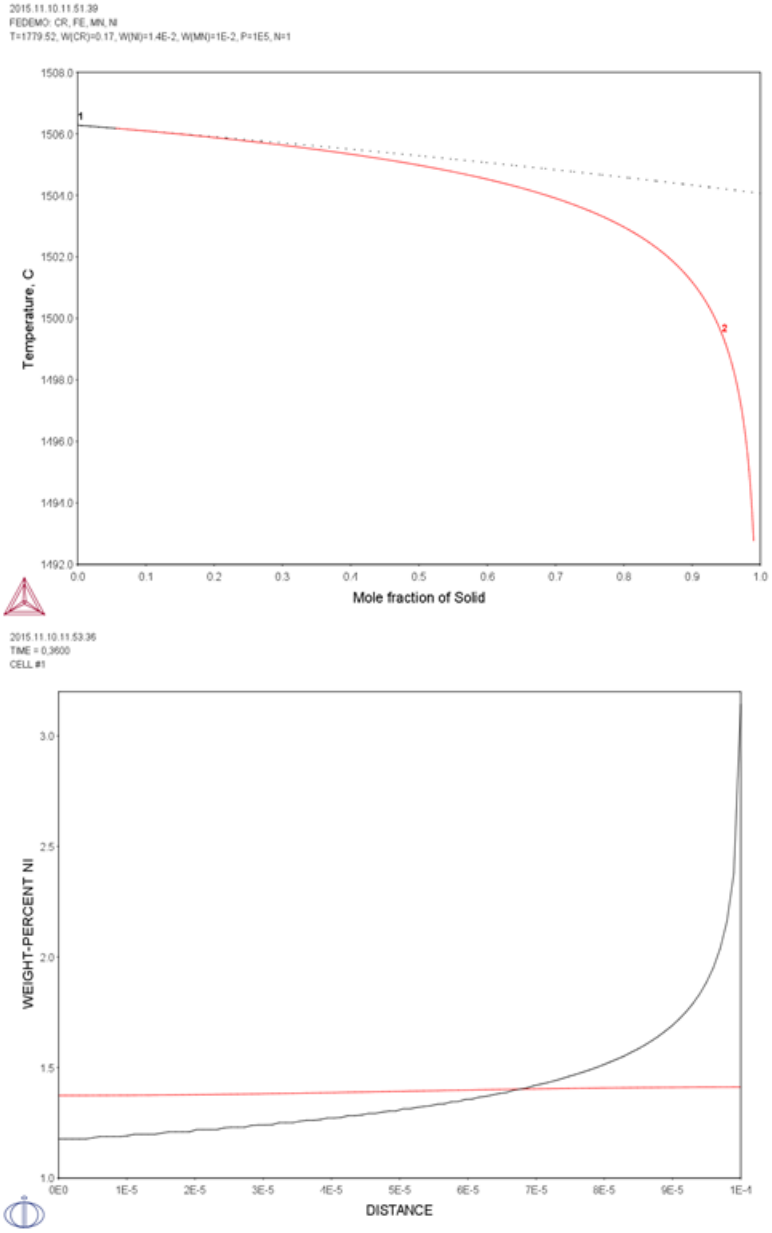


Press F1 in Thermo-Calc to search the help for more information.

Example a7

In the following example, taken from the Diffusion Module example collection (see About the Examples in the Thermo-Calc documentation), the Scheil segregation profile for a ferritic stainless steel (Fe-17Cr-1.4Ni-1Mn) was calculated in the Scheil module in Thermo-Calc.

The profile was then imported into the DICTRA module and a one hour homogenizing heat treatment at 1200° C was simulated. For the simulation a domain size of 100 µm was assumed, which approximately corresponds to the secondary dendrite arm spacing.



The plots show the initial (left) and final (right) Ni profile.

Models in the Diffusion Module

In this section:

About the Homogenization Model 60
About the Disperse Model 60
About the Para Equilibrium Model 61
About the Thermomigration Model 61
About the Grain Boundary Model (GB_Model) 61
Coarsening Processes 62
About the Coarsening Model 62
About the Pearlite Model 63
About Cooperative Growth 63
About Using Volume in the Diffusion Module (DICTRA) 64

About the Homogenization Model

This section or topic is specific to Console Mode.

If you enter a spheroid phase when you configure your calculation, then the homogenization model is automatically used. This is useful when you want to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point.

You can also explicitly set the DICTRA module to use the HOMOGENIZATION_MODEL. This way, you can use it when calculating a one phase or a moving boundary simulation.

When the homogenization model is used, simulations are run using an implicit finite volume method to increase numerical stability. Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations. You can increase or decrease the `Degree of implicity when integrating PDEs` with the command SET_SIMULATION_CONDITION.

There are several special commands for use with this model. The UTILITIES_ HOMOGENIZATION and SPECIAL_HOMOGENIZATION_OPTIONS commands are described individually in the *Diffusion Module Command Reference*. Search the help (press F1 in Thermo-Calc) for information.

If you have entered a spheroid phase in a region and want to use the older so-called dispersed system model, then you must explicitly disable the Homogenization Model after all phases have been entered.

About the Disperse Model

This section or topic is specific to Console Mode.

This model can be used to calculate diffusion of a phase that is dispersed in a matrix phase. However, it is recommended that you use the HOMOGENIZATION_MODEL for this type of calculation instead.

There is no specific command to activate this model. It is only available if a phase of type "spheroid" is entered in a region.

The disperse model has the following limitations:

- There must be a continuous matrix phase otherwise the simulation breaks down.
- There is no implicit integration of the partial differential equations (PDEs), leading to a lower accuracy.
- Only diffusion in the matrix phase can be simulated. It is assumed that no diffusion occurs in the dispersed phase.

After a spheroid phase is entered, the homogenization model must explicitly be *inactivated* in order to run the simulation with the dispersed model. To do this, enter the command HOMOGENIZATION_MODEL and then choose N to make it inactive.

About the Para Equilibrium Model

The model allows you to calculate a moving phase boundary simulation while assuming that para-equilibrium conditions hold at the boundary. You must explicitly set the DICTRA module to use this model with the PARA_EQUILIBRIUM_MODEL command.

When this model is used, it implies that the local equilibrium assumption is no longer valid and that substitutional components are regarded as one composite component. You can only simulate a single moving boundary in one cell.

About the Thermomigration Model



This section or topic is specific to Console Mode.

The thermomigration model allows you to simulate thermally induced diffusion in temperature gradients. To use the model, you must set the temperature to depend on the spatial coordinate (x) in your calculation. In addition, you must also enter the heat of transport quantity (Q*) using the ENTER_HEAT_TRANSFER_PARAMETER command. You must enter this parameter separately for each element in each phase.



The model is automatically used once this is done.



See Console Mode example exh3 in the *Diffusion Module Examples Guide*.

About the Grain Boundary Model (GB_Model)



This section or topic is specific to Console Mode.

You must explicitly set the DICTRA module to use this model with GB_MODEL. This model allows you to simulate grain-boundary and dislocation-assisted diffusion.

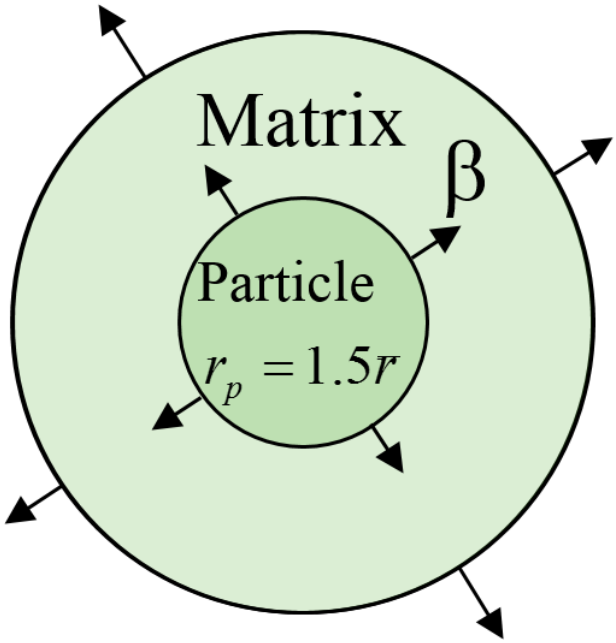
The grain boundaries and the dislocations contribute to the total amount of diffusion according to the weighted fractions. The parameters are entered separately for each region in order to allow for different expression for different phases.

Coarsening Processes

This type of simulation is available for Console Mode. See About the Coarsening Model for more information.

You can run a simulation of a coarsening process. In accordance with Lifshitz-Slyozov-Wagner theory, this is done by assuming that the coarsening can be simulated by calculating the growth of a single particle of the maximum size in the particle size distribution.

Simulate a coarsening process



About the Coarsening Model

This section or topic is specific to Console Mode.

The model is based on LSW theory (after Lifshitz and Slyozov (1961)[1.] and Wagner (1967)[2.]. The model is also described in Gustafson, Höglund, and Ågren (1998)[3.] and Björklund, Donaghey, and Hillert (1972)[4.].

LSW theory is strictly only valid for low volume fractions of the particle phase. The theory predicts that the normalized particle size distribution obtains a constant shape where the largest particles have a radius equal to 1.5 times the average particle radius.

The calculations are performed in one cell on a maximum size particle which thus is assumed to be 1.5 times the size of the average particle size. The matrix phase is on one side in contact with the maximum size particle and on the other the matrix phase is in local equilibrium with an average sized particle. The effect of the surface energy is such that both the maximum size particle as well as the matrix phase grows.

The model allows you to perform coarsening simulations. You must explicitly set the DICTRA module to use this model with the command COARSENING_MODEL.

To use this mode, configure the calculation as follows:

- Have one cell only, with a single particle that is 1.5 times larger than the average particle size.
- The matrix phase should be in contact with the maximum size particle on the left/lower side, and then the model specifies a local equilibrium with an average sized particle on the right/upper side.
- The surface energy then results in growth of both the maximum size particle and the matrix phase. Use the SET_SURFACE_TENSION command to enter the surface energy to enable coarsening.

About the Pearlite Model



This section or topic is specific to Console Mode.

The pearlite model is automatically used if there is lamellar phase in a region.

About Cooperative Growth



This section or topic is specific to Console Mode.

1. Lifshitz, I.M., and V.V. Slyozov. 1961. “The Kinetics of Precipitation from Supersaturated Solid Solutions.” Journal of Physics and Chemistry of Solids 19 (1–2): 35–50.
2. Wagner, Carl. 1967. “Theorie Der Alterung von Niederschlägen Durch Umlösen (Ostwald-Reifung).” Berichte Der Bunsengesellschaft Für Physikalische Chemie 65 (7–8): 581–91.
3. 'Simulation of carbo-nitride coarsening in multicomponent Cr-steels for high temperature applications'. In *Advanced heat resistant steels for power generation* (San Sebastian, Spain 27/04/1998
4. Björklund, Stig, L F Donaghey, and Mats Hillert. 1972. “The Effect of Alloying Elements on the Rate of Ostwald Ripening of Cementite in Steel.” Acta Metallurgica 20 (7): 867–74.

You can simulate the growth of pearlite in alloyed steels by calculating the Eutectoid reaction γ→α+β, where α and β grow cooperatively as a lamellar aggregate into the γ matrix.

About Using Volume in the Diffusion Module (DICTRA)

This section or topic is specific to Console Mode.

The following is applicable to the use of the classic models in the Diffusion Module (DICTRA). That is, all models *except* the homogenization model.

DICTRA uses a simplified treatment of volume, i.e. DICTRA does not use volume data from the thermodynamic databases. This implementation in the original software development was because most databases did not contain volume data at that time.

The basic rule to use when applying the classic model is that only substitutional phase constituents contribute to volume and the partial molar volume of such constituents are assumed to be constant and equal. The partial molar volume of interstitial phase constituents are assumed to be zero. The actual value used as partial molar volume of substitutional phase constituents is 10-5 [m^3/mol] and this is entered in databases as a constant `VS`.

The databases contain definitions of *zero volume species* and these species can then be interstitial phase constituents. Typically, C, N and O are entered as zero volume species.

There is, however, a rule that supersedes the basic rule, that is, for a phase that consists of a single sublattice, such as graphite, all constituents are considered to be substitutional. Another case is the liquid, which in most databases is described with a single sublattice. In such a liquid all constituents are then considered to be substitutional.

Thus, a given species can be interstitial in one phase but substitutional in another.

For the homogenization model the treatment of volume is, unfortunately, but for good reason, slightly different. The homogenization model only considers the elements of the system and regards each element as being either substitutional or interstitial. This status is the same in all phases. For many cases this treatment yields the same result as the rules for the classic model described above. However, it does not work for graphite, which has zero volume.

Plotting Simulations in the POST Module

You can plot or tabulate the results of your simulation in the POST_PROCESSOR module, also called the POST module and accessed within the DICTRA module. The resulting diagram is on a plot tab in the Console Results window. Once the simulation results are plotted, you can then change its appearance in the Plot Properties window.

In this section:

Plotting Simulation Results 66

Editing the Plot Properties 67

Tabulating Simulation Results 68

Plotting Simulation Results

Saving and Printing the Output in Console Mode

Plotting a diagram is to graphically represent how a dependent variable varies with an independent variable. The independent variable is either distance or time.

1. Complete all the steps to run your simulation.
2. At the `DIC` prompt type `POST_PROCESSOR` (or just `POST`).
3. Use SET_DIAGRAM_AXIS to specify the variables to plot on the X- and Y-axes of the diagram. One of the axes must be set to either TIME or DISTANCE.

   For example, to set the X-axis to plot the distance from the lower boundary of the calculation (rather than from the lower boundary of the current region) and the Y-axis to plot the weight-percent composition of the Si element, at the `POST` prompt type:

   ```
   SET_DIAGRAM_AXIS X DISTANCE GLOBAL
   SET_DIAGRAM AXIS Y WEIGHT-PERCENT SI
   ```

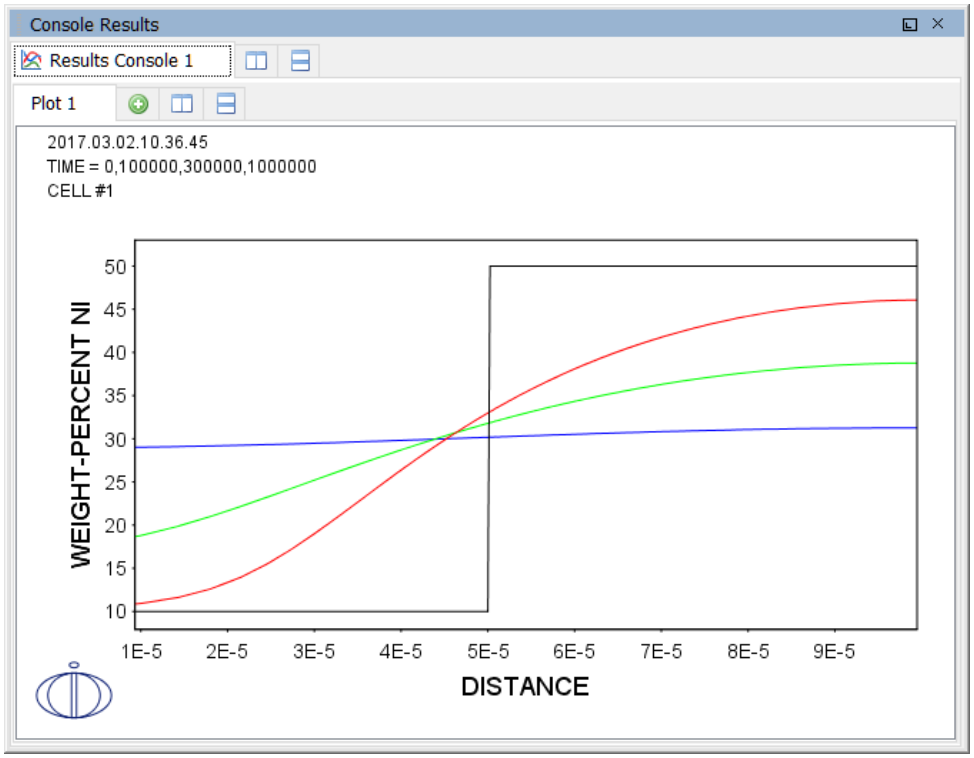
4. You can specify a Z-axis, which is represented as tick marks on the curve in the XY-plane.
5. When one of the axes is set to TIME or DISTANCE, the variable automatically becomes the independent variable. If you do not want the independent variable plotted along an axis, use SET_INDEPENDENT_VARIABLE and set it to `Time` or `Distance`.
6. Simulation calculations depend on both time and a spatial coordinate; these variables must be fixed during the plotting process. Use SET_PLOT_CONDITION to set the variable to keep fixed. These variables can be set as the fixed plot condition:
   - `Time`: The integration time. More than one value can be entered using commas or spaces to separate the values. One graph is plotted for each value.
   - `Distance`: The distance in the system (from the lower boundary).
   - `Interface`: At the location of a certain interface between two phases.
   - `Intergral`: The value of the plot condition is integrated over the phase, region or system volume.

7. Use PLOT_DIAGRAM to plot the results. The plot is added as a tab to the **Console Results** window.

   The plot example below is from example exa2a, which is part of the Diffusion Module example collection (see About the Examples in the Thermo-Calc documentation). Distance is set as the independent variable and the weight-percent of Ni is on the Y-axis. The plot condition is `TIME`: the plot shows four graphs, each with the spatial distribution of Ni in the region at the time steps 0, 1e5, 3e5, and 10e5.

8. To print the plotted graphs direct to a postscript-file, type `Plot` and a file name.
9. In the **Plot** window, right click the diagram and choose **Properties** to adjust its appearance and colors.

Editing the Plot Properties.



Editing the Plot Properties

To change the appearance of a plotted diagram, right click the diagram and select **Properties**. In the **Plot Properties** window you can change the fonts and colours, and add a title, for example.

You can also change the colour, stroke (solid/dashed/dotted/dash_dot) and line width of a particular series of lines in the plot by double-clicking one of the lines in the series. In this way, you can also toggle whether data points should be shown or not for a series of lines. The crosshair cursor turns into a cursor resembling a pointing hand when it is placed over a line that can be clicked but if you hold down the <Ctrl> key, this does not happen (the cursor continues to be shown as a crosshair).



To configure the default settings for plotting, from the main menu, select **Tools→Options**. For Console Mode click the **Plotting** tab.

Global Settings in the *Thermo-Calc User Guide*

Tabulating Simulation Results

DICTRA Commands

1. Complete all the steps to run your simulation.
2. At the DIC prompt type `POST_PROCESSOR` (or just `POST`).
3. Use ENTER_SYMBOL `Table` to specify the variables to be shown in the table columns. Separate the variables by commas (,).
4. Use SET_INDEPENDENT_VARIABLE to specify the variable that the rows in the table should represent.
5. Use TABULATE to generate the table.

Troubleshooting

The following topics contain some general advice to consider in order to avoid having your simulation fail to converge when you calculate different kinds of simulations in the Diffusion Module (DICTRA).

In this section:

Tips for a Successful Diffusion Simulation 70

Moving Boundary Simulations 73

Cell Calculations 74

Diffusion in Dispersed Systems 74

Cooperative Growth 74

Tips for a Successful Diffusion Simulation

Simplify Your Simulation

For example, if you have an alloy with five or six elements, first run a simulation with only the main elements. When this simulation works, you can then add more elements as necessary.

Start with a Low Accuracy and Refine It

If you start with a high accuracy setting, then computing the simulation takes much longer, and problems are more likely. Check the profiles and the overall mass balance, and if the accuracy is insufficient then you can improve the accuracy values.

To change the accuracy:



In Console Mode use SET_ACCURACY and increase or decrease `Max relative error` and `Max absolute error`.



In Graphical Mode the setting is on the Diffusion Calculator in the section *Time step control*.

Modify the Grid or Time Step

If you get large fluctuations in the composition or phase boundary profiles, then you can try modifying the grid or the time step of the simulation. You can increase the time step by lowering the accuracy if automatic time step control is used (the default).

If you increase the tolerated relative and/or absolute error then the automatic time step control increases the time step.



In Console Mode use the SET_ACCURACY command.



In Graphical Mode the setting is on the Diffusion Calculator in the section *Time step control*.

Integrate the PDEs

The composition or phase boundary profiles can often also be improved if the partial differential equations (PDEs) are integrated fully implicitly (i.e. Euler backward).

To integrate the PDEs in this way:



In Console Mode use SET_SIMULATION_CONDITION to set the parameter `Degree of Implicity when Integrating PDEs` to a value of `1`.



In Graphical Mode, the setting is on the Diffusion Calculator on the **Options** tab. Under *Simulation Conditions*, you can try a different **Time integration method**. The default method is Trapezoidal, which is equivalent to a 0.5 numerical setting in Console Mode. If you choose Euler backward, this is equivalent to a 1.0 numerical setting in Console Mode.

Debug (Console Mode)

If your Console Mode simulation fails to converge, then debugging may give you some clues about the source of the failure. To receive more detailed information about what is happening during the simulation use the command DEBUGGING.

Moving Boundary Simulations

Grid Distribution

Check the grid distribution at the interfaces. If the grid is too coarse or too fine-grained then the fluxes may not be defined well.

Use Activities Instead of Potentials

Use activities instead of potentials when the content of one or more of the elements becomes very low. If you do this, then the activity approaches zero, which is easier to handle than a potential that approaches infinity.

In Console Mode, use SET_SIMULATION_CONDITION to set the parameter `Vary potentials or activities` to `Activities`.

In Graphical Mode the setting is on the Diffusion Calculator in the section *Classic model specific*. From the list, choose **activity** [**Use the activity of a component in order to find the correct tieline at the phase interface**].

Starting Values

Use the automatic starting values when you run the simulation the first time. If the first time step does not converge try decreasing the starting values for the velocities. Alternatively, increase the duration of the first time step.

If the simulation fails during the first time step, then check how the starting values affect the residuals.

In Console Mode, use the command SET_SIMULATION_CONDITION and set the parameter `NS01A PRINT CONTROL` to `1`.

When you adjust this setting, the software then prints the tried unknown value and the residual for each flux balance equation in each iteration. The equations are organized so that the first unknown value is always the migration rate of the phase interfaces followed by the unknown potentials. All unknown values are scaled by the starting value or the calculated value in the previous time step.

Cell Calculations



This section or topic is specific to Console Mode.

In cell calculations, determine start values for each cell separately and thereafter connect the individual cells. You can even start out simulating in planar and/or cylindrical geometry in order to determine sufficient starting values if you want to use a spherical geometry.

Diffusion in Dispersed Systems



This section or topic is specific to Console Mode.

If you simulate diffusion in a dispersed system and the homogenization model is turned off, then time integration is explicit. The maximum time step allowed, or the highest time step actually taken in the calculation, affects the final result of the simulation. This effect is most evident if one or more of the diffusing species have low solubility in the matrix phase. When this is the case, a supersaturation is created in the matrix phase during a diffusion step and if too large a time step is allowed, then too much supersaturation is created. Consequently, always check your results by performing a second simulation with a maximum time step that is ten times lower than in the first run. If there is large difference in results between the first and the second run, then decrease the time step again with a factor of ten and perform a third run. Repeat this process until the results can be trusted.

If a simulation fails because the program is not able to calculate an equilibrium, then try to calculate the initial equilibrium yourself using Thermo-Calc and enter the composition and fraction of each phase separately instead of having the DICTRA module calculate it. Also enter starting values for each phase with the command SET_ALL_START_VALUES. Alternatively, you may force the software to use certain start values using SET_SIMULATION_CONDITION.

Cooperative Growth



This section or topic is specific to Console Mode.

If your simulation fails to converge, try calculating the A1e temperature with Thermo-Calc and start your simulation at a temperature slightly below that temperature. Use the equations given in the interactive help in order to estimate S0 and the growth rate.

Diffusion Module (DICTRA) Console Mode Examples

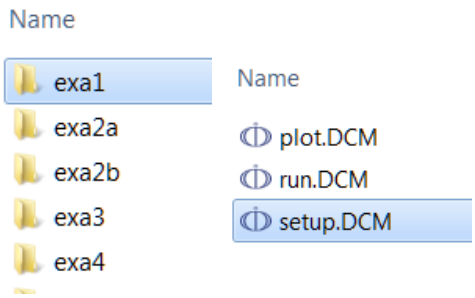
To learn more about how to use the add-on software you can open and run the example files. These macro files (with the extension *.DCM) include comments, which you can either run in the Thermo-Calc program or open and read in a text editor.

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

If you read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Opening the Setup, Run, and Plot Macro Files

For the main set of examples (this is different for the Quick Start examples), there are three macro files: a **setup**, **run** and a **plot**. You must run these macros in order.



To begin, double-click the **setup.DCM** file to open it. It launches a new session of Thermo-Calc and opens in Console Mode.

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

Quick Start Guide Examples

These examples are used in the *Diffusion Module Quick Start Guide (Console Mode)*. It is recommended you review this guide before going to the additional examples.

File Name	Description
simplest_ dictra.dcm	Simple homogenization of a binary Fe-Ni alloy. Initially it is assumed to have a linear Ni-concentration profile.
simple_moving_ boundary.dcm	Calculating a ferrite(bcc)/austenite(fcc) transformation in a binary Fe-C alloy
multiphase_ example.dcm	Shows the use of the homogenization model for multiphase simulations. It is taken from Larsson and Engström (2006), "A homogenization approach to diffusion simulations applied to α + γ Fe–Cr–Ni diffusion couples", *Acta. Mater.* 54, pp. 2431-2439. Experimental data is from Engström (1995), "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.* 243, p. 12.

One Phase Examples

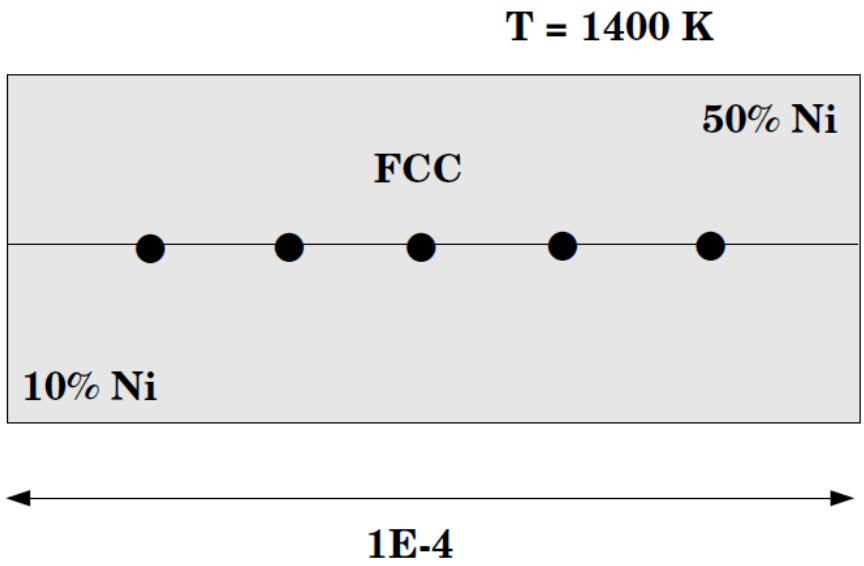
All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.



Example exa1

Homogenization of a binary Fe-Ni alloy: Linear concentration profile

Simple homogenization of a binary Fe-Ni alloy. It is assumed there is initially a linear Ni-concentration profile.

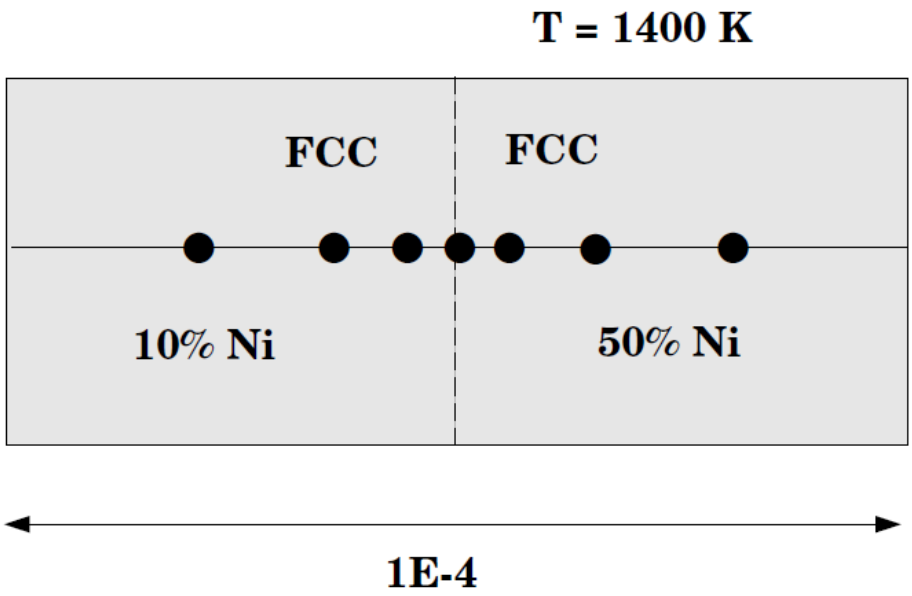


Example exa2a and exa2b

Homogenization of a binary Fe-Ni alloy

- Example exa2a **Step Profile:** Simple homogenization of a binary Fe-Ni alloy. A Ni rich and a Ni lean alloy are put together and initially there is a step profile.
- Example exa2b **Time Integration:** This example is identical to a2a but instead it uses implicit time integration instead of the trapezoidal method for solving the PDEs.

The exa2b example uses the TCFE and MOBFE databases. These licenses are required to run the example.



Example exa3

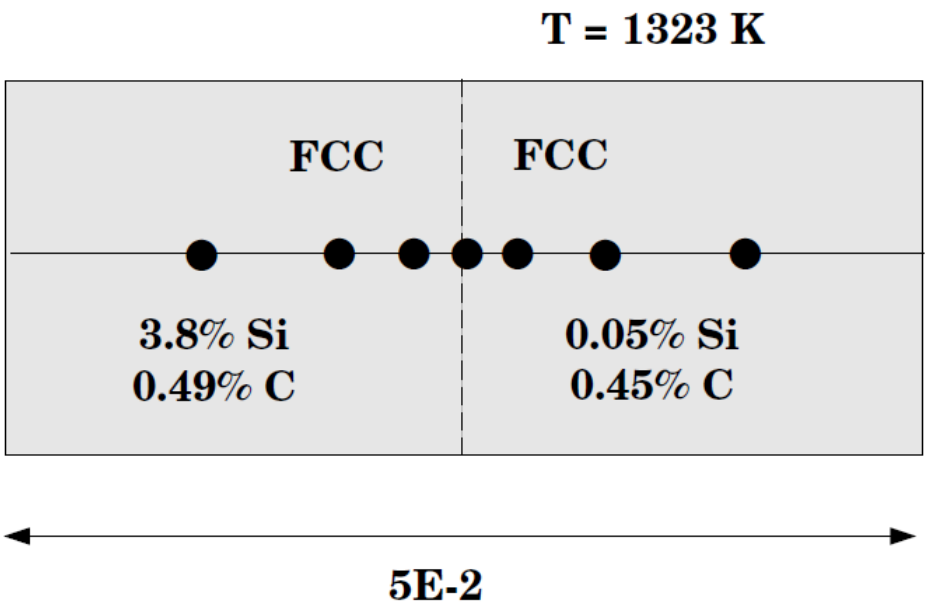
Uphill diffusion in an Fe-Si-C alloy

This is an example to simulate uphill diffusion in a ternary single phase austenite matrix due to the classical Darken experiment published by Darken, 1949: "Diffusion of Carbon in Austenite with a Discontinuity in Composition", *Trans. Amer. Soc. Metals, AIME*, 180, 430–438.

In this example, two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed at 1050 C for 13 days. As both pieces are austenite they must be entered into the same region. This is done by individually giving the compositions of Si and C in each grid point. These data are then stored to file.



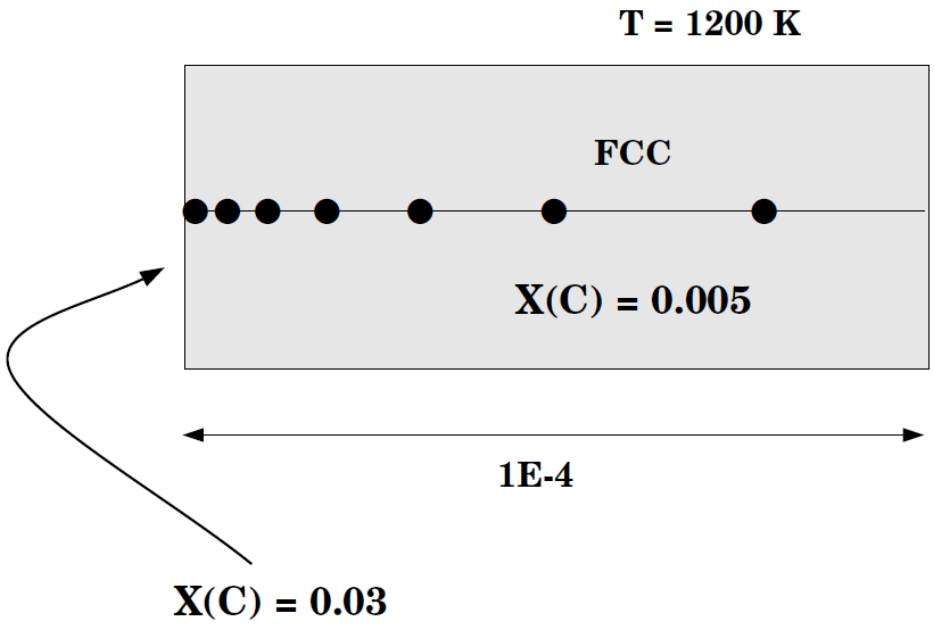
This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



Example exa4

Carburization of binary Fe-C alloy: Comparison to an analytical erf solution

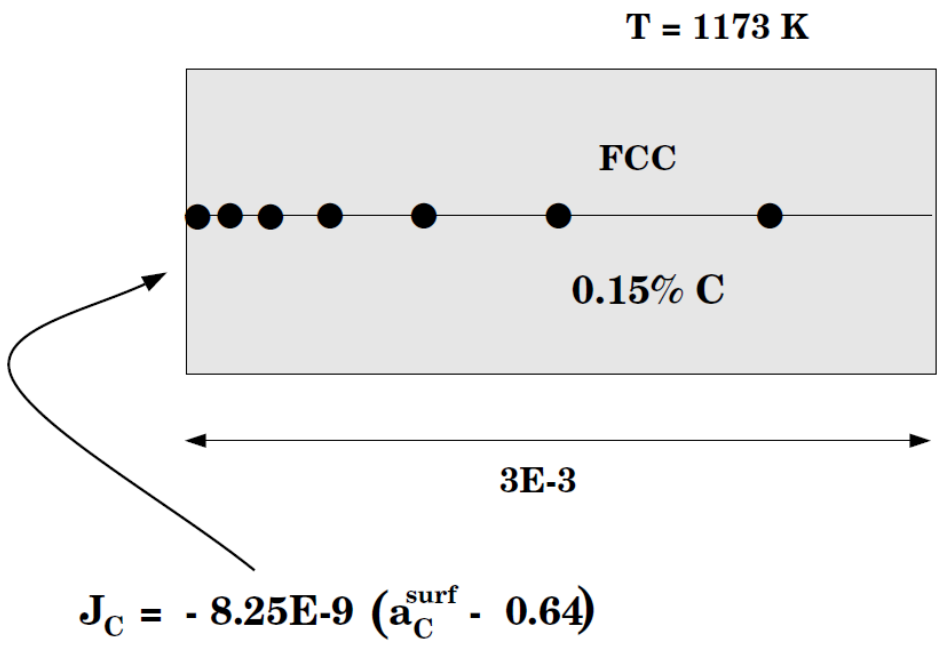
This is a simple binary simulation with one single phase region. The numerical simulation is compared with an analytical erf-solution. A special database is created (*erf.tdb*) where the diffusion coefficient is set to a concentration independent value.



Example exa5

Carburization of a binary Fe-0.15 wt% C alloy

A mixture of 40% N2 and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt% and a surface reaction controls the flux of C at the surface.

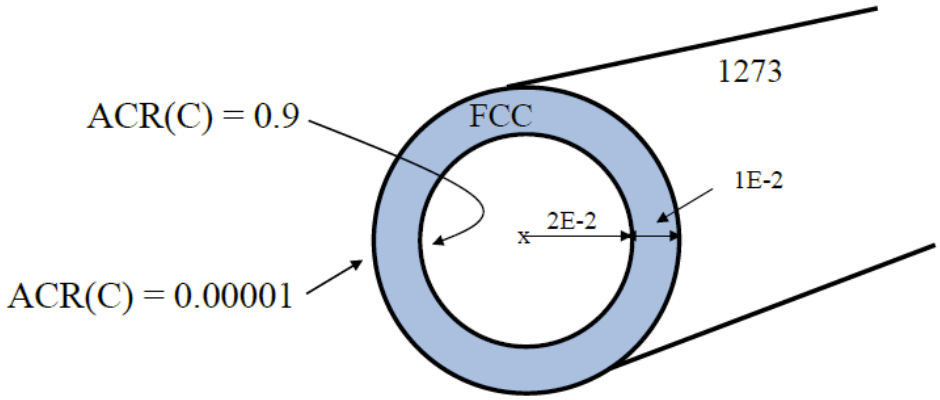


Example exa6

Diffusion through a tube wall

A simple example of diffusion through a tube wall. The tube material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the C-activity is very low. This example demonstrates the use of the command SET-FIRST-INTERFACE as well as the use of MIXED boundary conditions.

This example uses the TCFE and MOBFE databases. These licenses are required to run the example.

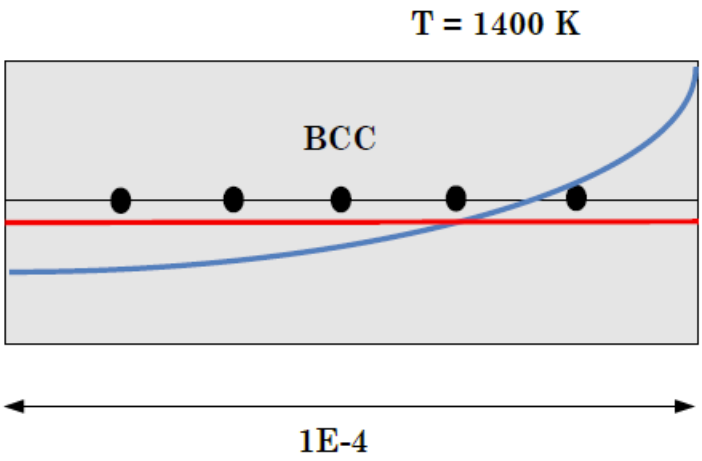


A modified version of this example is also available in Graphical Mode as example D_06. For Graphical Mode you do not need a Diffusion Module (DICTRA) license. You can open the example from Thermo-Calc when in Graphical Mode (**File → Examples Files → Diffusion Module**).

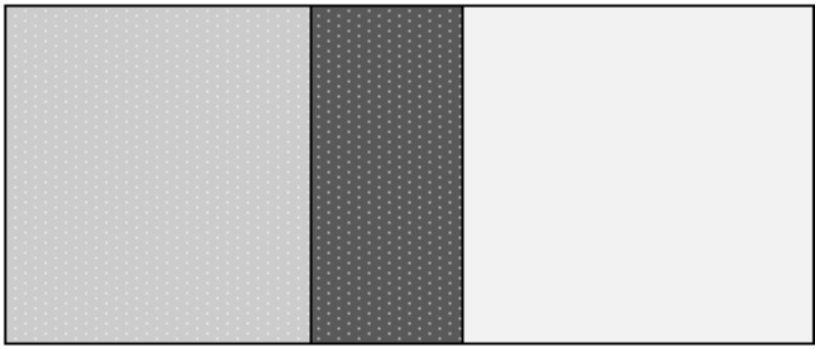
Example exa7

Homogenization heat treatment

The initial segregation profile is created from a Scheil calculation (see `macro create_initial_profile.TCM`). The command INPUT_SCHEIL_PROFILE in the DICTRA monitor performs most of the setup. Only time and temperature must be entered after the INPUT_SCHEIL_PROFILE command is executed.



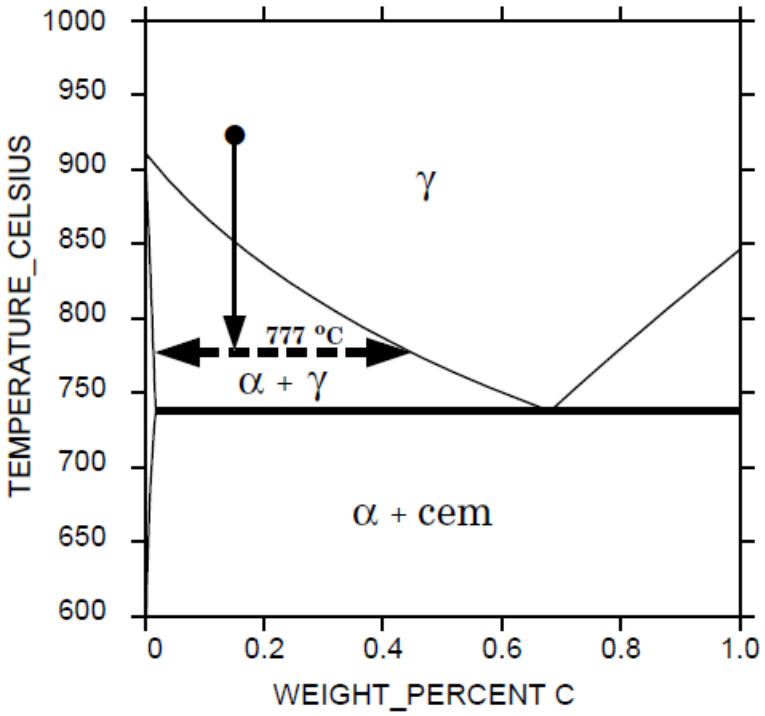
Moving Boundary Examples

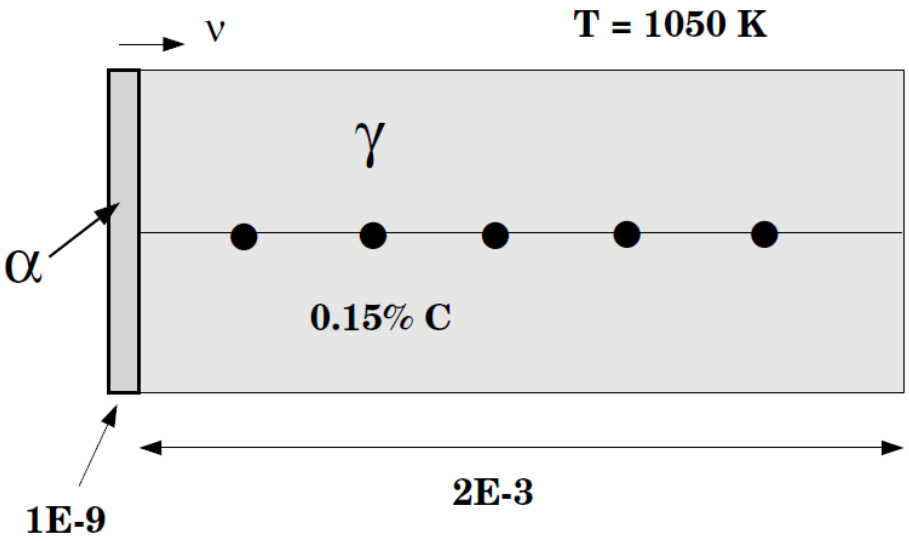


Example exb1a

Austenite (γ) to ferrite (α) transformation in a binary Fe-C alloy

This example calculates a ferrite (BCC)/austenite (FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2 mm thickness. The composition of the austenite is Fe-0.15wt%C. After austenitization the specimen is quenched down to 1050K. The system is assumed closed, so no boundary conditions are set (a closed system is the default). Ferrite is expected to grow into the austenite. For this reason you start with a thin region with ferrite adjacent to the austenite.

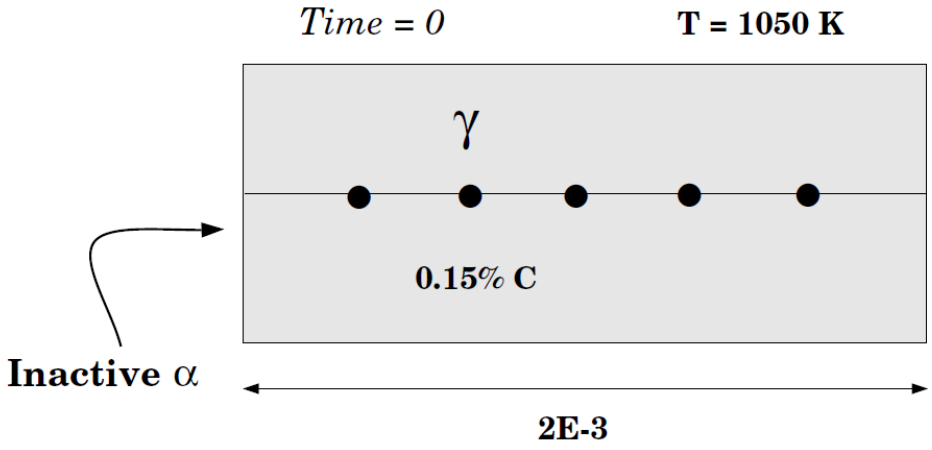


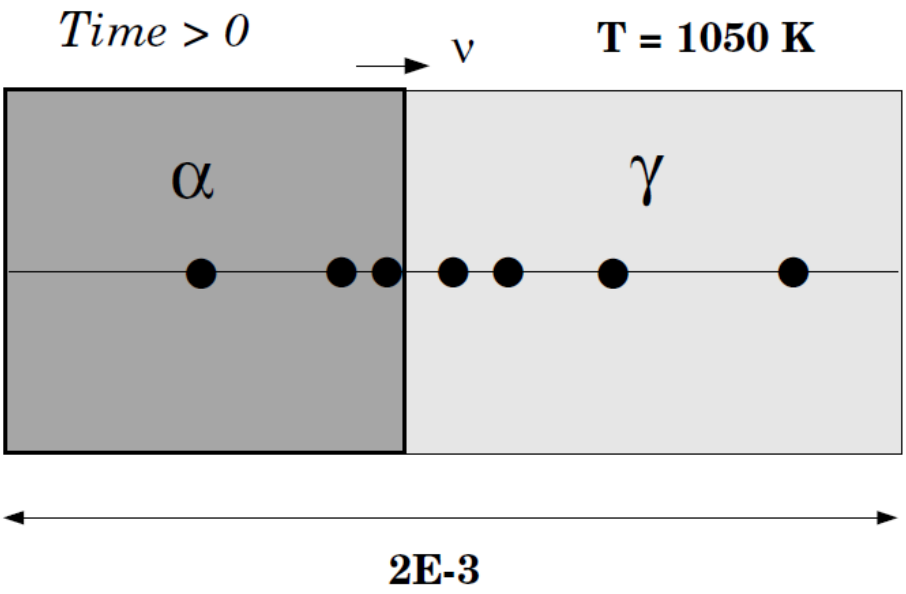


Example exb1b

Austenite (γ) to ferrite (α) transformation in a binary Fe-C alloy: Inactive α

This is the same example as in exb1a but now the problem is with ferrite as an inactive phase adjacent to the initial austenite.



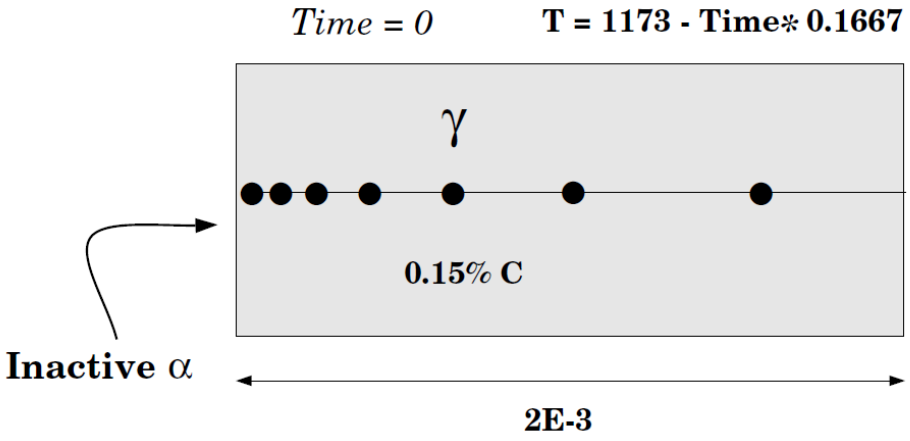


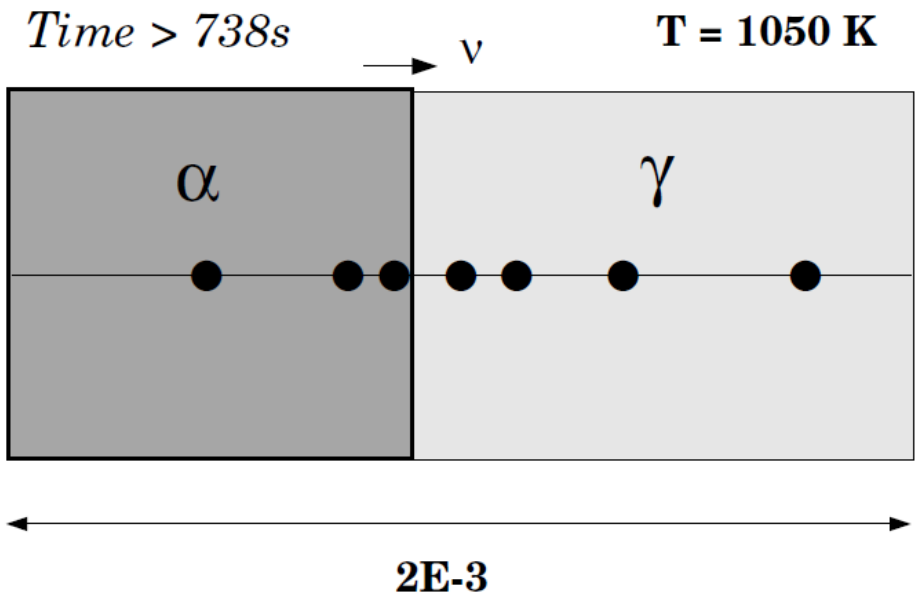
Example exb1c

Austenite (γ) to ferrite (α) transformation in a binary Fe-C alloy: Gradual cool down to 1050K

This is the same example as in exb1a and exb1b but now the simulation starts at a higher temperature and assumes a gradual cooling down to 1050 K.

When 1050 K is reached, the temperature is kept constant and thus has an isothermal transformation. As in exb1b, ferrite is in an inactive phase adjacent to the initial austenite.





Example exb2

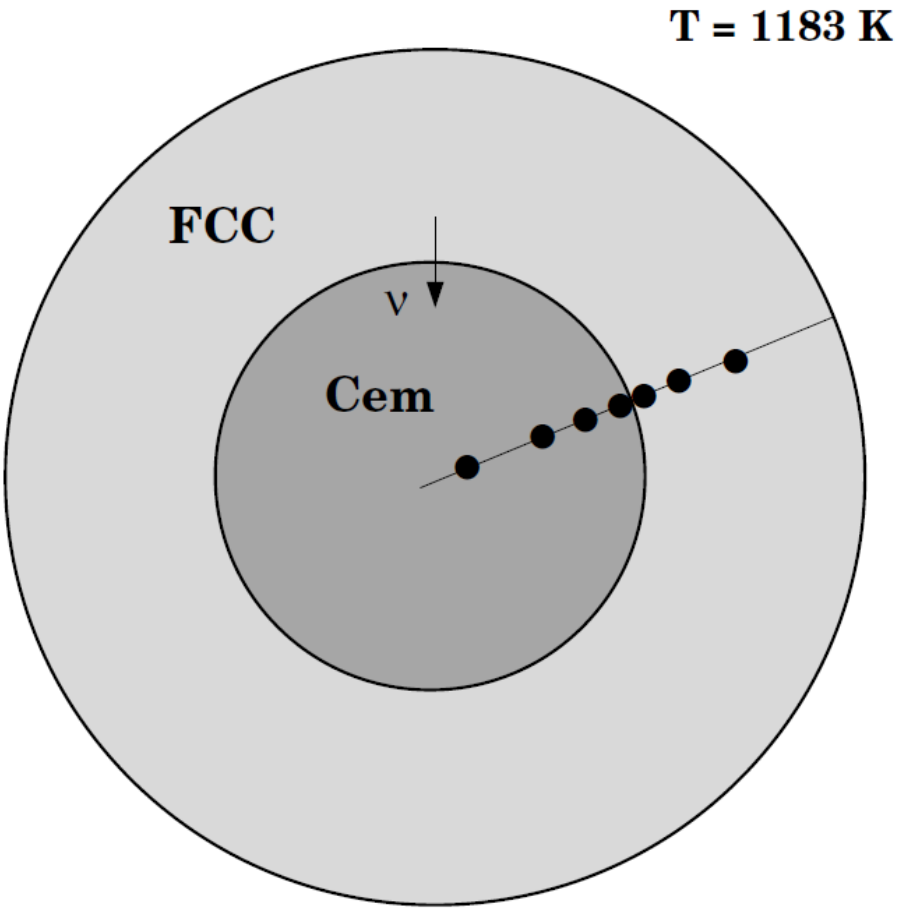
Cementite dissolution in an Fe-Cr-C alloy

This example calculates the dissolution of a spherical cementite particle in an austenite matrix.

This case is from Liu, Höglund, Jönsson, and Ågren, 1991:, "An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy", *Met. Trans. A*, 22(8), 1745–1752.

In order to achieve the correct average composition in the calculation it is necessary to take into account the fact that the calculation is set up using the volume fraction of the phases. To calculate the initial state at the heat treatment temperature we need first to determine the state at the normalizing temperature. To calculate the volume fraction of the phases we need to enter a number of functions that calculate these quantities.

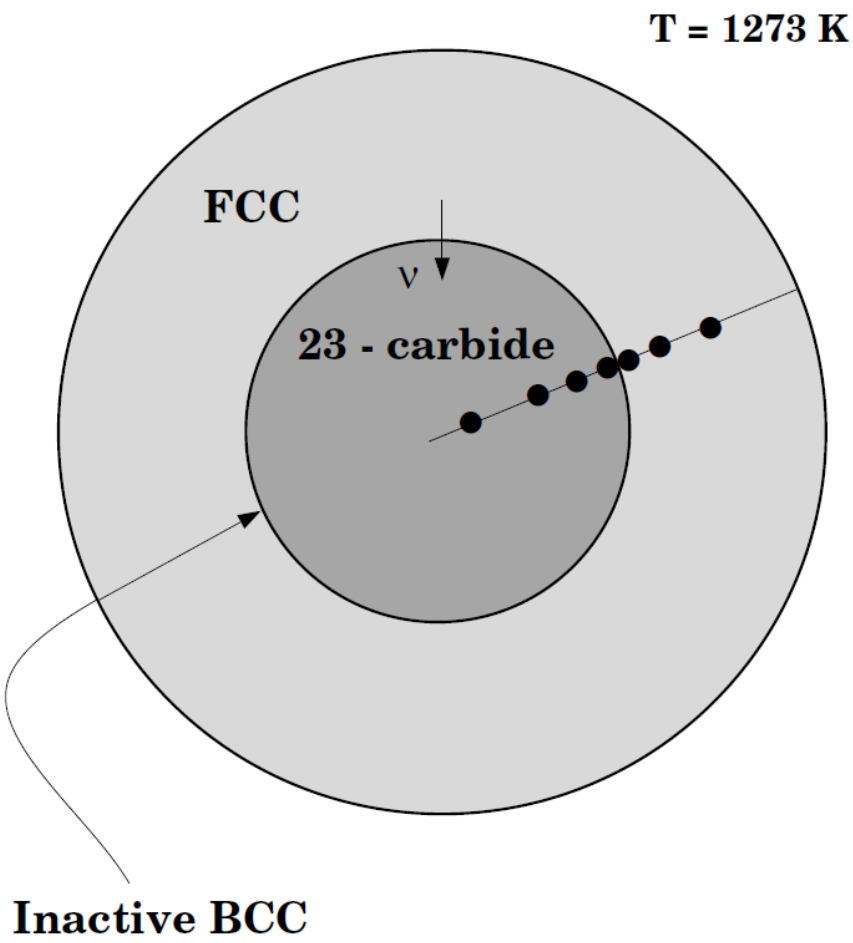
This example uses the MOBFE database. This license is required to run the example.



Example exb3

Dissolution of 23-carbide in an austenitic matrix

This example calculates the dissolution of an M23C6 particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.

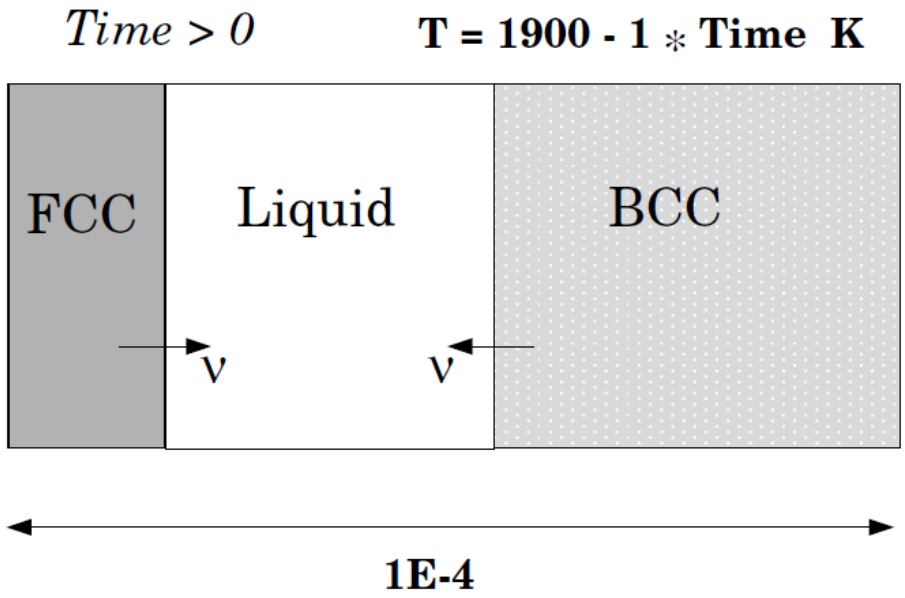


Example exb4a

Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction

This example demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the BCC and FCC regions should be on separate sides of the liquid region. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

This example uses the MOBFE database. This license is required to run the example.

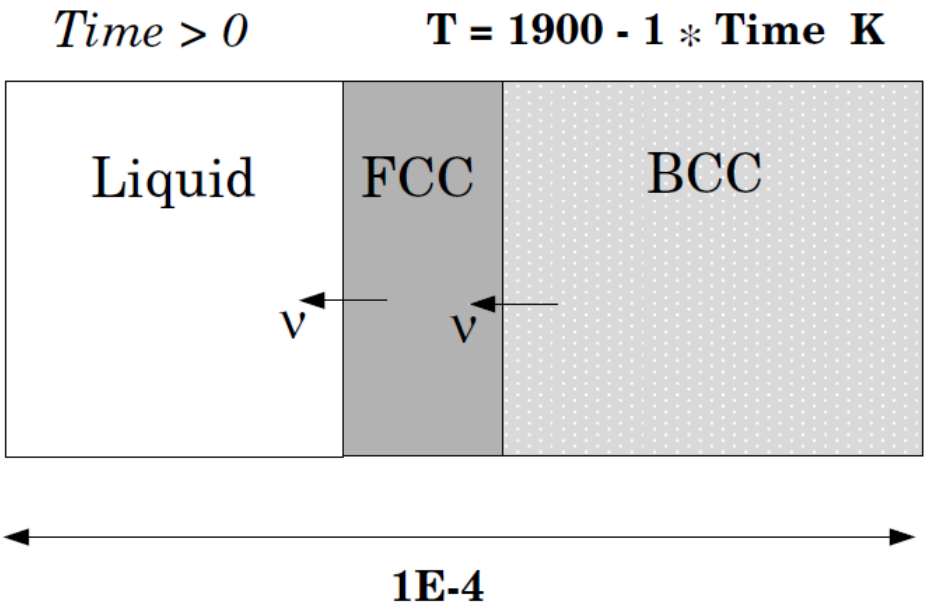


Example exb4b

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction

This example is the same as exb4a but now a peritectic reaction is assumed: LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

This example uses the MOBFE database. This license is required to run the example.

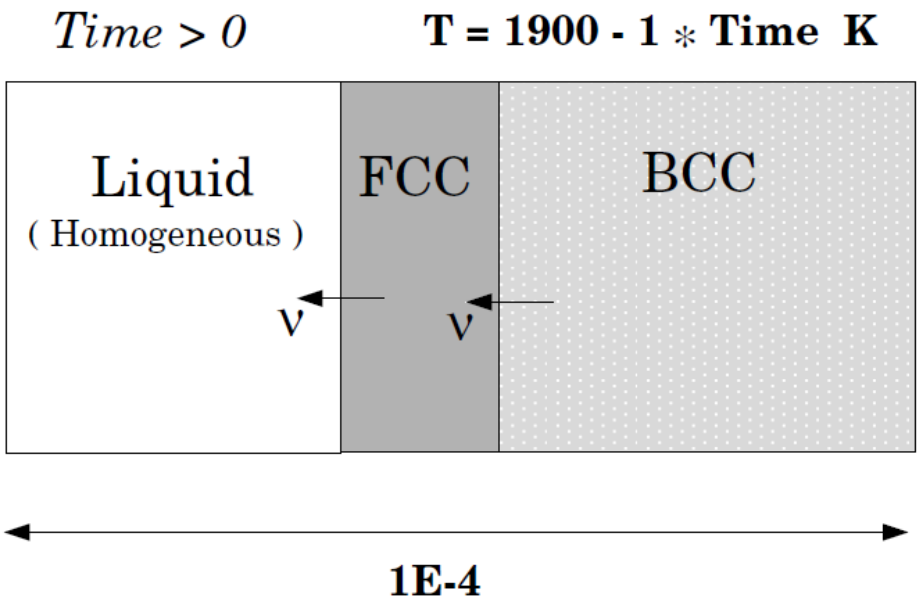


Example exb4c

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, homogeneous liquid

This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a very high value for the diffusivity is used in order to simulate a case where we assume that the composition in the LIQUID is always homogeneous. This case should be considered less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

This example uses the MOBFE database. This license is required to run the example.

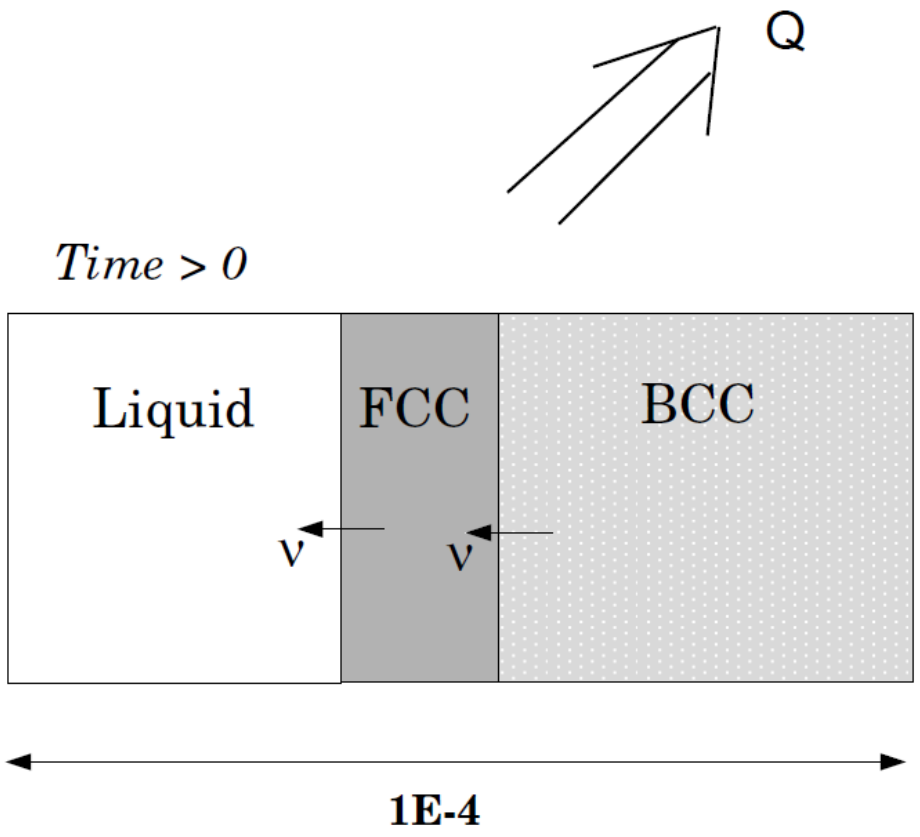


Example exb4d

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, heat-flux controls the temperature

This example is the same as exb4b but instead of controlling the temperature the amount of heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

This example uses the MOBFE database. This license is required to run the example.

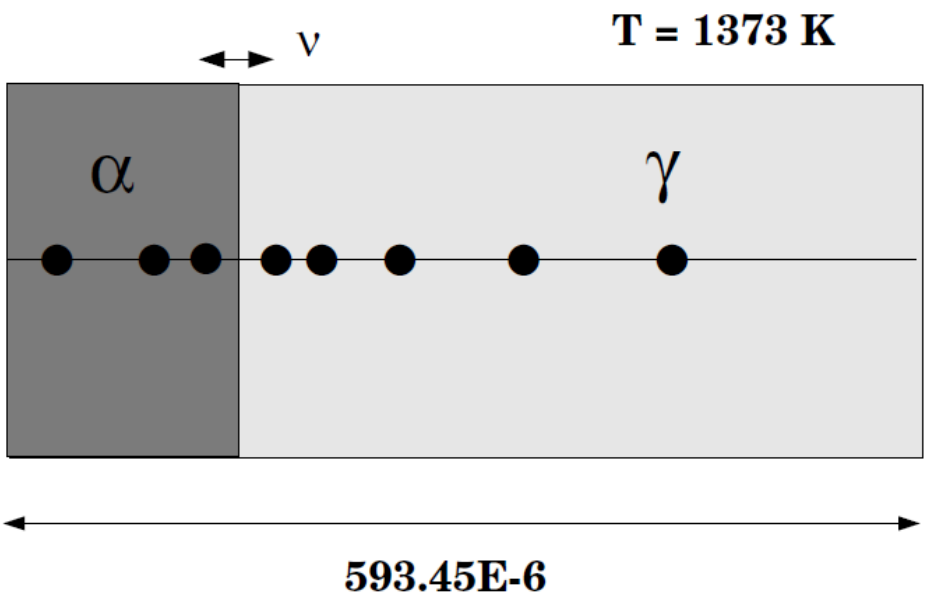


Example exb5

γ/α/γ Diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of α phase (38%Cr,0%Ni) is clamped between two thicker slices of γ phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373K.

This set up corresponds to diffusion couple in Kajihara, Lim, and Kikuchi, 1993: "Experimental Study on Dissolution of ALPHA Phase in GAMMA/ALPHA/GAMMA Diffusion Couples of the Fe-Cr-Ni System", *ISIJ Int.*, 33(4), 498–507. Also see Kajihara and Kikuchi, 1993: "Numerical analysis of dissolution of α phase in γ/α/γ diffusion couples of the Fe-Cr-Ni system", *Acta Metall. Mat.*, 41(7), 2045–2059.

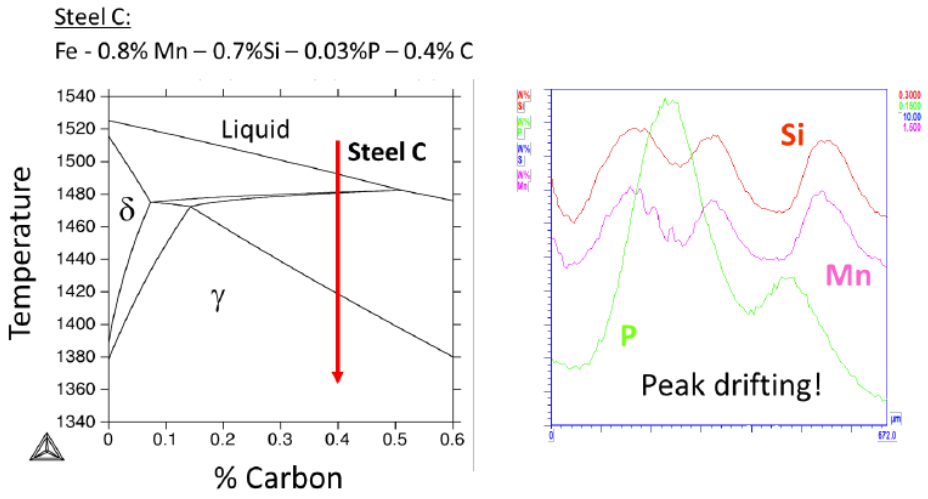


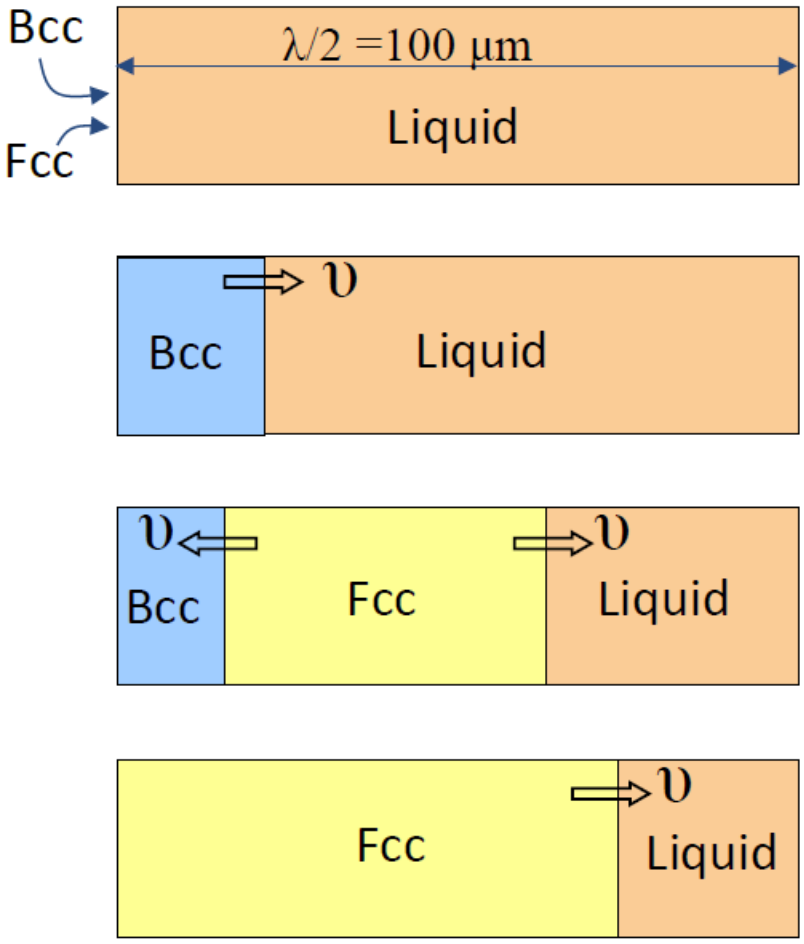
Example exb6

Microsegregation of phosphorus

This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.

This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



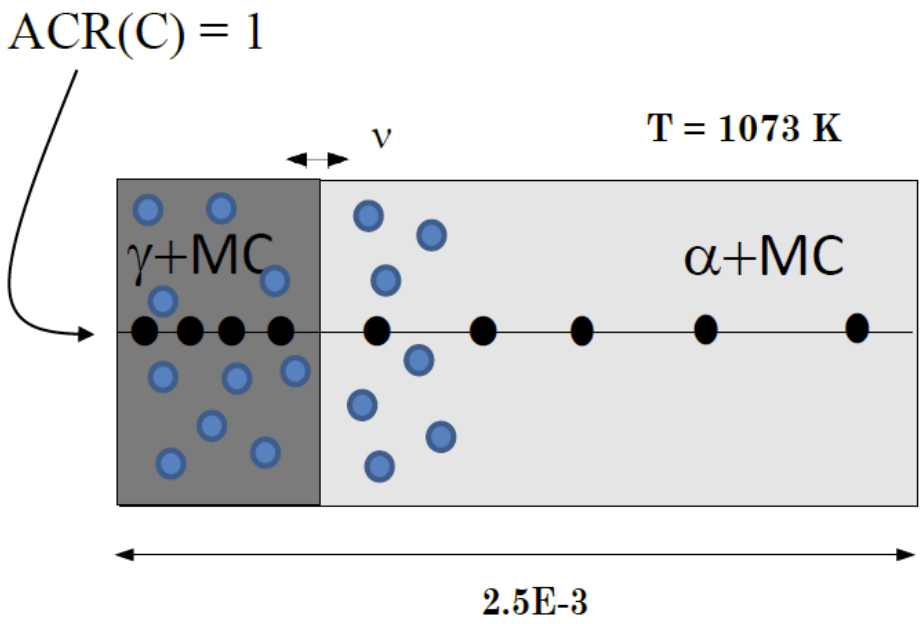


Example exb7

Moving boundary problem with multiple phases on each side of the boundary

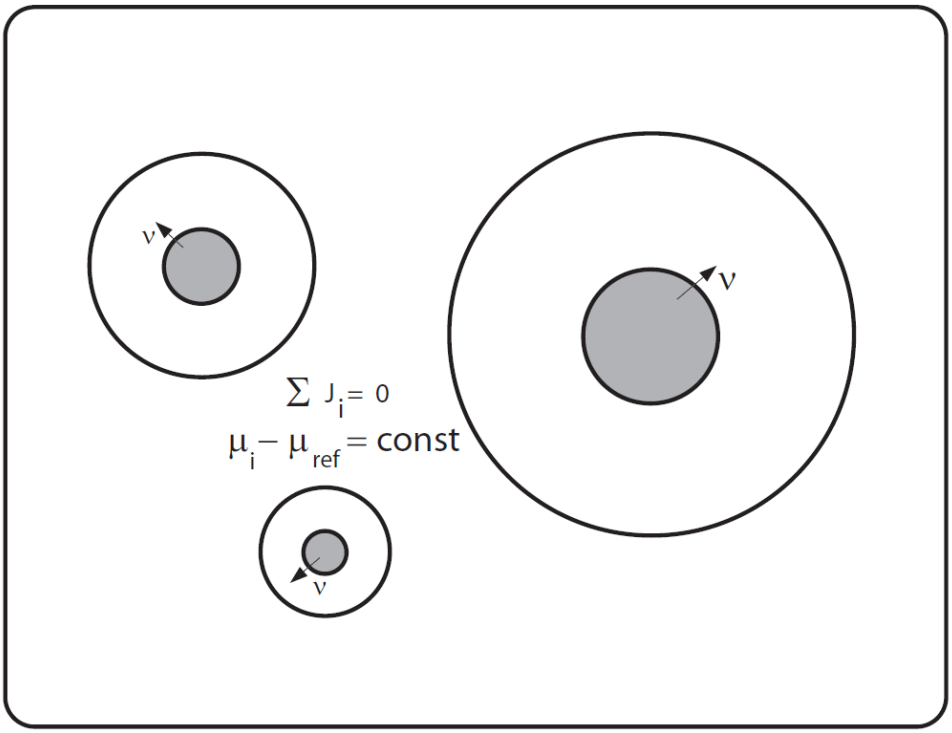
This example shows how to enter dispersed phases on either side of a phase interface. The particular case shows how the kinetics of a ferrite to austenite transformation is affected by simultaneous precipitation of niobium carbide. The transformation is caused by carburization.

This example uses the TCFE, SSUB and MOBFE databases. These licenses are required to run the example.



Cell Calculation Examples

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

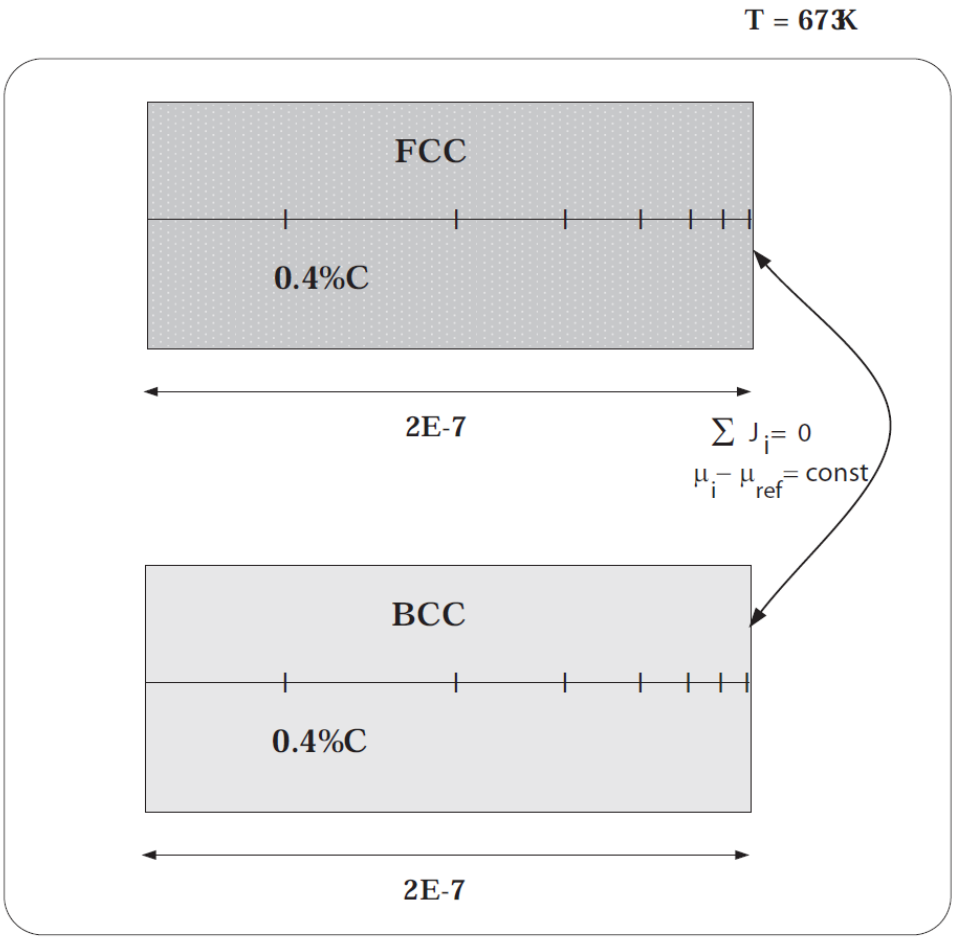


Example exc1

Carbon cannon in ferrite/austenite (α/γ): Fe-C system, two-cell calculation

This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells[1.] .

1. Also see Hillert, Höglund, and Ågren (1993) "Escape of carbon from ferrite plates in austenite", *Acta Metallurgica et Materialia*, 41(7), 1951–1957.



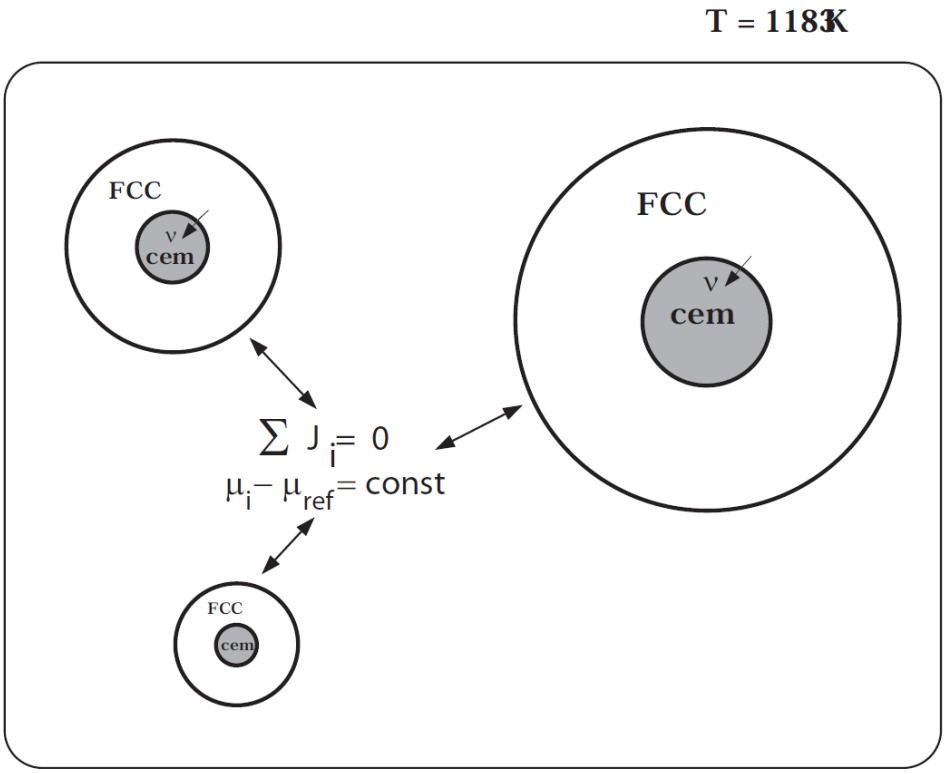
Example exc2

Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells

This example calculates the dissolution of cementite particles in an austenite matrix. This is the same as exc1 except that there are three particle sizes. Altogether six particles are considered using three different cells. This is to be able to represent some size distribution among the cementite particles.

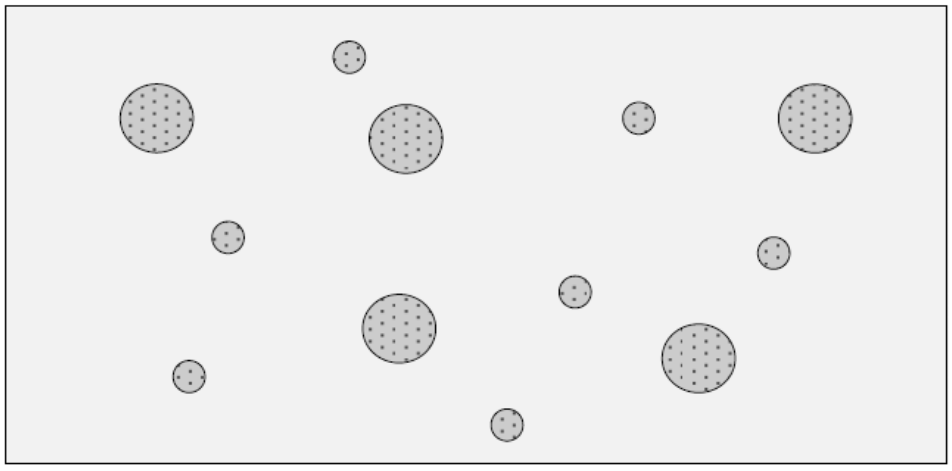
This example uses the MOBFE database. This license is required to run the example[1].

1. Also see Liu, Höglund, Jönsson, and Ågren (1991) "An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy", *Met. Trans. A*, 22(8), 1745–1752.



Diffusion in Dispersed Systems Examples

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.



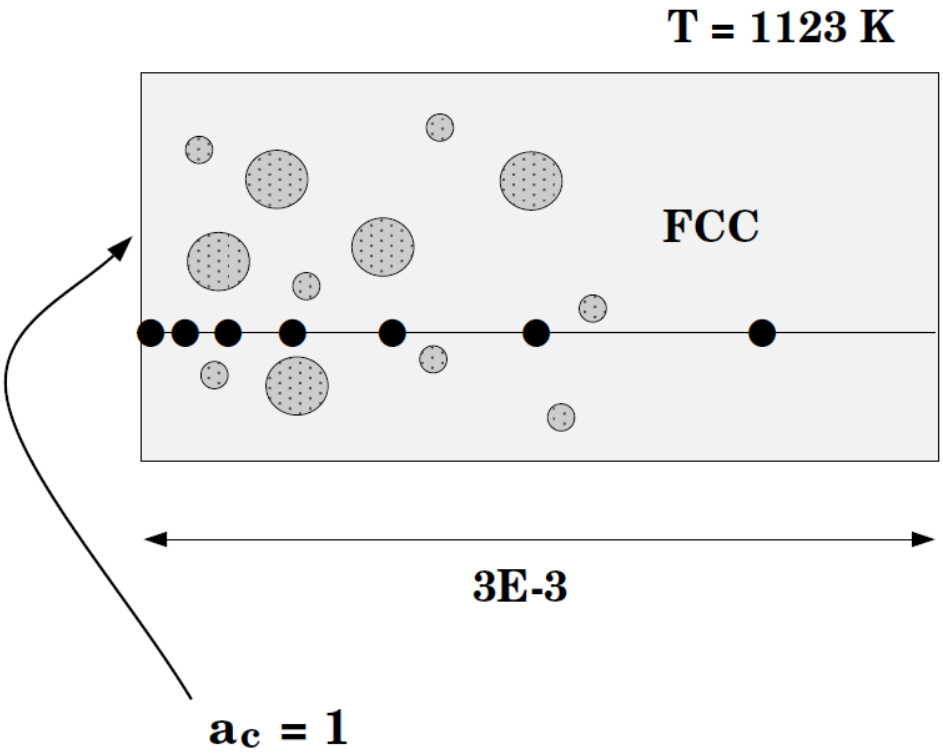
Example exd1a

Carburization of Ni-25%Cr alloy: Dispersed system model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used.

This case is from Engström, Höglund, and Ågren (1994), "Computer simulation of diffusion in multiphase systems", *Met. Mat. Trans. A*, 25(6), 1127–1134.

This example uses the SSOL and MOB databases. These licenses are required to run the example.



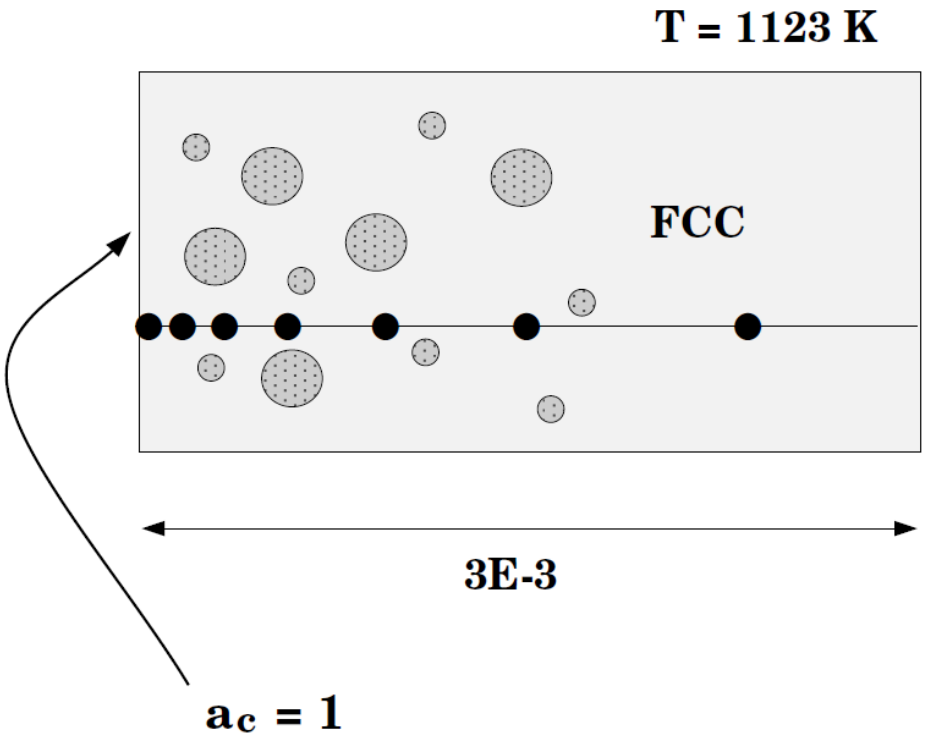
Example exd1b

Carburization of Ni-25%Cr alloy: Homogenization model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. It is similar to exd1a except the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION.

This case is from Engström, Höglund, and Ågren (1994), "Computer simulation of diffusion in multiphase systems", *Met. Mat. Trans. A*, 25(6), 1127–1134.

This example uses the SSOL and MOB databases. These licenses are required to run the example.



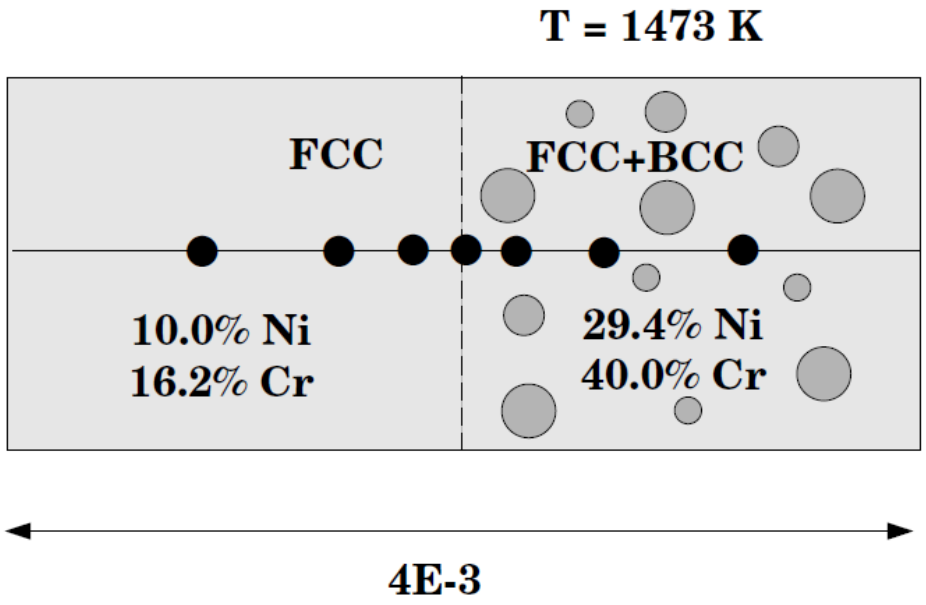
A modified version of this example is also available in Graphical Mode as example D_07. For Graphical Mode you do not need a Diffusion Module (DICTRA) license. You can open the example from Thermo-Calc when in Graphical Mode (**File →Examples Files → Diffusion Module**).

Example exd2a

Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used.

This case is from Engström, 1995. "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24(1), 12–20.

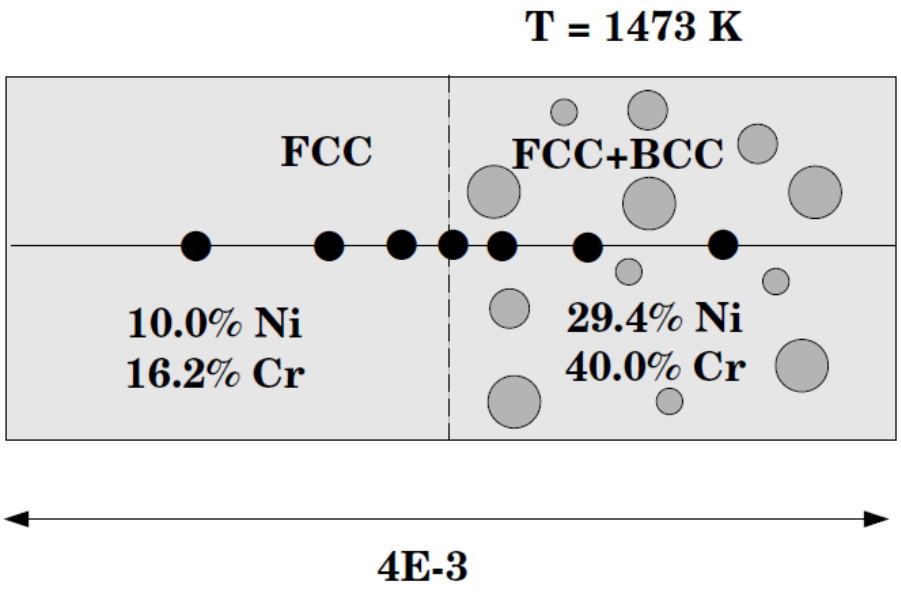


Example exd2b

Diffusion couple of Fe-Cr-Ni alloys: Homogenization model

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. It is similar to exd2a except the default HOMOGENIZATION MODEL is used and then ENTER_ HOMOGENIZATION_FUNCTION is used instead of ENTER_LABYRINTH_FUNCTION.

This case is from Engström, 1995. "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24(1), 12–20.

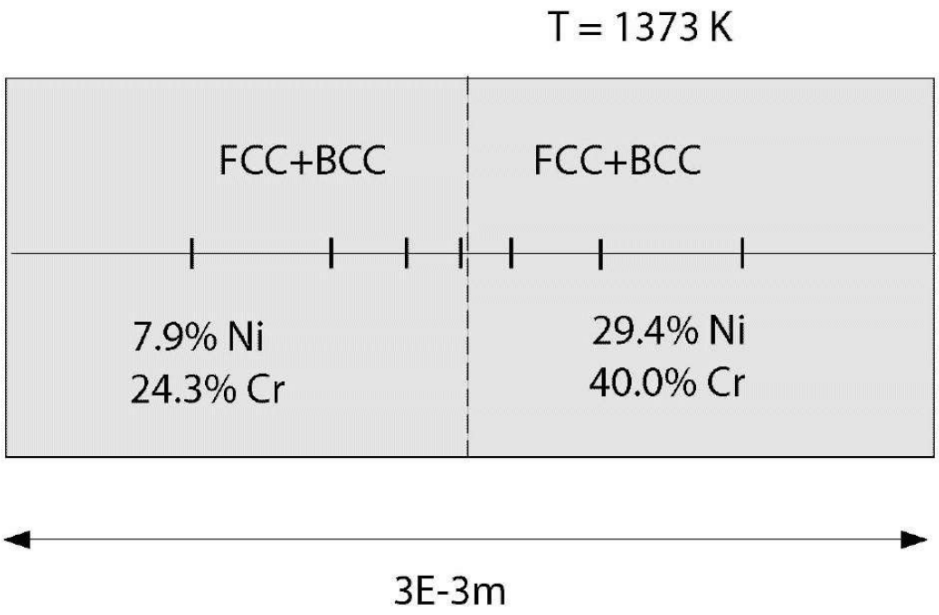


Example exd3

Diffusion couple of Fe-Cr-Ni alloys: Homogenization model

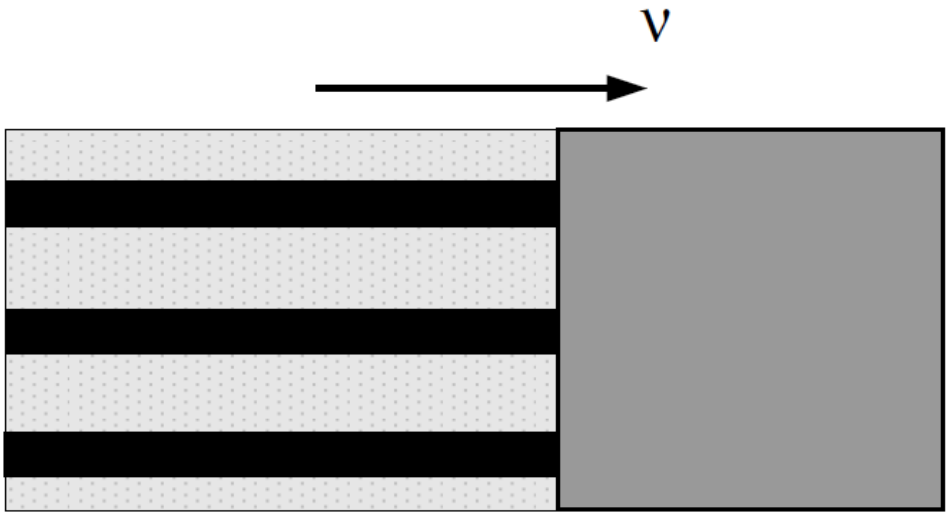
This example uses the homogenization model. It is taken from Larsson and Engström, 2006: "A homogenization approach to diffusion simulations applied to α + γ Fe–Cr–Ni diffusion couples", *Acta Mat.*, 54(9), 2431–2439. Experimental data is from Engström, 1995. "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24(1), 12–20

The homogenization model can be used for multiphase simulations like the dispersed system model, but unlike the dispersed system model there is no need to have a single continuous matrix phase and, furthermore, there is no need to limit the size of time-steps. The set-up is performed in the same manner as for the dispersed system model, which means that a certain phase is entered as the matrix phase and the other phases are entered as spheroidal, but the choice of matrix phase does not affect the simulation.



Cooperative Growth Example

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

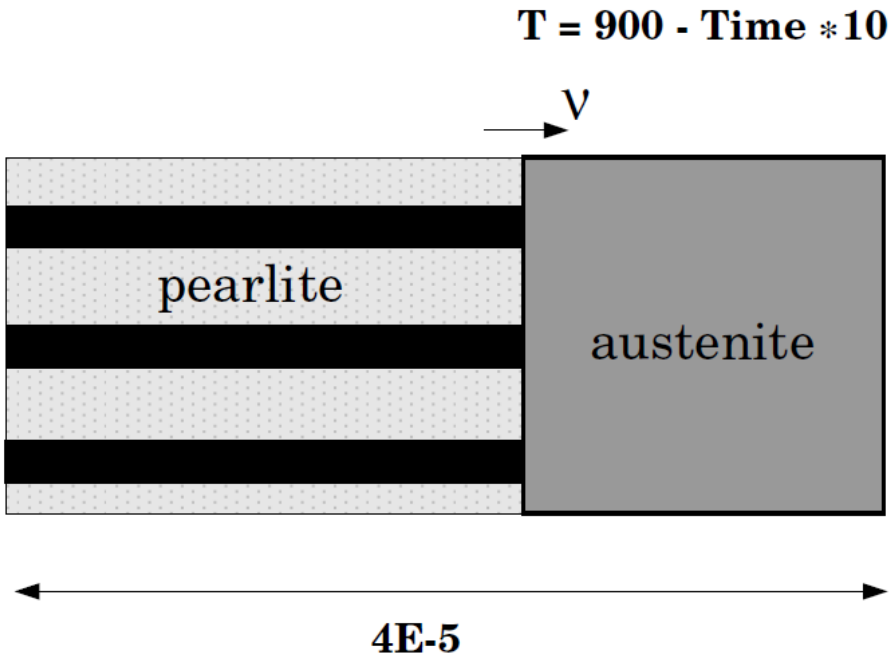


Example exe1

Growth of pearlite in an Fe-Mn-C alloy

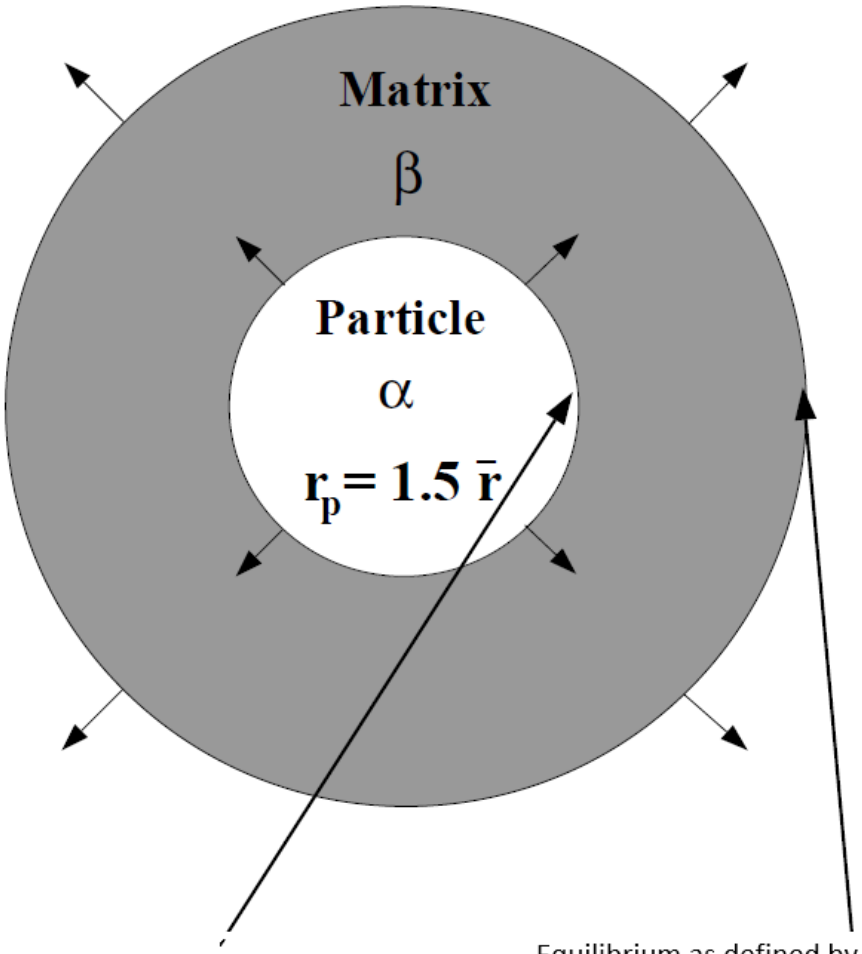
This is an example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel.

This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



Coarsening Example

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

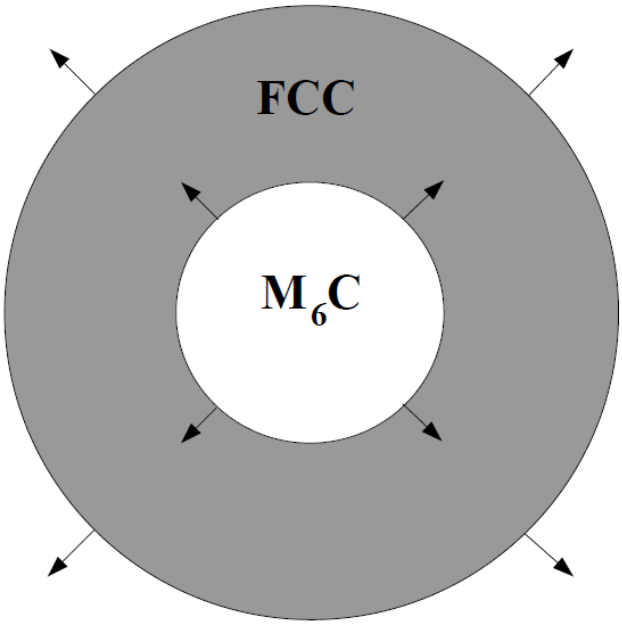


Example exf1

Coarsening of M6C precipitate in an Fe-Mo-C alloy

This example calculates the Ostwald-ripening of a spherical M6C carbide in an austenite matrix.

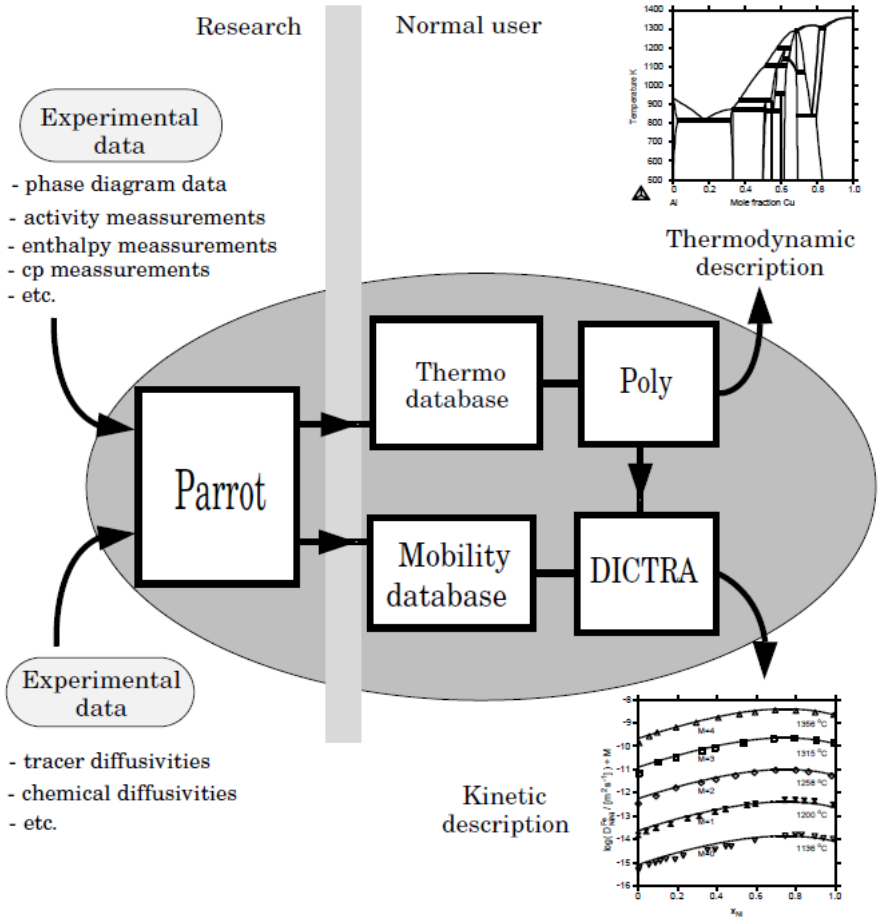
This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



T = 1173K **r_p= 0.228 μm**

Kinetic Data Examples

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

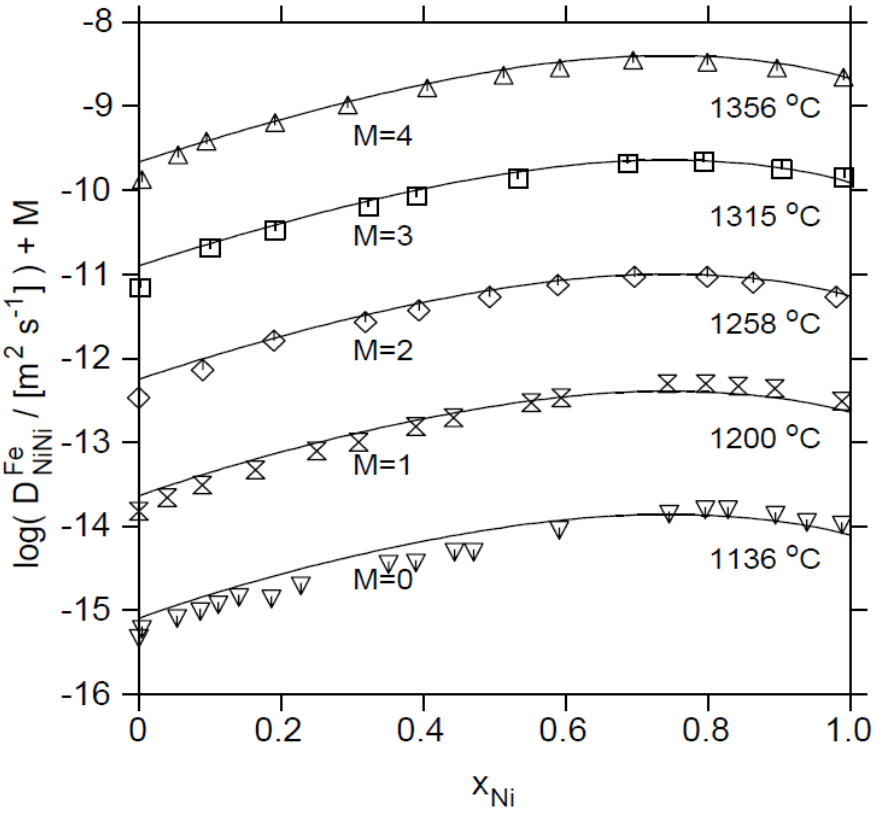


Example exg1

Checking mobilities and diffusivities in an Fe-Ni alloy

This is an example file to check the mobilities and diffusivities in an Fe-Ni alloy.

This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



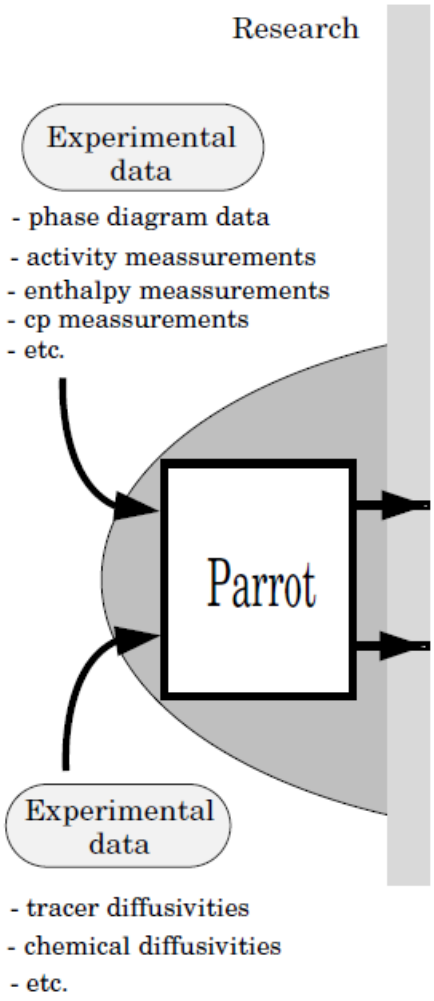
Example exg2

Optimization of mobilities in Ni-Al fcc alloys

A file for reading thermodynamic data and setting up the kinetic parameters that are needed for an optimization of the FCC phase in the binary Ni-Al system.

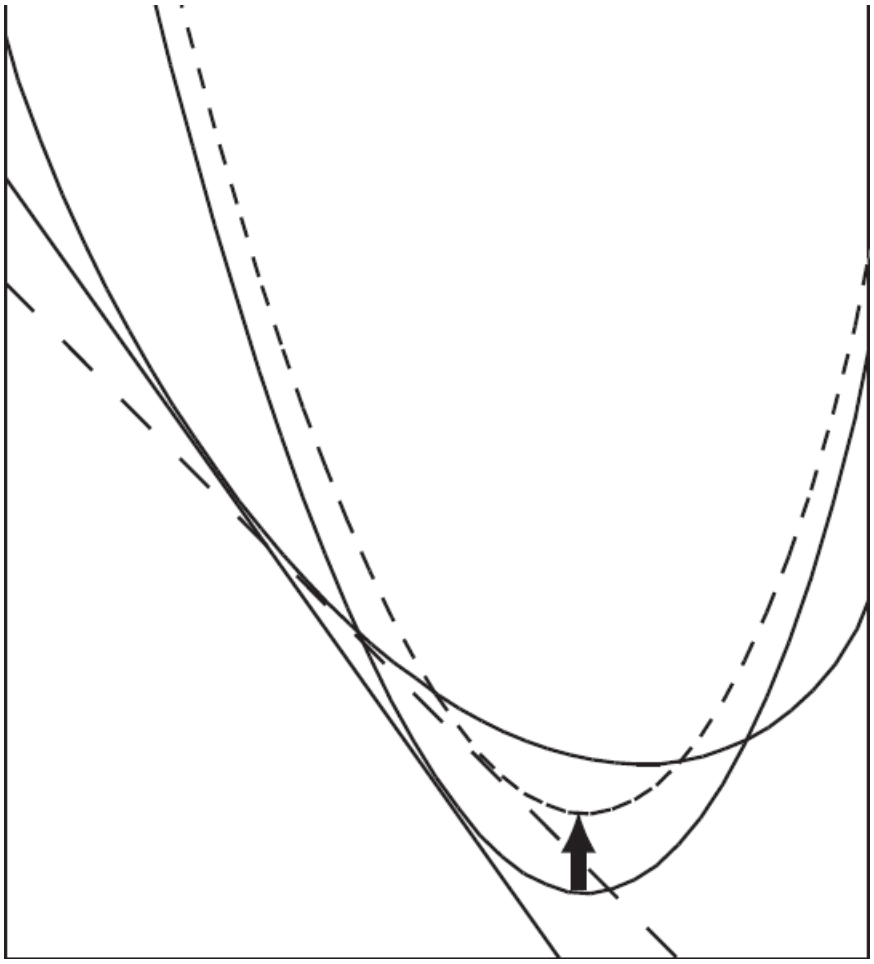
Also see Engström and Ågren, 1996: "Assessment of Diffusional Mobilities in Face-centered Cubic Ni-Cr-Al Alloys", *Z. fur Metall.*, 87(2), 92–97.

This example uses the MOB database. This license is required to run the example.



Deviation from Local Equilibrium Examples

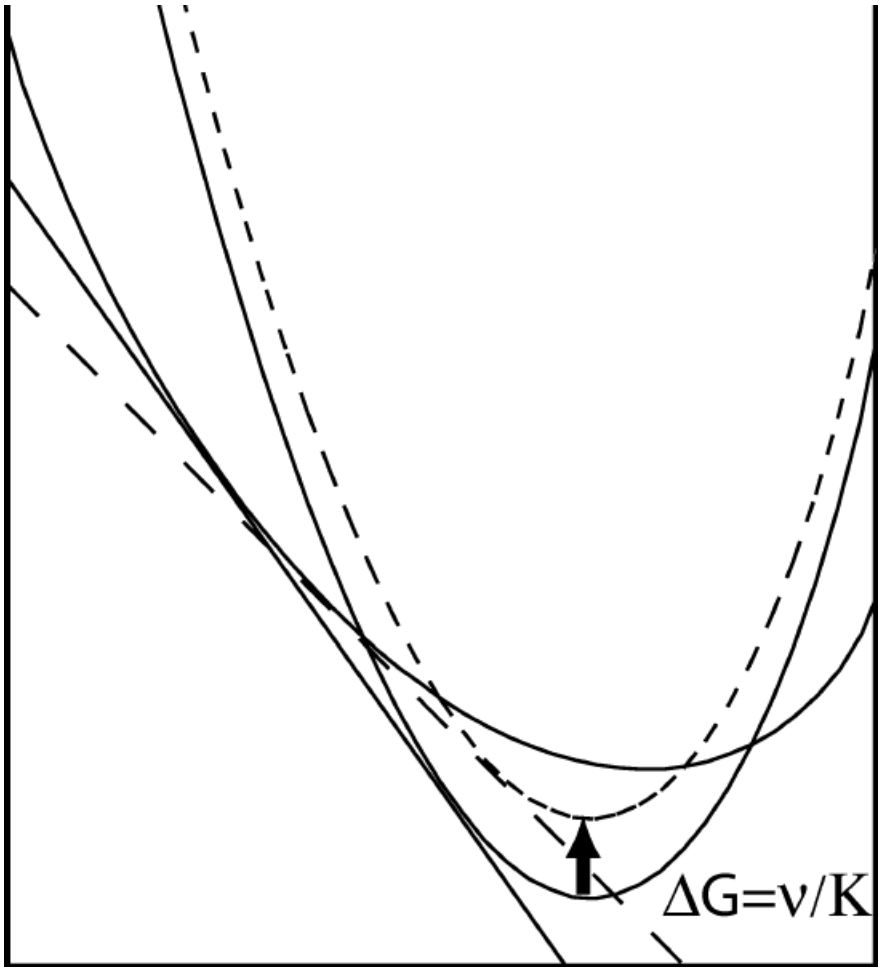
All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.



Example exh1

Ferrite/austenite (α/γ) diffusion couple with interface mobility

This example calculates the growth of ferrite (α) into austenite (γ) with a limited interface mobility. This is done by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command.

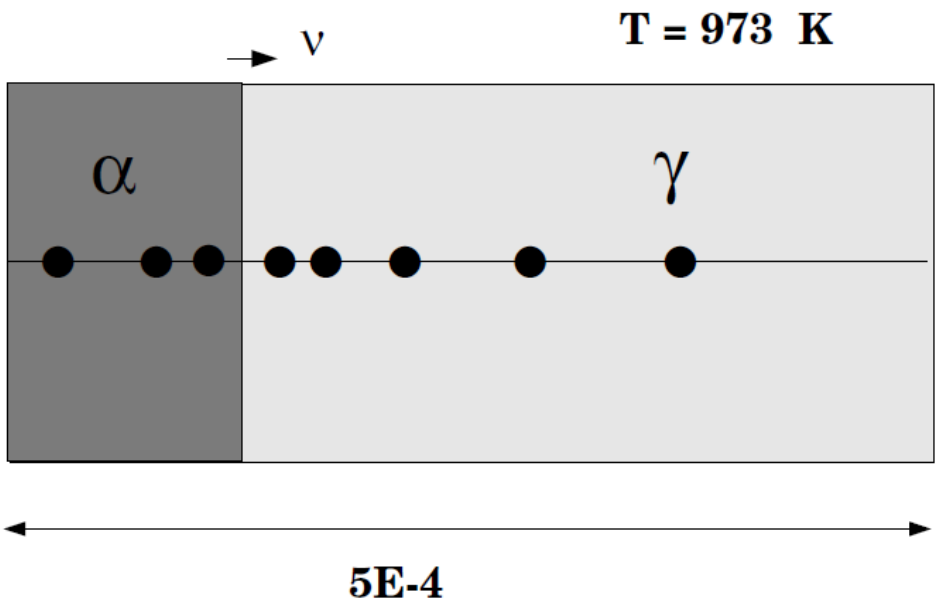


Example exh2

Ferrite/austenite (α/γ) para-equilibrium in an Fe-Ni-C alloy

This example calculates the growth of ferrite (α) into austenite (γ) in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model. The results are compared with experimental information from Hutchinson, Fuchsmann, and Brechet (2004)[1.] .

1. Hutchinson, Fuchsmann, and Brechet. 2004. "The diffusional formation of ferrite from austenite in Fe-C-Ni alloys", Met. Mat. Trans. A, 35(4), 1211–1221.

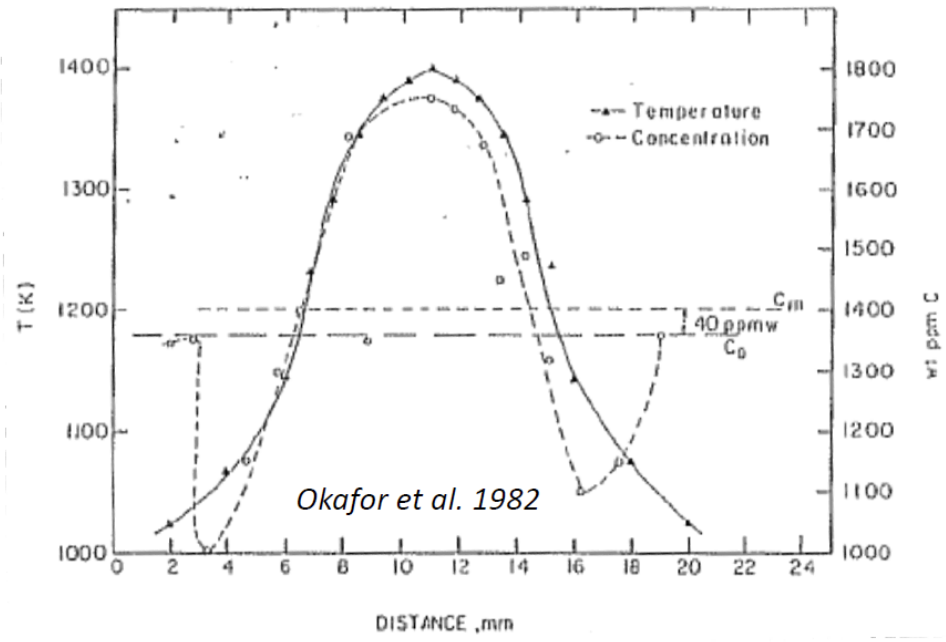


Example exh3

Diffusion induced by a temperature gradient (thermomigration)

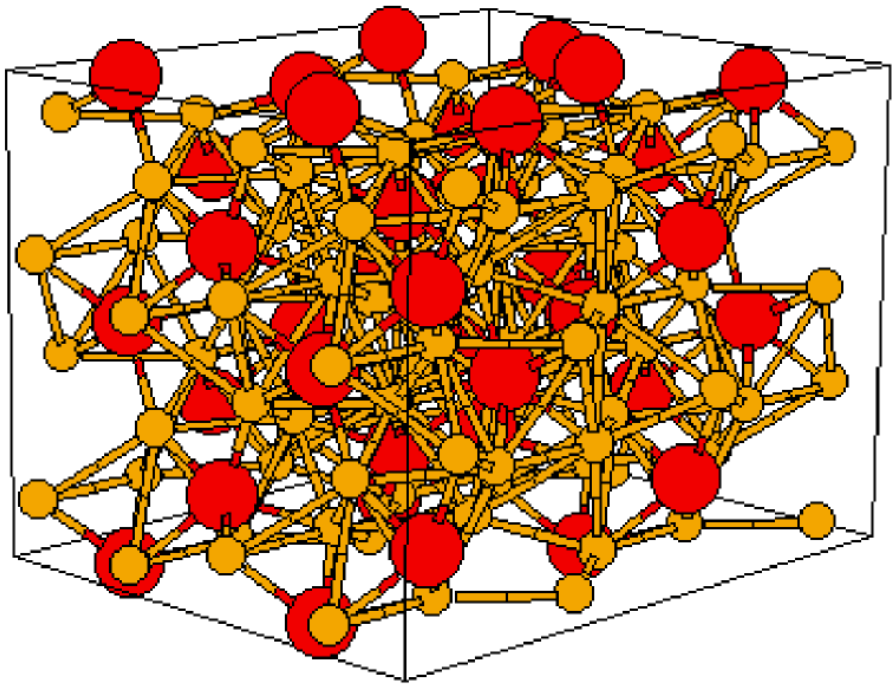
This calculation shows how a temperature gradient induces diffusion.

$$J_C = -\frac{u_C}{V_s} y_{Va} M_{CVa} \left(\frac{\partial \mu_C}{\partial x} + \frac{Q_C^*}{T} \frac{\partial T}{\partial x} \right)$$



Diffusion in Complex Phases Examples

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.



Example exi1

Diffusion in a system with B2 ordering

In this example folder, there is also a datafile `AlFeNi-data.TDB`, which contains both a thermodynamic and kinetic description for the ordered and disordered bcc.

Example exi2

Diffusion of carbon in cementite

This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component.

This calculation is compared with experimental data where a sample of pure iron has been exposed to a gas atmosphere with a certain carbon activity. The weight gain is then measured as a function of time.

The experimental data is obtained from Ozturk, B., Fearing, V. L., Ruth, J. A., and Simkovich, G. (1982)[1.] .

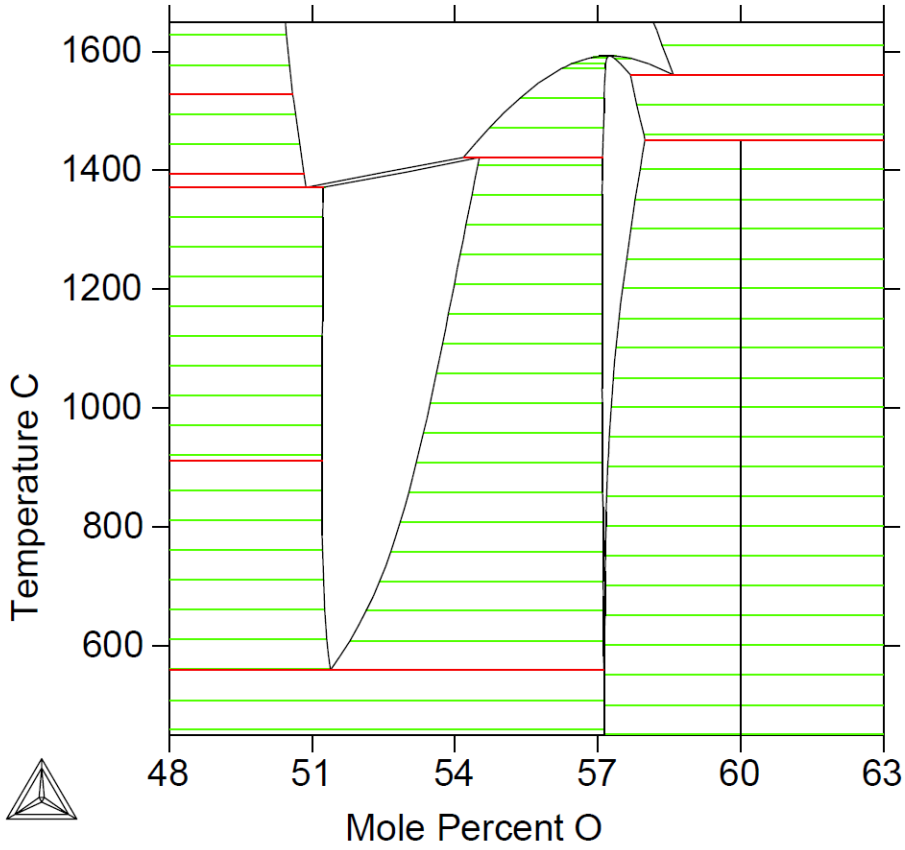
$J \sim \Delta\mu$

1. "Self-Diffusion Coefficients of Carbon in Fe3C at 723 K via the Kinetics of Formation of This Compound", *Met. Trans. A*, 13 (10), 1871–1873.

Example exi3a

Diffusion in iron oxide (FeO)

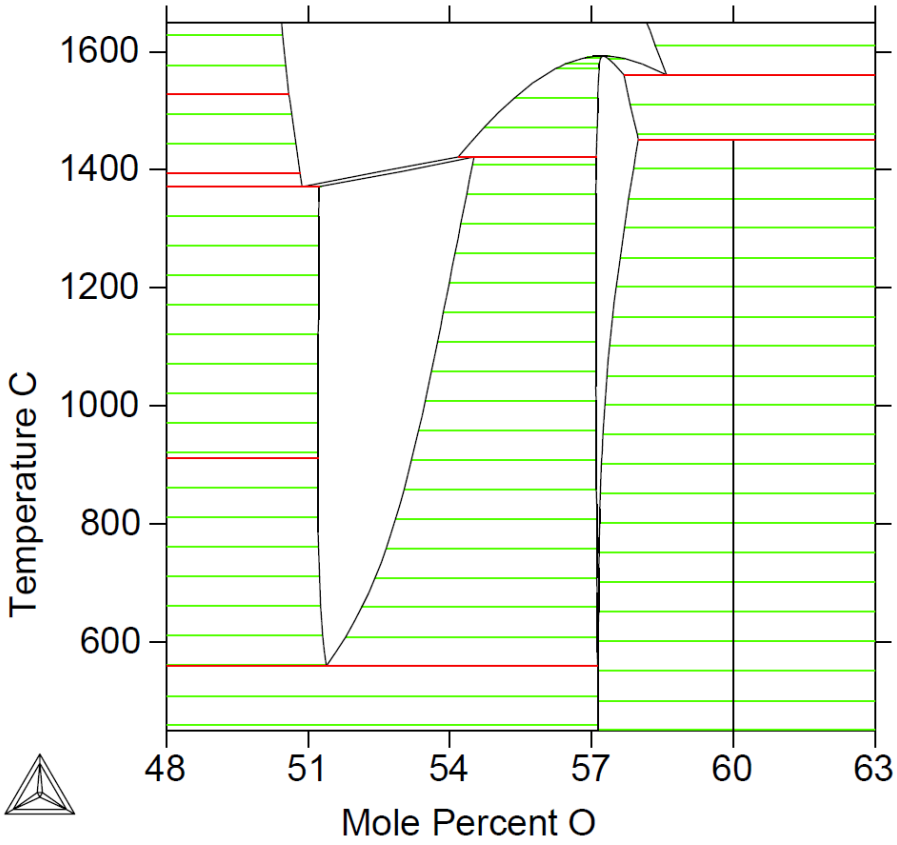
This example shows the oxidation of an iron sample and the consequent growth of an oxide layer.



Example exi3b

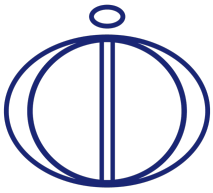
Diffusion in iron oxide (FeO) with a grain boundary contribution

This example shows the oxidation of an iron sample and the consequent growth of an oxide layer using the grain boundary diffusion contribution model.


1600
1400
1200
1000
800
600
Temperature C
48
51
54
57
60
63
Mole Percent O

Diffusion Module (DICTRA) Quick Start Guide - Graphical Mode

Thermo-Calc Version 2021b



Thermo-Calc Software

Introduction to the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to the Thermo-Calc software package. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulations are both time- and space-dependent.

The Diffusion Module (DICTRA) is suitable for solving diffusion problems that include a moving boundary (so-called *Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. The concentration fields only vary along one spatial coordinate, but the geometry may be either planar, cylindrical or spherical.

In this section:

About this Quick Start Guide 3

Diffusion Module Terminology in Graphical Mode 4

Setting up a Diffusion Simulation in Graphical Mode 6

About this Quick Start Guide

The following introduces you to the basic concepts, steps and theory to start using the Diffusion Module (DICTRA). An understanding of this information is necessary to ensure accurate calculations.

- More details about the use of DICTRA can be found in Andersson et. al (2002)[1.] and Borgenstam et al. (2000)[2.] .



If you are not familiar with Graphical Mode, it is recommended you review the available documentation and training material.

1. Andersson, J.-O., Helander, T., Höglund, L., Shi, P., and Sundman, B., *Calphad*, 26 (2), pp. 273–312.

2. Borgenstam, Al, Höglund, L., Ågren, J. and Engström, A., *J. Ph. Equilib.*, 21 (3), pp. 269–280.

Diffusion Module Terminology in Graphical Mode

The following definitions are useful to help you understand the examples in this guide. For more detailed information search or browse the online help (**Help →Online Help**).

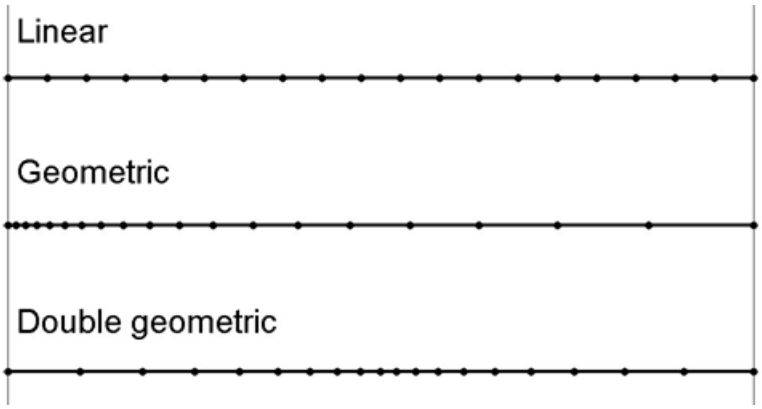
These terms are specific to working in Graphical Mode. The overall simulation in Console Mode is comparable but there are some differences in terminology and functionality.

Region

In Graphical Mode, a system consists of one *cell* with one or multiple *regions* in which the diffusion problem is to be solved.

Grid Types

These grid types are used in diffusion simulations: linear, geometric and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region must contain at least one *phase*. The so-called *homogenization model* is used if multiple phases are added inside a region, then the average properties of the local phase mixture is used. Phase(s) can also be added to interphases of region(s) and then only participate in the simulation if the driving force for precipitation of the phase exceeds a predefined value. A new region is then created where the name of the region is set to the name of the phase but with `R_` added as a prefix.

Composition

These types of composition variables are used in the configuration of the Diffusion Calculator: *mass (weight) fraction*, *mass (weight) percent*, *mole fraction*, or *mole percent*.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$\mu_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume. Weight fraction, mole fraction or u-fraction can be used when plotting the results from a simulation.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where compositions vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical* or *spherical*.

The *planar* geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Setting up a Diffusion Simulation in Graphical Mode

When you are using the Graphical Mode version of the Diffusion Module (DICTRA), the steps to set up a simulation are a combination of adding *Activity* nodes (the System Definer, Diffusion Calculator and Plot Renderer) and then defining the applicable settings for each of these nodes in a Configuration window.

The following is a general overview of the steps to set up the simulation.

1. Use the **Diffusion Simulation** template to add the System Definer, Diffusion Calculator and Plot Renderer activity nodes.
2. On the **System Definer**, you select the thermodynamic and kinetic databases, add elements and phases, and generally define the system.
3. On the **Diffusion Calculator**, you set the geometry (by default the geometry is planar), add region(s) and enter grid(s) and phase(s) in the region(s). You then enter composition(s) of phase(s).
4. On the **Plot Renderer** or **Table Renderer**, you choose how to visualize your diagrams, and then run the simulation, i.e. you **Perform** the sequence of nodes you have defined in the tree to produce the output simulation.



Go to Working in Graphical Mode for links to the relevant content to continue.

Single Phase Simulations

In this section:

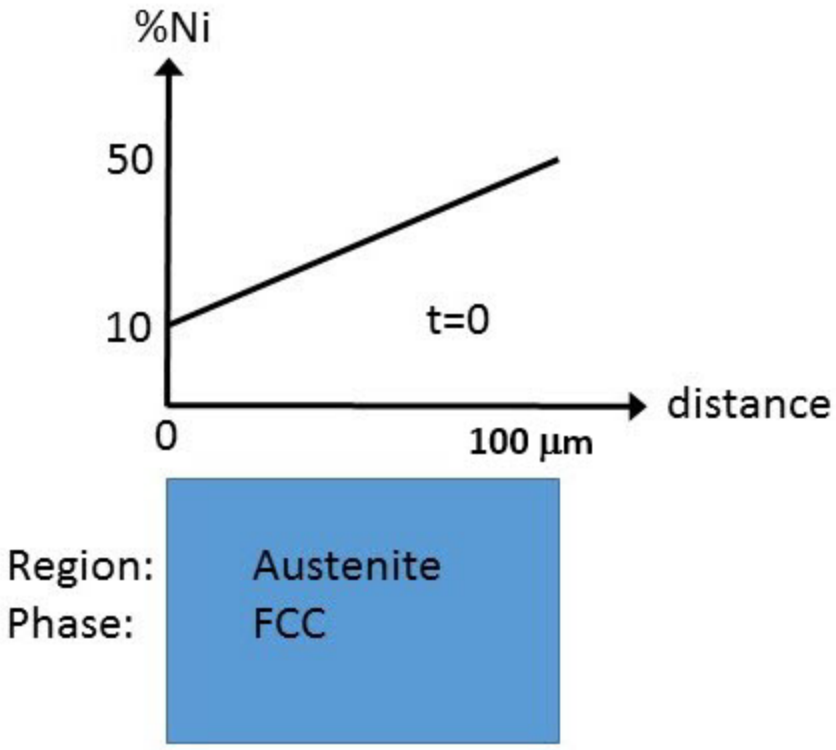
About the Single Phase Simulation 8
Theory for the Single Phase Simulation 9
Setting Up the Single Phase Simulation 11
System Definer Settings 13
Diffusion Calculator Settings 16
Plot Renderer Settings 19
Renaming the Nodes and Saving the Project 21

About the Single Phase Simulation

In a 100 µm wide planar domain, the single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase (in Thermo-Calc the name of this phase is FCC_A1). Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

The simulation time is slightly different between the modes. For Console Mode it is 10^5 s and for Graphical Mode it is 30 hours.

By default the boundaries are closed. The plot generated shows the initial and final Ni profile.



Schematic view of the initial state of Single Phase Diffusion example. The width of the domain is 100 µm and there is a linear gradient in composition going from 10 to 50 mass-% Ni. There is a single region named Austenite that consists of an fcc phase.

Theory for the Single Phase Simulation

The flux of a component k in the z-direction in an isobarothermal system is in general given by

$$J_k = \sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z}$$

where L_{ki} is a matrix of kinetic coefficients and μ_i is the chemical potential of component *i*. The correlation effects, i.e. the coupling of the flux of *k* component to the chemical potential gradients of the other elements, are normally neglected

$$(L_{ki} = 0, k \neq i)$$

and thus

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

where c_k is the concentration and M_k the mobility of component *k*.

The equation for the flux is combined with the equation of continuity, which takes the following form in a planar domain,

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z}(-J_k)$$

which relates the local evolution of the concentration of k to the divergence of the flux.

The expression for the flux can be expanded in terms of concentration gradients

$$J_k = -\sum_{i=1}^{n} M_k c_k \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z} = -\sum_{i=1}^{n} D_{kj} \frac{\partial c_j}{\partial z}$$

where the diffusion coefficient of component k with respect to the concentration gradient of component j has been introduced.

$$D_{kj} = M_k c_k \frac{\partial \mu_k}{\partial c_j}$$



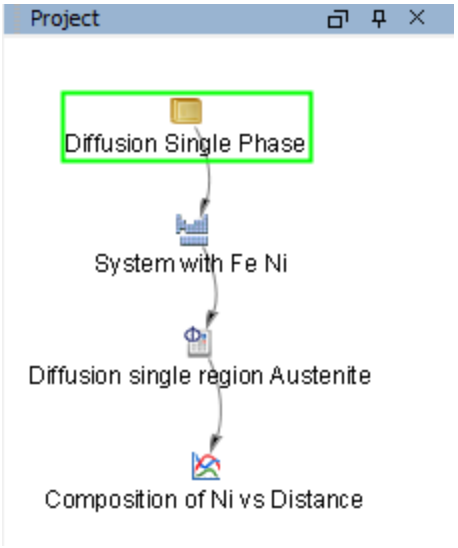
The flux expressions above are given in the so-called lattice-fixed frame of reference. In practical calculations it is more common to use a volume-fixed frame of reference. For a discussion of these concepts, see Andersson and Ågren (1992)[1.] .

1. Andersson, Jan-Olof, and John Ågren. 1992. "Models for Numerical Treatment of Multicomponent Diffusion in Simple Phases." Journal of Applied Physics 72 (4): 1350–55.

Setting Up the Single Phase Simulation

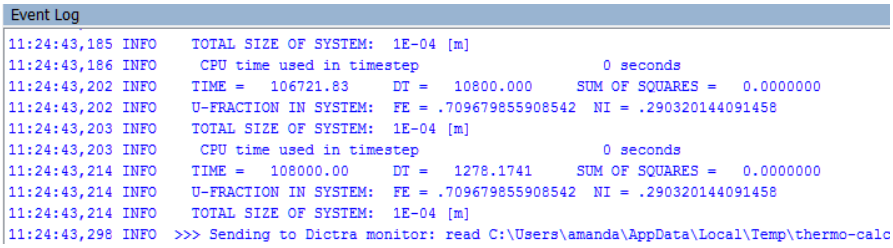
For the single phase example, you can open the example project file included with your installation to first see how it is set up:

1. Open Thermo-Calc.
2. From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
3. Open the **Diffusion Module - DICTRA** folder and locate the `D_01_Diffusion_Single_Phase.tcu` file and double-click to open it.
4. The project opens in Thermo-Calc and adds this tree structure:

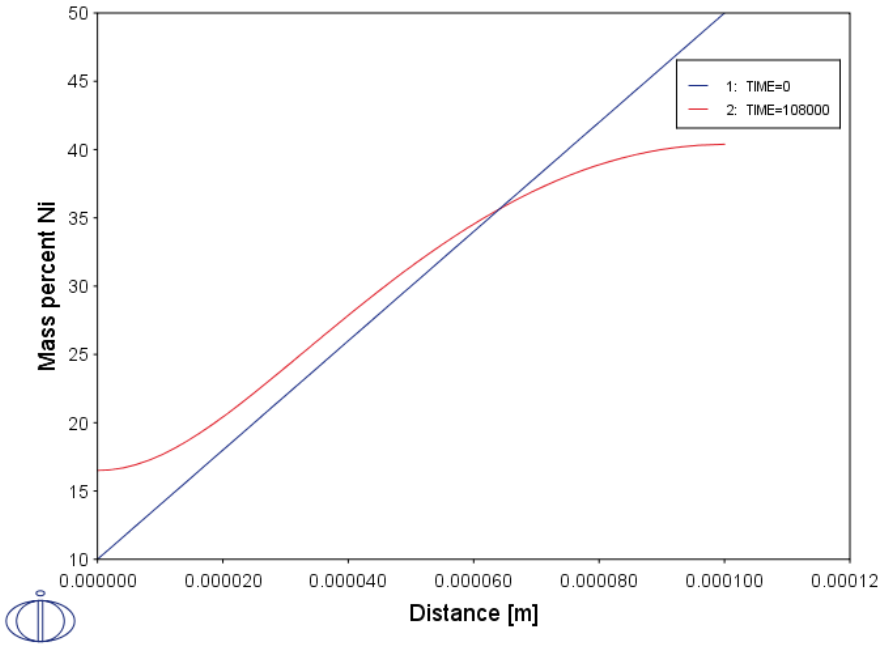


5. Click the top Project node (renamed to *Diffusion_Single_Phase*). At the bottom of the **Configuration** window click **Perform Tree**.

   The **Event Log** shows the progress of the calculations:



   When completed, the results are plotted in the **Results** window as shown below.



Output from the Single Phase example showing the initial and final Ni profile.

For the rest of the exercise, you will learn how to build this example step-by-step.

System Definer Settings

To learn more about the activity nodes and tree structure see 'Project Activities and the Tree Structure' in the *Thermo-Calc User Guide*.

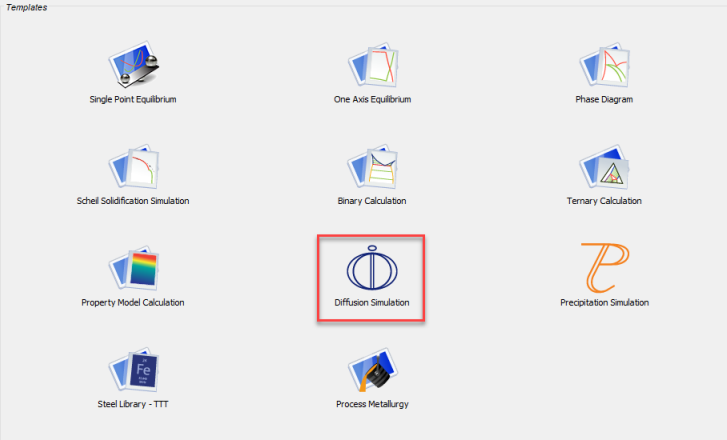
The following describes how to set up the *D_01_Diffusion_Single_Phase.tcu* example from the beginning.

Add a System Definer Node

1. Open Thermo-Calc.
2. In the **Project** window, right-click **My Project** and select **Create New Activity → System Definer**.
3. In the **System Definer Configuration** window, you select the thermodynamic and kinetic databases to use and select the elements.

Tip: The Diffusion Simulation Template

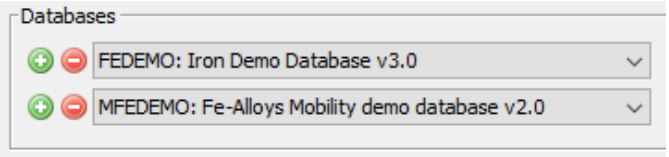
For this first example the activity nodes are added one at a time. A faster way to add all the nodes you need is to use the **Diffusion Simulation** template.



Choose the Databases

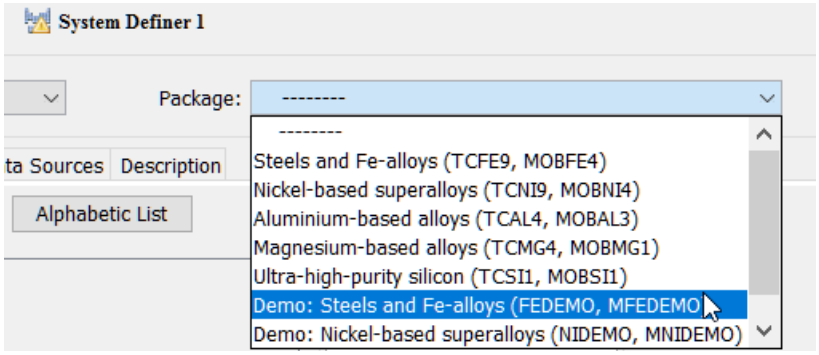
There are databases for different purposes and material types. This example uses two demonstration databases: **FEDEMO** (the thermodynamic iron-base database) and **MFEDEMO** (the kinetic/mobility iron-base database).

1. In the System Definer **Configuration** window click the **Databases** list and select the **FEDEMO** database.
2. Click the **Add a database** button .
3. Select the **MFEDEMO** database.



Tip: Database Packages

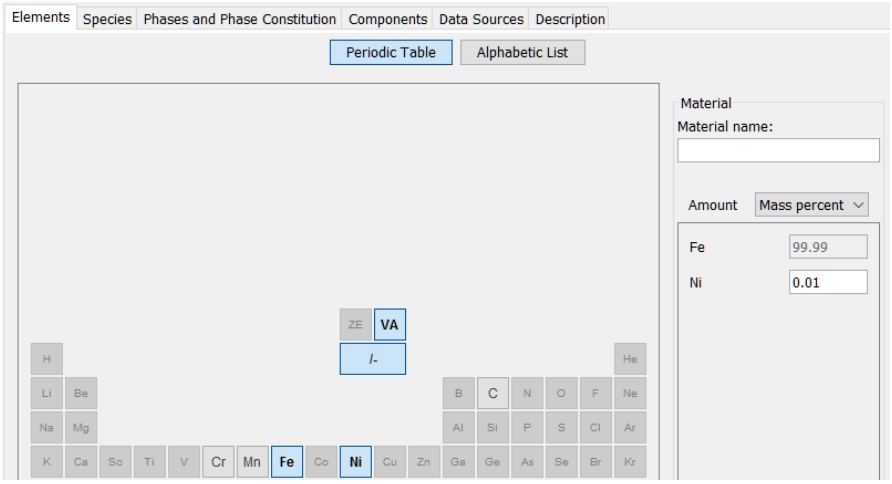
For this first example the databases are added one at a time. A faster way to add both the databases is to add a predefined database **Package**.



Choose the Elements

On the **Elements** tab, and based on the databases selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. The demonstration databases have only a small number of elements to choose from.

1. In the **Periodic Table**, click **Fe**.
2. Click **Ni**.



When using the System Definer with the Diffusion Calculator, you can keep all phases selected on the **Phases and Phase Constitution** tab.

Diffusion Calculator Settings

After you have completed the settings for the System Definer you start defining the diffusion parameters on the Diffusion Calculator.

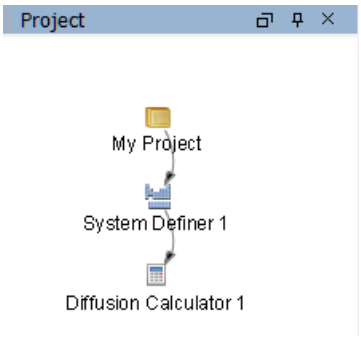
In any simulation at least one *region* must be defined. This is a named container that designates a certain part of the domain. In this case it is the whole domain. The name of a region is arbitrary and specified by you.

The use of regions becomes clearer in the context of moving phase boundary simulations.

A region must contain a numerical *grid* specified by width and type. In this example, a 10^{-4} m (1e-4 m) wide, linear (i.e. equidistant) grid is used with 50 grid points.

Define the Region and Composition Profiles

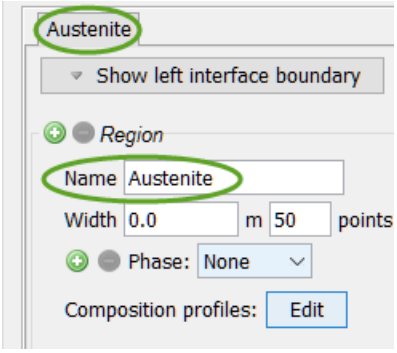
1. In the **Project** window, right click the **System Definer** node and select **Create New Successor → Diffusion Calculator**. A Diffusion Calculator node is added to the tree structure.



If you used the **Diffusion Simulation** template, then this activity node is already there. Click the **Diffusion Calculator** node to access the **Configuration** window settings.

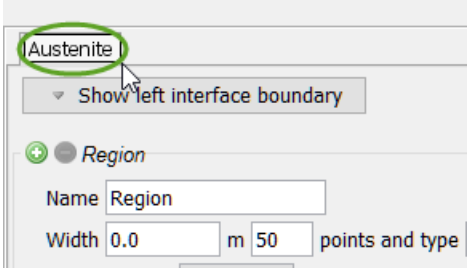
2. You are now going to add the settings to the Configuration window on the **Conditions** tab. Keep the defaults for *Composition unit* (**Mass percent**) and *Length unit* (**m**). A **Planar** geometry is used for all the examples.

3. In the *Region* **Name** field, enter `Austenite`. This name is automatically updated on the tab.



Tip: Double-click the Region *Tab to Name a Region*

Another way to enter the region name is to double-click the tab, enter a name and then press enter.

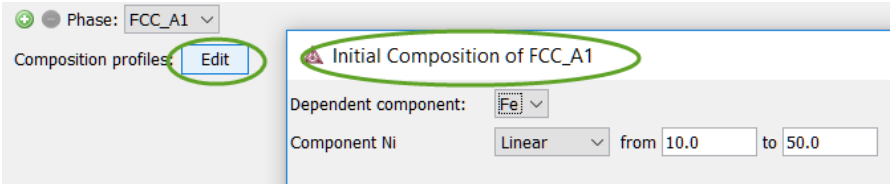


4. In the **Width** field replace the default with `1e-4`. Keep the defaults for number of points (**50**) and type of grid (**Linear**).

5. From the **Phase** list, select **FCC_A1**.

   The initial composition profile must be specified for all regions. Since there are only two elements, Fe and Ni, the initial composition profile must only be given for one of them.

6. Click **Edit** next to **Composition profiles**. Fe is chosen as the *Dependent component*.



There are many ways to specify the composition profile, e.g. an arbitrary position dependent function. In this example, the default *Linear* type is used.

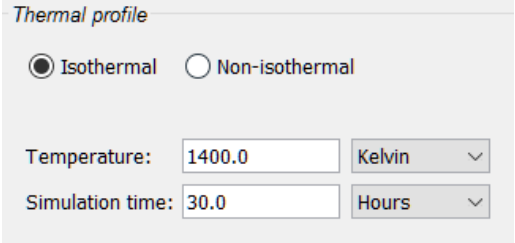
7. The initial profile for Ni is a **Linear** variation. In the **from** field enter `10` and in the **to** field enter `50`. Click **Apply**.

   These settings mean that the profile goes from 10 (mass-%) on the lower/left hand side of the system to 50 (mass-%) on the upper/right hand side of the system.

Define the Thermal Profile

The default **Isothermal** profile is used for this example. A constant temperature of 1400 K is used during the simulation, which is run for 30 hours. Enter these values in the fields:

1. In the **Temperature** field, enter `1400`. Keep **Kelvin** as the default unit.
2. In the **Simulation time** field, enter `30`. Select **Hours** from the list.



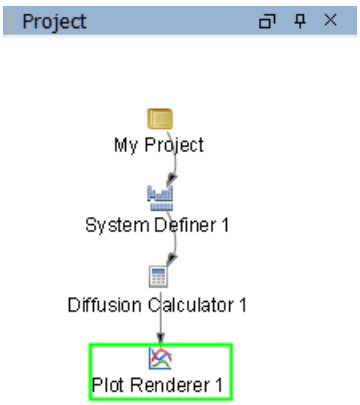


There are no changes to the default settings on the **Options** tab. You can click the tab to see what settings are available and then search the Online Help for more information.

Plot Renderer Settings

After you have completed the settings for the System Definer and Diffusion Calculator you define the plot parameters and run (perform) the simulation.

1. In the **Project** window, right click the **Diffusion Calculator** node and select **Create New Successor → Plot Renderer**. A Plot Renderer node is added to the tree structure.

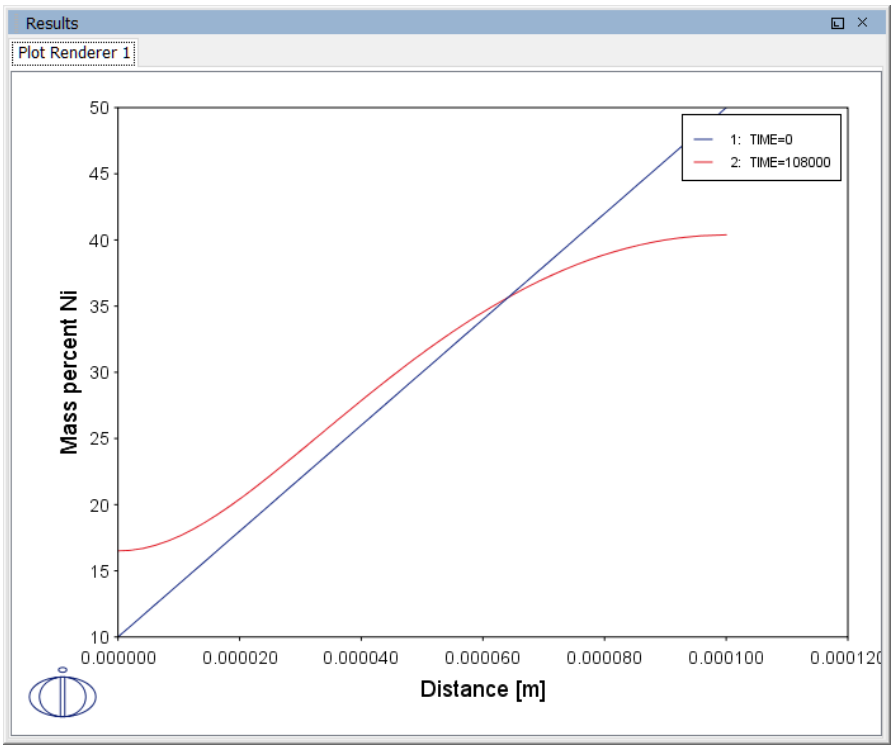


If you used the **Diffusion Simulation** template, then this activity node is already there. Click the **Plot Renderer** node to access the **Configuration** window settings.

For this first example, all the defaults are kept and there is only one setting to add. In most cases, either a specific position in the domain or one or more specific times must be specified depending on whether time or spatial position is chosen as independent (x-axis) variable.

2. In the time field, enter `0.0` before the `30.0`, which is automatically taken from the Diffusion Calculator setting.
3. Click **Perform**. If you have entered everything correctly, you should get this plot showing the composition profile of Ni at the initial (0 hours) and final time (30 hours

or 108,000 seconds).



Renaming the Nodes and Saving the Project

You can rename the nodes in the tree at any time during the creation of a project. For this first example it was left until the end so you could become familiar with the System Definer, Diffusion Calculator and Plot Renderer settings. It is also important at this point to save the project. You can do this at any time and it is good practice to save your project often.

The following renaming can be done to match the example file included with your installation:



When you rename a node, associated tabs are also renamed automatically. For example, when the Plot Renderer is renamed, so is the tab in the Results window.

1. Right-click the **My Project** node and select **Rename**.
2. In the **New name** field enter `Diffusion_Single_Phase`. Click **OK**. Continue renaming the other nodes.
3. Right-click the **System Definer**, select **Rename** and enter `System with Fe Ni`.
4. Right-click the **Diffusion Calculator**, select **Rename** and enter `Diffusion single region Austenite`.
5. Right-click the **Plot Renderer**, select **Rename** and enter `Composition of Ni vs Distance`.
6. Save the project. To do this, click the **Save** button and navigate to a location on your computer where you can easily find this project file.

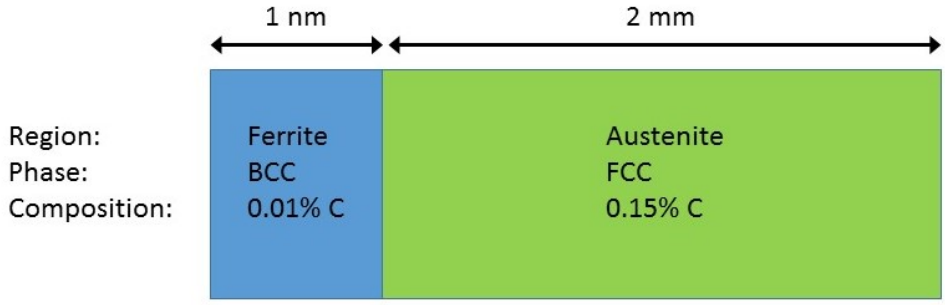
Moving Phase Boundary Simulations

In this section:

About the Moving Phase Boundary Simulation 23
Theory for the Moving Phase Boundary Simulation 25
Moving Phase Boundary Example Project 26
System Definer Settings 28
Diffusion Calculator Settings 29
Plot Renderer Settings 32

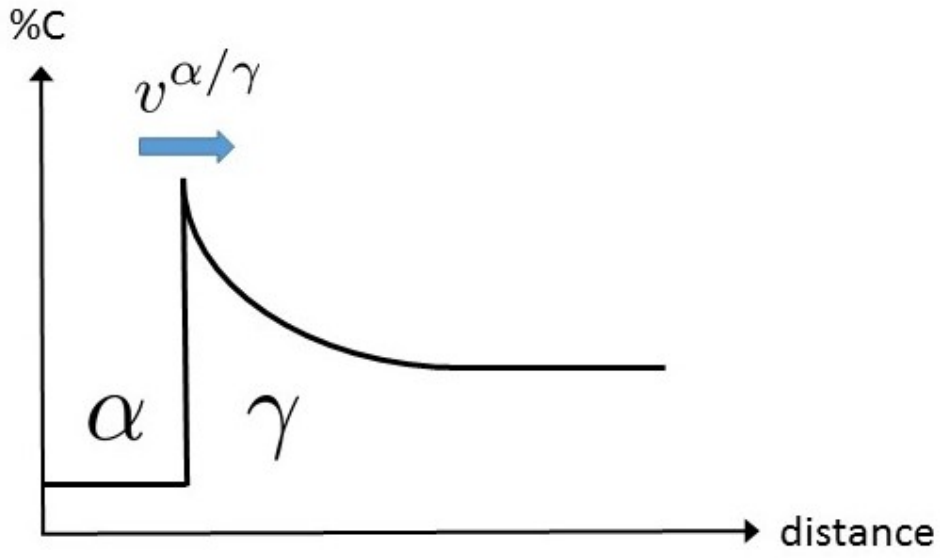
About the Moving Phase Boundary Simulation

The growth of ferrite (bcc) into austenite (fcc) is simulated in this example. The austenite is assumed to be initially homogeneous with the composition Fe - 0.15 mass-% C and the transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation. The initial state is as below.



The set-up of the Moving Boundary example. There are two regions, Ferrite and Austenite, consisting of bcc and fcc, respectively.

A schematic graph of the carbon profile during the transformation is shown in the image below. Crusius et al. (1992)[1.] is recommended as further reading.



1. Crusius, Sabine, Lars Höglund, Ursula Knoop, Gerhard Inden, and John Ågren. 1992. "On the Growth of Ferrite Allotriomorphs in Fe-C Alloys." Zeitschrift Fur Metallkunde 83 (10): 729–38.

Schematic view of the carbon profile during the transformation from austenite (γ) to ferrite (α) in the Moving Boundary example.

Theory for the Moving Phase Boundary Simulation

It is assumed that local equilibrium holds at the phase interface, i.e. the chemical potentials of all elements are continuous across the boundary, but the chemical potential gradients are in general discontinuous.

In order to maintain mass balance a set of flux balance equations must be satisfied at the phase interface:

$$v^{\alpha/\gamma}(c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma \qquad k = 1, \ldots, n-1$$

where v is the interfacial velocity. The concentrations and the fluxes c and J are those at the interface on the α and γ sides, respectively.

In the present case there are no degrees of freedom at the interface and the concentrations can be taken directly from a phase diagram. There is only one flux balance equation and the interface velocity can be evaluated once the fluxes at the interface are known. However, for ternary and higher systems the state at the interface must be found by some iterative procedure.

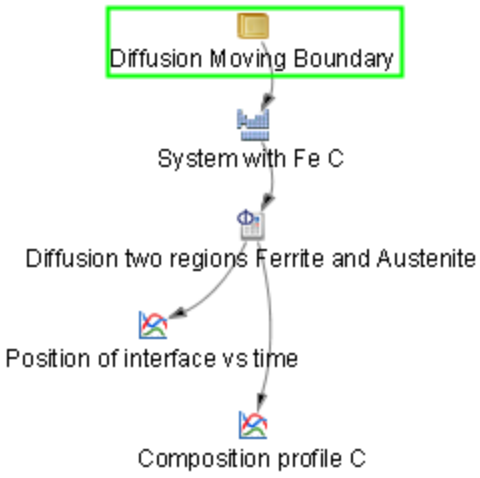
For more information on moving phase boundary problems, see, for example, Ågren (1982)[1.] ,Crusius et al. (1992)[2.] and Höglund (1997)[3.] .

1. Ågren (1982) "Numerical Treatment of Diffusional Reactions in Multicomponent Alloys," *J. Phys. Chem. Solids*, 43 (4), pp. 385–391.
2. Crusius, Sabine, Gerhard Inden, Ursula Knoop, Lars Höglund, and John Ågren. 1992. "On the Numerical Treatment of Moving Boundary Problems." Zeitschrift Fur Metallkunde 83 (9): 673–78.
3. Höglund (1997).*Computer simulation of diffusion controlled transformations in multicomponent alloys*, PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden.

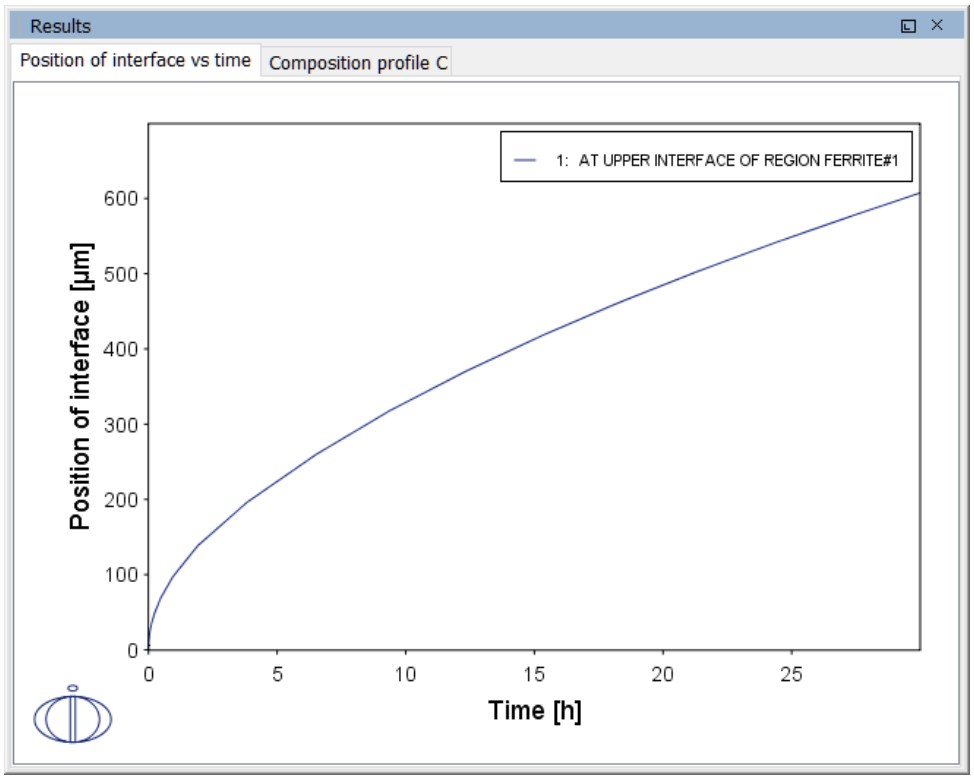
Moving Phase Boundary Example Project

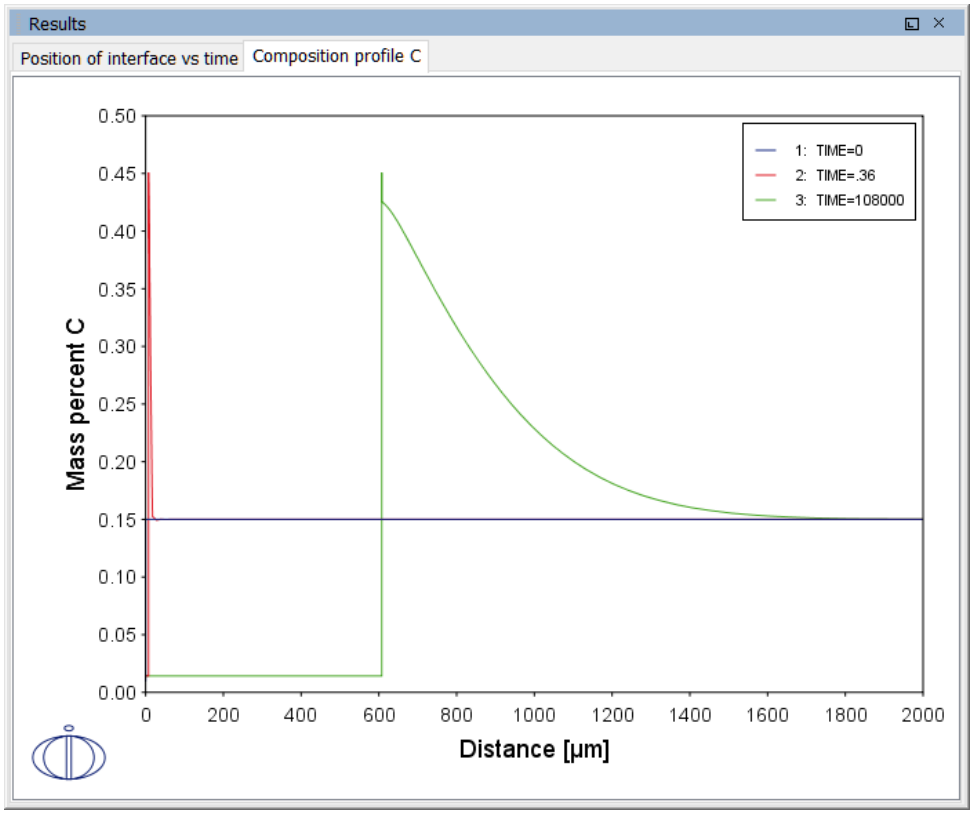
For the moving phase boundary simulation, you can open the example project file included with your installation to see how it is set up.

1. Open Thermo-Calc.
2. From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
3. Open the **Diffusion Module - DICTRA** folder and locate the file `D_02_Diffusion_Moving_Boundary.tcu` and double-click to open it.
4. The project opens in Thermo-Calc. Click the top Project node (renamed to *Diffusion_Moving_Boundary*). At the bottom of the **Configuration** window click **Perform Tree**.



When completed, the results are plotted in the **Results** window. There are two plot nodes, which creates two plots: The ferrite/austenite phase interface position as a function of time and the composition profile for Carbon.


Results
Position of interface vs time
Composition profile C
1: AT UPPER INTERFACE OF REGION FERRITE#1
Position of interface [µm]
0
100
200
300
400
500
600
0
5
10
15
20
25
Time [h]


Results
Position of interface vs time
Composition profile C
1: TIME=0
2: TIME=.36
3: TIME=108000
Mass percent C
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Distance [µm]

System Definer Settings

This is a continuation from the Single Phase simulation and it describes how to set up the example file *D_02_Diffusion_Moving_Boundary.tcu*. In this example, the shortcuts explained for the Single Phase System Definer are used.

Add the Databases and the Elements

1. Open a new instance of Thermo-Calc.
2. In the **My Project** window click the **Diffusion Simulation** template icon.
3. In the System Definer **Configuration** window click the **Package** list and choose **Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)**.
4. In the **Periodic Table**, click **Fe** then **C**.
5. Rename the nodes. Right-click **System Definer** and rename it to **System with Fe C**.
6. Right-click **My Project** and give it the same name as the project e.g. *Diffusion_Moving_Boundary*.
7. Save the project file with a new name, such as *DiffusionMovingBoundary*.

Diffusion Calculator Settings

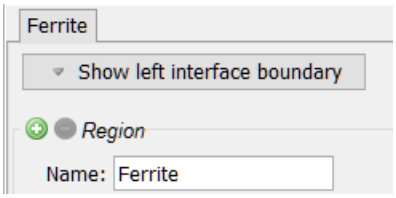
After you have completed the settings for the System Definer you define the diffusion calculation parameters.

The phase interface between ferrite and austenite is created by introducing an austenite region that is attached to the ferrite region. Regions are always separated by phase interfaces and must therefore always contain different phases.

In this simulation both the FCC_A1 and BCC_A2 phases are included. Both phases are assumed to be initially homogeneous, the bcc phase having 0.01 mass-% C and the fcc phase 0.15 mass-% C. These settings are entered on the Diffusion Calculator.

Add a Ferrite Region

1. In the **Project** window, click the **Diffusion Calculator** node.
2. Keep the default for *Composition unit* (**Mass percent**). Choose **µm** for the **Length unit**. A **Planar** geometry is used for all the examples.
3. Double-click the **Region** tab and enter `Ferrite`. Press <Enter>.

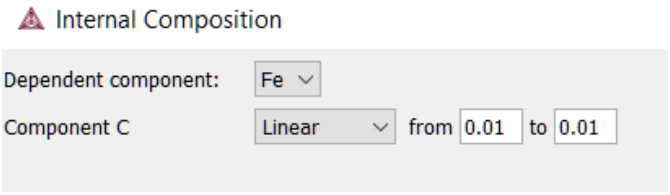


4. In the **Width** field enter `0.001` µm and change the default number of points to `10`. Keep the default **Linear** grid type.

   The grid type for the ferrite region is the same as in the single-phase simulation example, i.e. equidistant.

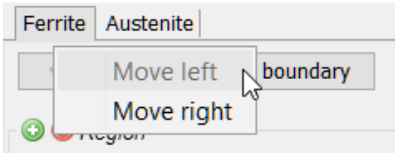
5. From the **Phase** list select **BCC_A2**.
6. Click **Edit** next to **Composition profiles**. **Fe** is chosen as the **Dependent component** and the initial profile for **Component C** is a **Linear** variation.
7. Enter `0.01` in both fields to represent C going from 0.01 (mass-%) on the lower, left-hand side of the system to 0.01 (mass-%) on the upper, right-hand side of the

system. Click **Apply**.



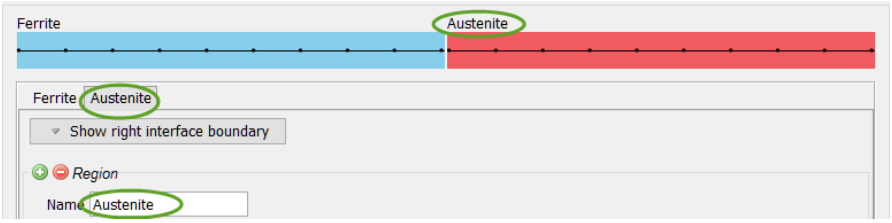
Add an Austenite Region

1. Next to *Region*, click the green add button. A new tab called **Region** is added.



If you add a region and then need to change the order, right-click the applicable tab and choose **Move left** or **Move right**.

2. In the *Region* **Name** field, enter `Austenite`. This name is automatically updated on the tab and above the grid points in a new section for the second region.



3. In the **Width** field enter `2000` µm.
4. In the next field (the number of points), enter `50`.
5. Select a **Geometric** type of grid and enter `1.05` for the **Ratio**.

   For the austenite region the grid type is *geometric*. For these grids the grid point spacing changes by a constant factor between every grid point. In this case the spacing increases by 5%, i.e. a factor of 1.05, from the lower, left side for each grid point. It is usually good practice to have a denser grid close to moving boundaries where the composition profiles are expected to vary a lot during the simulation.

6. From the **Phase** list, select **FCC_A1**.
7. Click **Edit** next to **Composition profiles**. Enter `0.15` in both fields to represent **Component C** going from 0.15 (mass-%) on the lower, left-hand side of the system to 0.15 (mass-%) on the upper, right-hand side of the system. Click **Apply**. The Austenite grid shows the points.

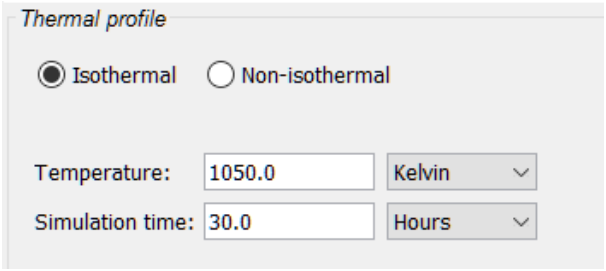


The domain now consists of two regions: Ferrite and Austenite.

Define the Thermal Profile

The default **Isothermal** profile is used.

1. In the **Temperature** field, enter `1050`.
2. In the **Simulation time** field, enter `30`. Choose **Hours** from the list.
3. Right-click **Diffusion Calculator** and rename it to **Diffusion two regions Ferrite and Austenite**.



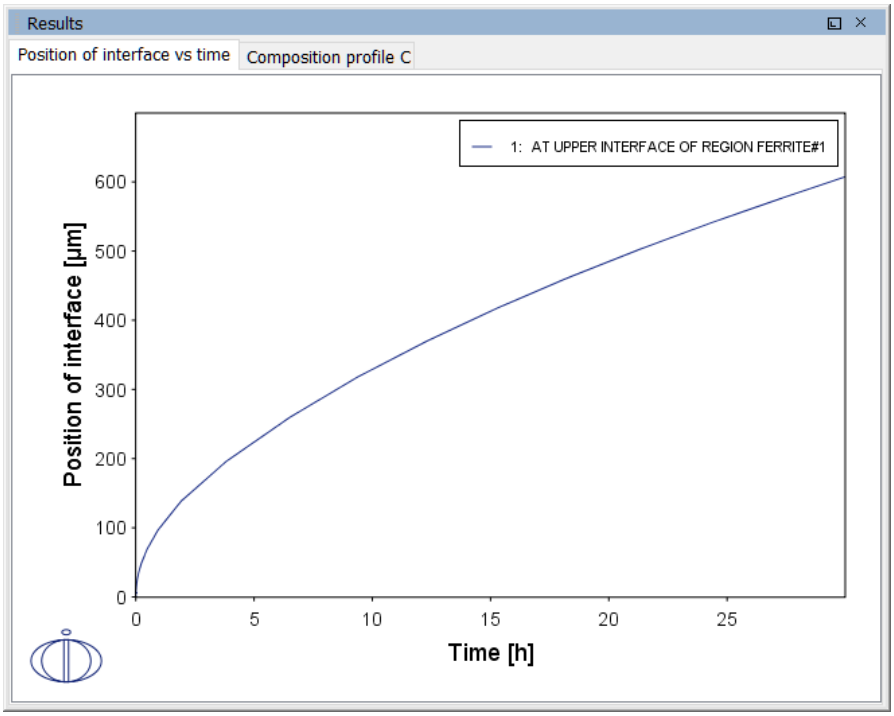
As with the single phase example, the **Options** tab keeps all the defaults.

Plot Renderer Settings

After you have completed the settings for the System Definer and Diffusion Calculator you define the plot parameters.

1. In the **Project** window, click the **Plot Renderer** node.
2. Choose **Time** as the *X*-**Axis variable** and select **Hours**.
3. Choose **Position of interface** as the *Y*-**Axis variable**.
4. In the **Interface** list, keep the default **Ferrite/Austenite**.
5. Right-click **Plot Renderer** and rename it to **Position of interface vs time**.
6. Click **Perform** If you have entered the same settings the plot shows the ferrite/austenite phase interface position as a function of time. The plot has the parabolic appearance characteristic for many types of diffusion simulations.

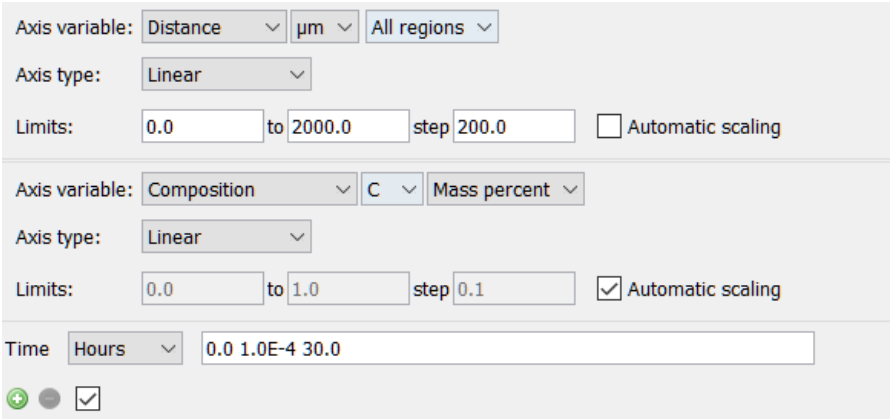
   Plot result from the example showing the phase interface position as a function of time.



Add a Second Plot

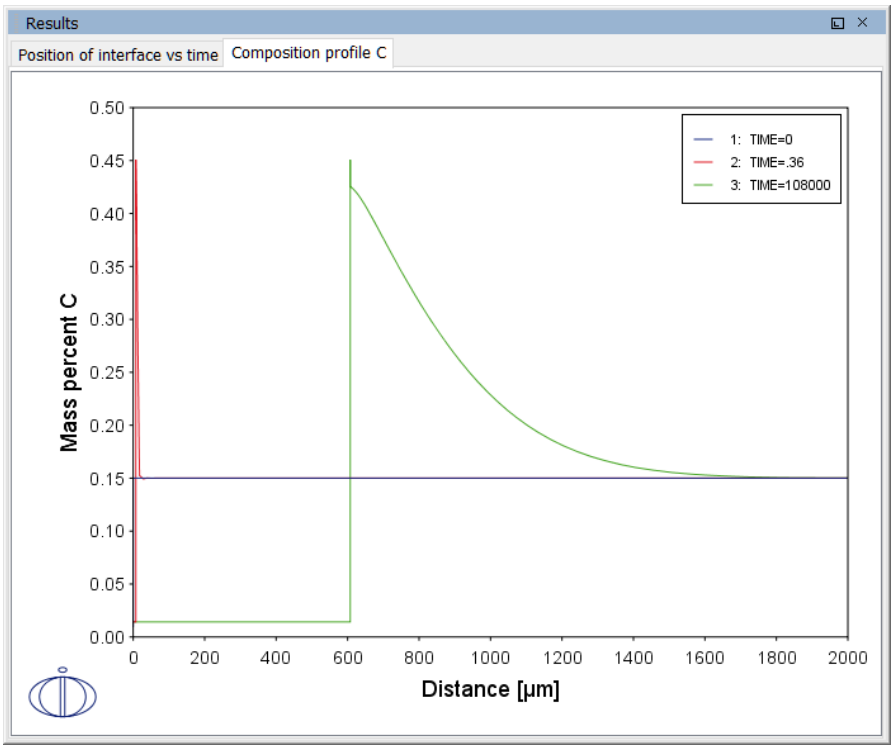
1. Right-click the **Diffusion Calculator** node. Remember it is renamed to *Diffusion two regions Ferrite and Austenite*.
2. From the **Create New Successor** list, click **Plot Renderer**.

3. In the new Plot Renderer node **Configuration** window, for the *X*-**Axis variable**, change the Distance units to **µm**.
4. Click to clear the **Automatic scaling** check box.
5. In the **Limits** fields, keep `0` as the lower limit, enter `2000` for the upper limit and `200` for **step**.
6. For the *Y*-**Axis variable**, keep the default Composition and choose **C** from the list.
7. Choose **Hours** as the **Time** unit and enter `0.0 1.0E-4 30.0` in the field.



8. Right-click **Plot Renderer** and rename it to **Composition profile C**.

9. Click **Perform** If you have entered the same settings the plot shows the composition profile of C.



Multiphase Simulations

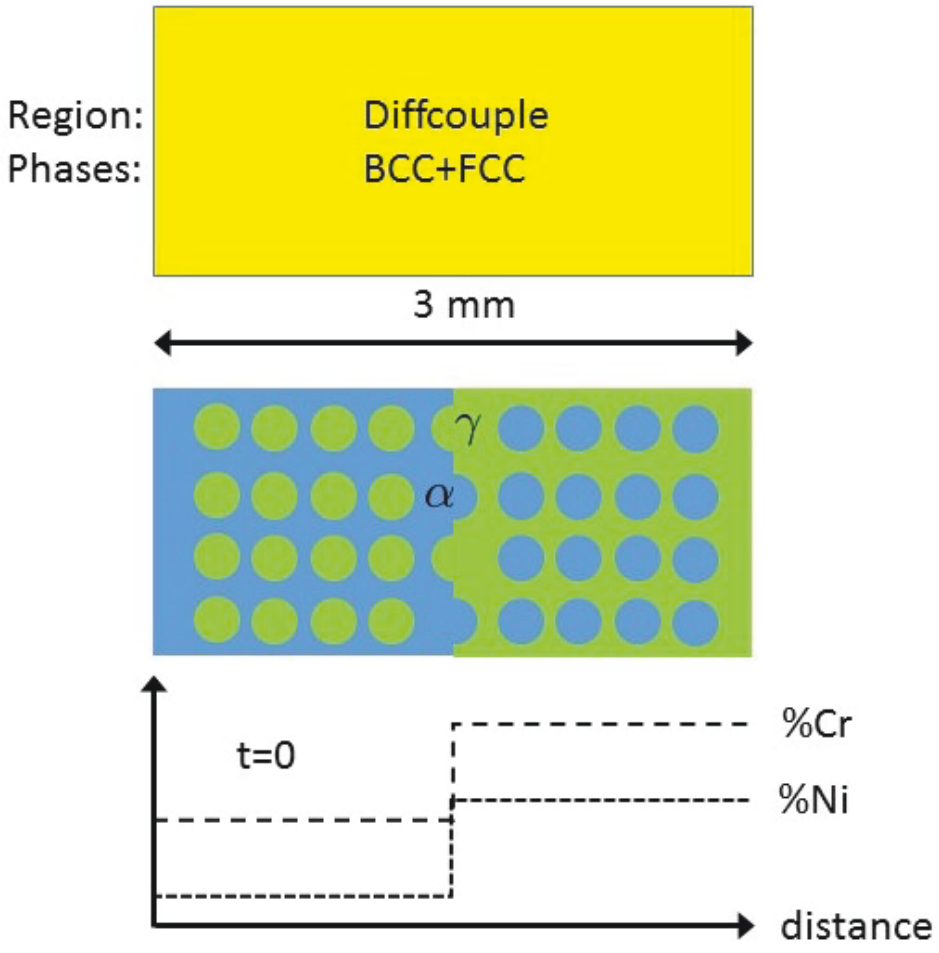
In this section:

About the Multiphase Simulation 36
Theory for the Multiphase Simulation 37
Multiphase Example Project 38
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About the Multiphase Simulation

This example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.



Schematic view of the initial state of the Multiphase example. Two ternary Fe-Cr-Ni alloys form a diffusion couple. There is a single region (diffcouple) where both the bcc and fcc phases are entered. Both alloys are duplex bcc+fcc, but the majority phase is bcc (α) in the left-hand side alloy and fcc (γ) in the right.

Theory for the Multiphase Simulation

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström (2006)[1] and Larsson and Höglund (2009)[2]. As mentioned in the description of this simulation, it is assumed that the material is locally fully equilibrated and that the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition. From a numerical point of view the homogenization model treats the multiphase material as a single phase having the "average", or "effective", properties of the local phase mixture.

When estimating the effective kinetics of a multiphase mixture the product of solubility and mobility in each phase is considered. It is therefore convenient to define

$$\Gamma_k^\phi = M_k^\phi c_k^\phi$$

for each phase ϕ. The effective kinetics of the multiphase mixture is denoted and in this example it was evaluated using the lower Hashin-Shtrikman bound. The default method is a simple rule of mixtures

$$\Gamma^\star = \sum_\phi f^\phi \Gamma_k^\phi$$

where f^ϕ is the volume fraction of ϕ. The flux is obtained as

$$J_k = -\Gamma_k^\star \frac{\partial \mu_k}{\partial z}$$

which replaces the single-phase equation

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

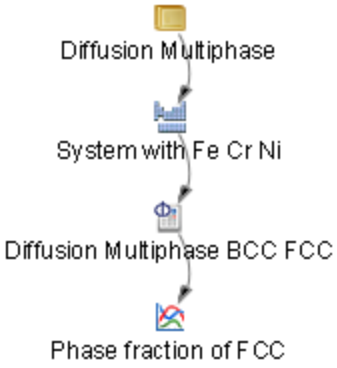
for multiphase simulations.

1. Larsson, Henrik, and Anders Engström. 2006. "A Homogenization Approach to Diffusion Simulations Applied to α + γ Fe–Cr–Ni Diffusion Couples." Acta Materialia 54 (9): 2431–39.
2. Larsson, Henrik, and Lars Höglund. 2009. "Multiphase Diffusion Simulations in 1D Using the DICTRA Homogenization Model." Calphad 33 (3): 495–501.

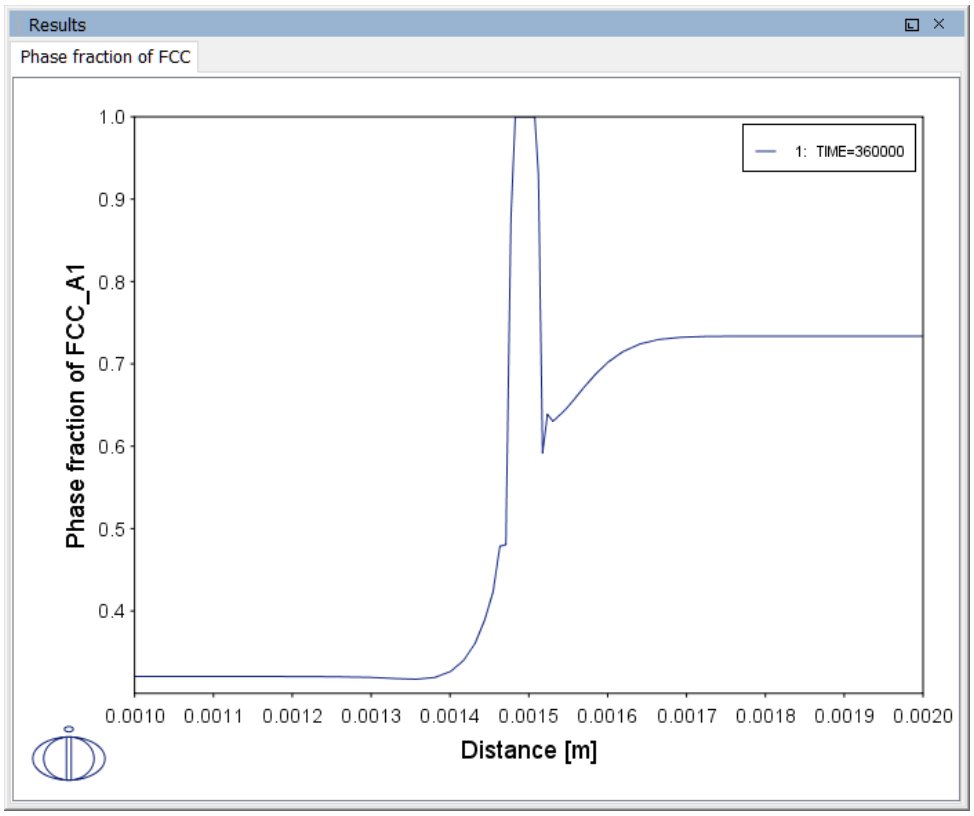
Multiphase Example Project

For the multiphase simulation, you can open the example project file included with your installation to see how it is set up.

1. Open Thermo-Calc.
2. From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
3. Open the **Diffusion Module - DICTRA** folder and locate the `D_03_Diffusion_Multiphase.tcu` file and double-click to open it.
4. The project opens in Thermo-Calc. Click the top Project node (renamed to *Diffusion_Multiphase*). At the bottom of the **Configuration** window click **Perform Tree**.



When completed, the results are plotted in the Results window.


Results
Phase fraction of FCC
1: TIME=360000
Phase fraction of FCC_A1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.0010
0.0011
0.0012
0.0013
0.0014
0.0015
0.0016
0.0017
0.0018
0.0019
0.0020
Distance [m]

System Definer Settings

This is a continuation from the previous examples and uses the short cuts already described. You can alternatively open a saved project and edit the settings.

Add the Databases and the Elements

1. Open a new instance of Thermo-Calc.
2. In the **My Project** window click the **Diffusion Simulation** template icon.
3. In the System Definer **Configuration** window click the **Package** list and choose **Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)**.
4. In the **Periodic Table**, click **Fe**, then **Cr** and **Ni**.
5. Right-click **System Definer** and rename it to **System with Fe Cr Ni**.
6. Save the project file with a new name, e.g. *DiffusionMultiphase*.

Diffusion Calculator Settings

After you have made the settings to the System Definer, you add the diffusion calculation parameters.

Define the Ferrite and Austenite Regions

1. In the **Project** window, click the **Diffusion Calculator** node.
2. For *Composition unit* select **Mole fraction**.

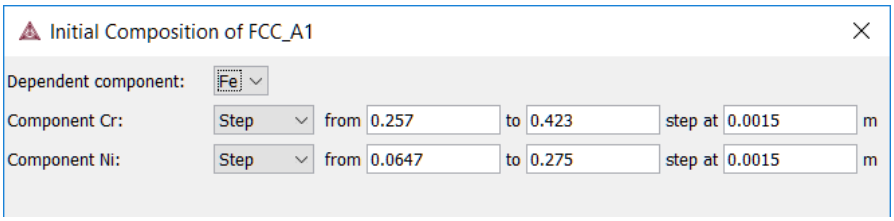
   Keep the default Length unit (**m**). A **Planar** geometry is used for all the examples.

3. In the *Region* **Name** field, enter `Diffcouple`.
4. In the *Width* field enter `0.003` and enter `60` points.
5. Select **Double geometric** as the grid type.

   A double geometric grid is similar to the geometric grid used in the moving phase boundary example. The difference is that two geometrical factors are entered: one for the lower and one for the upper half of the region. In the lower half of the region the distance between subsequent grid points decreases by 15 % (0.85) and in the upper half it increases by 15 % (1.15). The resulting grid has a much larger grid point density toward the middle of the domain where there are sharp changes in composition.

6. Enter these values as follows. In the **Lower ratio** field enter `0.85` and `1.15` in the **Upper ratio** field.
7. Choose **FCC_A1** from the **Phase** list.
8. Next to *Phase* click the **Add quantity** button. From the *Phase* list select **BCC_A2**.
9. Click **Edit** next to *Composition profiles*. **Fe** is chosen as the **Dependent component**. Define **Component Cr** and **Component Ni**.
10. Choose **Step** for both the Cr and Ni elements.
11. In each of the fields for Cr (**from**, **to**, **step at**) enter `0.257`, `0.423` and `0.0015`, respectively.

12. In each of the fields for Ni (**from**, **to**, **step at**) enter `0.0647`, `0.275` and `0.0015`, respectively. Click **Apply**.



The resulting Cr profile is thus 0.257 on the left half of the domain and 0.423 on the right with a sharp step at the center (as shown in About the Multiphase Simulation).

Define the Thermal Profile

1. The default **Isothermal** profile is used for this example.
2. In the *Temperature* field, enter `1100` and choose **Celsius** from the list.
3. In the *Simulation time* field, enter `100` and choose **Hours** from the list.
4. Right-click **Diffusion Calculator** and rename it to **Diffusion Multiphase BCC FCC**.

Choose the Homogenization Function

The local kinetics of the multiphase mixture must be estimated by means of some function that may depend on the local phase fractions, phase compositions and the mobilities of the individual phases.

There are many such homogenization functions to choose from. In this particular example the **General lower Hashin–Shtrikman bound**[1] is a good choice.

1. To choose this homogenization function, go to the **Diffusion Calculator** and click the **Options** tab.



Homogenization is already automatically selected as the **Default solver** because multiple phases are selected in a region.

2. Go to the section *Homogenization Model Specific* from the **Homogenization function** list select **General lower Hashin–Shtrikman bound**.

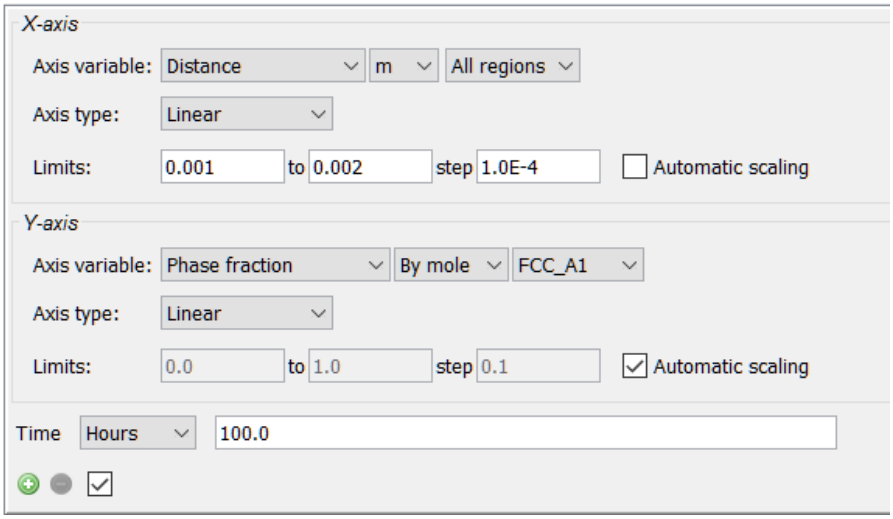
[1] Z. Hashin and S. Shtrikman (1962), "A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials", *J. Appl. Phys.*,33(10), pp. 3125–3131.

Plot Renderer Settings

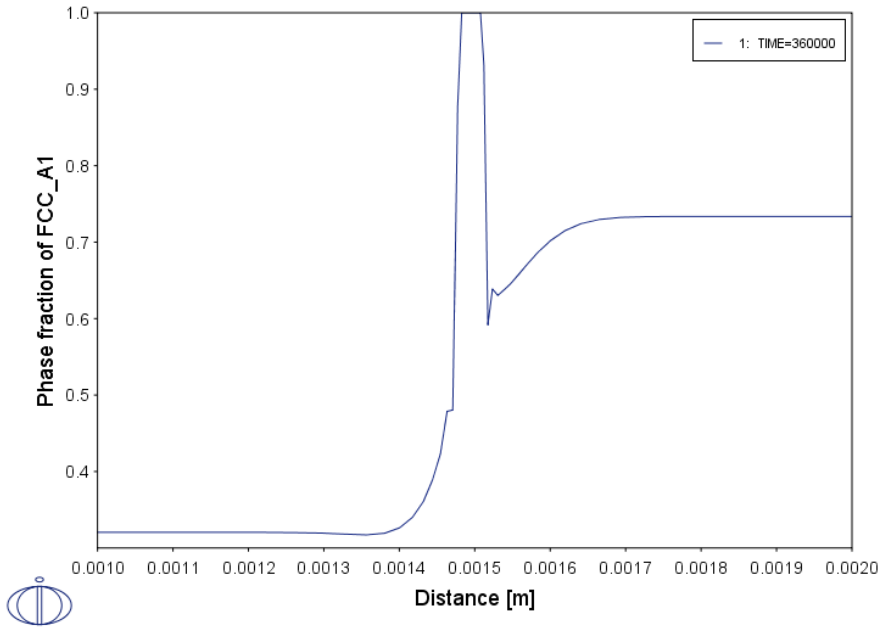
After you enter the settings for the System Definer and Diffusion Calculator, you define the plot parameters. For this example you want to plot the mole fraction fcc phase as a function of distance at the end of the heat treatment.

The plot of phase fraction vs distance shows that a single phase fcc zone has formed and this was also observed experimentally, see A. Engström, 1995: "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24 (1), pp. 12–20.

1. Click the **Plot Renderer** node.
2. Click to clear the **Automatic scaling** check box.
3. Enter the **Limits**: `0.001` **to** `0.002` **step** `1.0E-4`.
4. From the second **Axis variable** list, choose **Phase fraction** and **FCC_A1**.



5. Click **Perform** If you have entered the same settings you will get this plot result.



6. Right-click **Plot Renderer** and rename it to **Phase fraction of FCC**.

References

1. J.-O. Andersson, T. Helander, L. Höglund, P. Shi, and B. Sundman, "Thermo-Calc and DICTRA, computational tools for materials science," *Calphad*, vol. 26, no. 2, pp. 273–312, Jun. 2002.
2. A. Borgenstam, L. Höglund, J. Ågren, and A. Engström, "DICTRA, a tool for simulation of diffusional transformations in alloys," *J. Phase Equilibria*, vol. 21, no. 3, pp. 269–280, May 2000.
3. J.-O. Andersson and J. Ågren, "Models for numerical treatment of multicomponent diffusion in simple phases," *J. Appl. Phys.*, vol. 72, no. 4, pp. 1350–1355, Aug. 1992.
4. S. Crusius, L. Höglund, U. Knoop, G. Inden, and J. Ågren, "On the growth of ferrite allotriomorphs in fe-c alloys," *Zeitschrift für Met.*, vol. 83, no. 10, pp. 729–738, 1992.
5. J. Ågren, "Numerical Treatment of Diffusional Reactions in Multicomponent Alloys," *J. Phys. Chem. Solids*, vol. 43, no. 4, pp. 385–391, 1982.
6. S. Crusius, G. Inden, U. Knoop, L. Höglund, and J. Ågren, "On the numerical treatment of moving boundary problems," *Zeitschrift für Met.*, vol. 83, no. 9, pp. 673–678, 1992.
7. L. Höglund, *Computer simulation of diffusion controlled transformations in multicomponent alloys*, PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden, 1997.
8. Z. Hashin and S. Shtrikman, "A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials," *J. Appl. Phys.*, vol. 33, no. 10, pp. 3125–3131, 1962.
9. A. Engström, "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples," *Scand. J. Metall.*, vol. 24, no. 1, pp. 12–20, 1995.
10. H. Larsson and A. Engström, "A homogenization approach to diffusion simulations applied to α + γ Fe–Cr–Ni diffusion couples," *Acta Mater.*, vol. 54, no. 9, pp. 2431–2439, May 2006.
11. H. Larsson and L. Höglund, "Multiphase diffusion simulations in 1D using the DICTRA homogenization model," *Calphad Comput. Coupling Phase Diagrams Thermochem.*, vol. 33, no. 3, pp. 495–501, 2009.

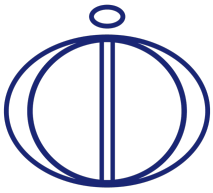
Next Steps

Below are suggestions for you to learn more about using the Diffusion (DICTRA) Module.

- Browse the Online Help (Help → Online Help) or open one of the available PDFs included with your installation (Help → Manuals Folder).
- You have been working with in Graphical Mode. You might also want to try the *Diffusion Module Console Mode Quick Start Guide* (Help → Manuals Folder). This will further prepare you to work with the Console Mode examples (Help → Examples Files), which contain many simulation types and advanced functionality not available in Graphical Mode.
- You can also go to the Thermo-Calc website to see if there are other options suited to you, such as a course or video tutorials. (Help → Video Tutorials and Help → Thermo-Calc Website).

Diffusion Module (DICTRA) Quick Start Guide - Console Mode

Thermo-Calc Version 2021b



Thermo-Calc Software

Introduction to the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to the Thermo-Calc software package. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulations are both time- and space-dependent.

The Diffusion Module (DICTRA) is suitable for solving diffusion problems that include a moving boundary (so-called *Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. The concentration fields only vary along one spatial coordinate, but the geometry may be either planar, cylindrical or spherical.

In this section:

About this Quick Start Guide 3

About the DICTRA File Formats 4

Opening the Module and Macro Files 6

Basic Terminology 9

Setting up a Simulation in Console Mode 12

About this Quick Start Guide

The following introduces you to the basic concepts, steps and theory to start using the Diffusion Module (DICTRA). An understanding of this information is necessary to ensure accurate calculations.

- More details about the use of DICTRA can be found in Andersson et. al (2002)[1.] and Borgenstam et al. (2000)[2.] .



If you are not familiar with Graphical Mode, it is recommended you review the available documentation and training material.

1. Andersson, J.-O., Helander, T., Höglund, L., Shi, P., and Sundman, B., *Calphad*, 26 (2), pp. 273–312.

2. Borgenstam, Al, Höglund, L., Ågren, J. and Engström, A., *J. Ph. Equilib.*, 21 (3), pp. 269–280.

About the DICTRA File Formats

The Diffusion Module (DICTRA) in Console Mode uses different file formats: *log*, *macro* and *workspace* files.



When working with the DICTRA module in Graphical Mode, the file formats are the same as when using Thermo-Calc.

Log Files

Log files (*.TCM) are plain text files and are just macro files used to save a sequence of commands. These files can be edited in a text editor.

- To start saving your input into a file, in the SYS module type `SET_LOG_FILE`, followed by the name of the file that you want to save your command sequence to.
- When creating a command sequence, and if you want to save the output in the log file, type `SET_ECHO` before SET_LOG_FILE. This is useful if you later want to use the log file as a macro file because the macro file lists the full commands instead of only the short names.

Macro Files

Macro files (*.DCM) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

- To run a macro file, in the SYS or DICTRA module type `MACRO_FILE_OPEN`, followed by the name of the macro file. DICTRA runs the MACRO_FILE_OPEN sequence that the file contains.
- To remain in the console and keep working in the DICTRA module, in the SYS, DICTRA, POLY, or POST module add the command SET_INTERACTIVE at the end of the macro file. Alternatively, use `EXIT` as the final command.

Workspace Files

Workspaces files for the Diffusion Module (DICTRA) have the file extension *.DIC, which allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations.

- At the `DIC` prompt use SAVE_WORKSPACES.
- To load the data and calculation results of a workspace file, at the `DIC` prompt use READ_WORKSPACES.

Opening the Module and Macro Files

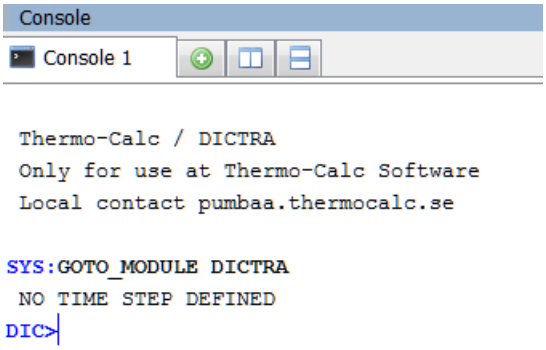
You can go to into the Console Mode to explore the command options, or continue with this quick start guide, which uses macro files to demonstrate how to use the software.

How to Open the DICTRA Module in Thermo-Calc

1. Open Thermo-Calc in Console Mode.

   By default, Thermo-Calc opens in the most recently used state. If it opens in Graphical Mode, on the toolbar, click **Switch to Console Mode**.

2. In the `SYS` module, type `GOTO_MODULE DICTRA`. For a list of all the available commands in the current module, at the prompt type a question mark (?) and press <Enter>. For a description of a specific command, type `Help` followed by the name of the command.



How to Open the Beginner Guide Examples

For the Console Mode examples included with your installation, you can open the .DCM files from the main menu. You can also open any macro file with a command or by dragging it into the Console window.

How to Open a Macro File from the Examples Folder

To open a specific macro file from the Examples folders included with your installation:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens (these are the Thermo-Calc macro files).
4. Double-click the **Diffusion Module - DICTRA** folder and navigate to an example folder.

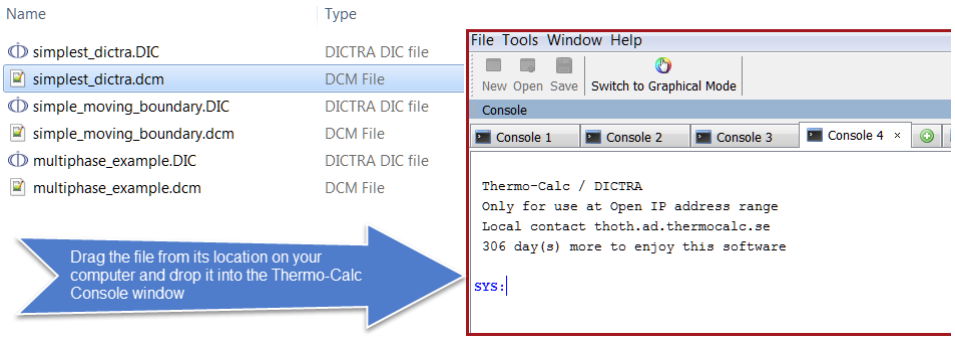
   The three Quick Start example macros and the PDF guide are in the first folder called **Beginner Guide**.

How to Use a Command in Console Mode

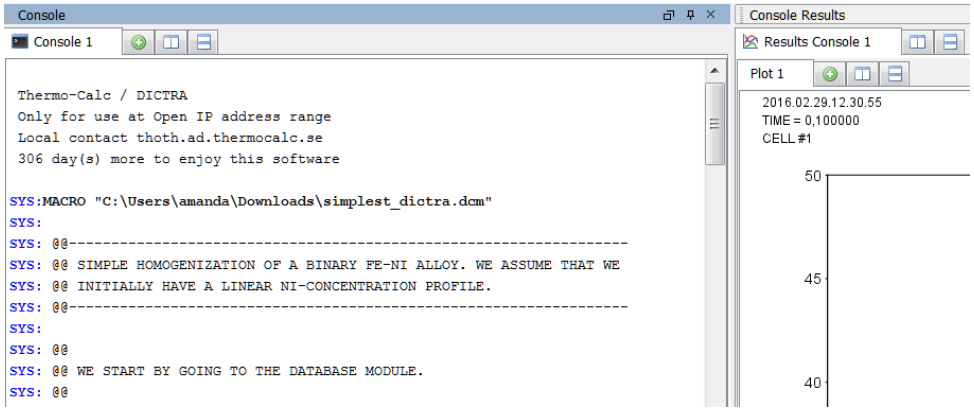
At the `SYS` prompt, type MACRO_FILE_OPEN and press <Enter>. In the file dialogue window that opens, locate and select the macro file on your computer.

Drag and Drop a Macro File into Console Mode

For example, navigate to the **Beginner Guide** folder and then drag the file from its location into Thermo-Calc Console window.



The macro automatically runs after you drop it into the Console window.



Double-click to Open a File

Navigate to the macro file location, for example where each set of file examples is in its own folder. When you double-click, it opens the file in a new instance of Thermo-Calc.

Basic Terminology

The following definitions are useful to help you understand the examples and commands in this guide. For more detailed information search or browse the online help (**Help →Online Help**).

Cells and Regions in a System

A system normally consists of one *cell*. This cell contains one or several *regions* in which the diffusion problem is to be solved. A system of diffusion equations is solved for each region. The size of the system is the sum of sizes of all the regions in all the system's cells.

The interface between two regions typically moves as the result of a simulation, that is, the regions grow or shrink. Such an interface is called an *inner interface*. The boundary of a cell is called an *outer interface* and the condition of this type of interface may be affected by the choice of boundary conditions.

For some simulations it is useful to have several cells in a system. Matter can move between cells. However, it is assumed that there is diffusional equilibrium between all cells (this means that there are no differences in diffusion potentials between cells). In other words, the size of a cell is fixed during the simulation.

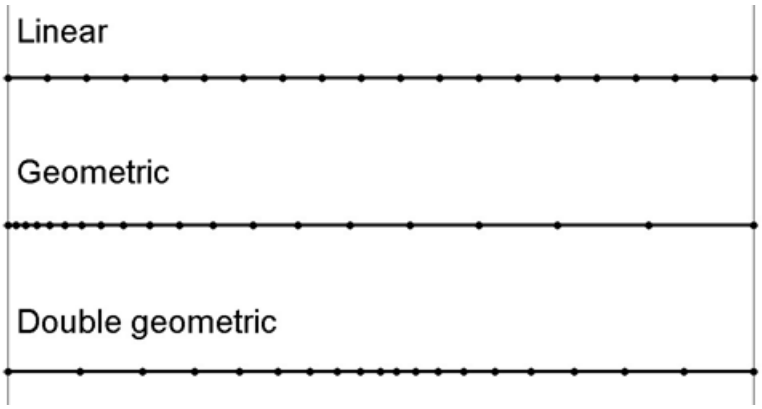
By default this is a *closed system*, which means that matter cannot move across its boundaries. However, you can change this setting for both the *lower boundary* (left side/centre) and the *upper boundary* (right side/surface) of the system. You can also set these boundary conditions to vary as a function of time, temperature and/or pressure.

Regions and Grids

A *region* contains one or more phases. If a region contains several phases one of those must be entered as a *matrix phase* whereas the others are entered as *spheroid*.

A region must also contain a number of *grid points*. The composition is only known at these grid points and the software assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

These grid types are used in diffusion simulations: linear, geometric and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region contains one or more *phases*. A phase can be of the *matrix*, *spheroid* or *lamellar* type. A phase can be introduced with the status *active* (the default) or *inactive*.

An inactive phase is a phase which does not participate in the calculations until it is stable. If a phase is inactive, then the driving force for precipitation of the phase is continuously monitored. When the driving force exceeds a predefined positive value, the phase take parts in the simulation and the phase automatically becomes active. A new region is then created and the formerly inactive phase is entered as the matrix phase of the new region. The name of the region is set to the name of the phase that just became active but with `R_` added as a prefix.

Composition

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Two types of composition variables are used within the program: site-fractions and u-fractions, although you can also use weight fraction or mole fraction, for example.

The *site-fractions* are used to set up the problem and interface with POLY-3 (in Console Mode). The site fraction of a species *k*, y_k, is the fraction of equivalent lattice sites occupied by species k. It is the only concentration variable that uniquely defines the composition and the constitution of a phase and it is necessary to use the site fraction in the storage of the data during a simulation.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$u_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where composition vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical* or *spherical*.

Planar Geometry

This geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Cylindrical and Spherical Geometries

- Cylindrical geometry corresponds to an infinitely long cylinder of a certain radius.
- Sypherical geometry corresponds to a sphere with a certain radius.

By default for both geometries, the lower boundary (the zero coordinate) is at the centre of the cylinder/sphere. The upper boundary (the coordinate with the highest value) is at the *surface* of the cylinder/sphere. You can enter a left most coordinate that is larger than zero to allow for tube and hollow sphere geometries.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Setting up a Simulation in Console Mode

Although there are several commands to learn to correctly set up a DICTRA module simulation, the sequence in which to proceed is basically the same:

1. Define and read **thermodynamic** and **kinetic** data.
2. Set **global conditions** (i.e. temperature, *T*, and pressure, *P*).
3. Enter **region(s)**.
4. Enter **grid(s)** in region(s).
5. Enter **phase(s)** in region(s).
6. Enter **composition(s)** of phase(s).
7. Set **geometry** (optional – by default, the geometry is planar).
8. Set **boundary conditions** (optional – by default, the boundaries are closed).
9. Set the simulation **time**.
10. **Run** the simulation.

For definitions of the above, see Basic Terminology.

The following sections describe each step in more detail for these simulation types:

- About the Single Phase Simulation
- About the Moving Phase Boundary Simulation
- About the Multiphase Simulation

Single Phase Simulations

In this section:

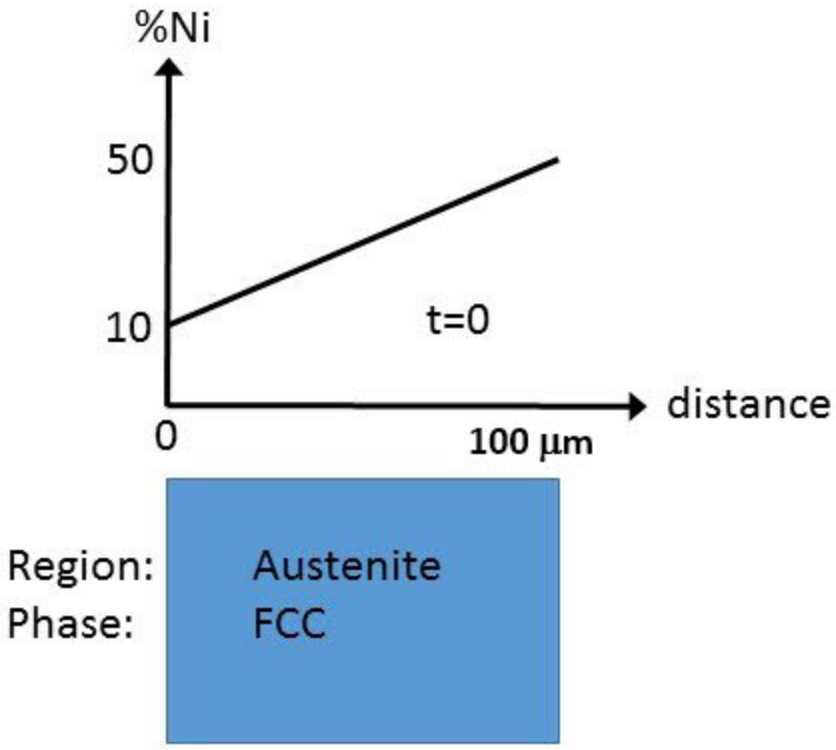
About the Single Phase Simulation 14
Theory for the Single Phase Simulation 15
Running the Single Phase Simulation 17
Single-Phase Command Details 18

About the Single Phase Simulation

In a 100 µm wide planar domain, the single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase (in Thermo-Calc the name of this phase is FCC_A1). Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

The simulation time is slightly different between the modes. For Console Mode it is 10^5 s and for Graphical Mode it is 30 hours.

By default the boundaries are closed. The plot generated shows the initial and final Ni profile.



Schematic view of the initial state of Single Phase Diffusion example. The width of the domain is 100 µm and there is a linear gradient in composition going from 10 to 50 mass-% Ni. There is a single region named Austenite that consists of an fcc phase.

Theory for the Single Phase Simulation

The flux of a component k in the z-direction in an isobarothermal system is in general given by

$$J_k = \sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z}$$

where L_{ki} is a matrix of kinetic coefficients and μ_i is the chemical potential of component *i*. The correlation effects, i.e. the coupling of the flux of *k* component to the chemical potential gradients of the other elements, are normally neglected

$$(L_{ki} = 0, k \neq i)$$

and thus

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

where c_k is the concentration and M_k the mobility of component *k*.

The equation for the flux is combined with the equation of continuity, which takes the following form in a planar domain,

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z}(-J_k)$$

which relates the local evolution of the concentration of k to the divergence of the flux.

The expression for the flux can be expanded in terms of concentration gradients

$$J_k = -\sum_{i=1}^{n} M_k c_k \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z} = -\sum_{i=1}^{n} D_{kj} \frac{\partial c_j}{\partial z}$$

where the diffusion coefficient of component k with respect to the concentration gradient of component j has been introduced.

$$D_{kj} = M_k c_k \frac{\partial \mu_k}{\partial c_j}$$



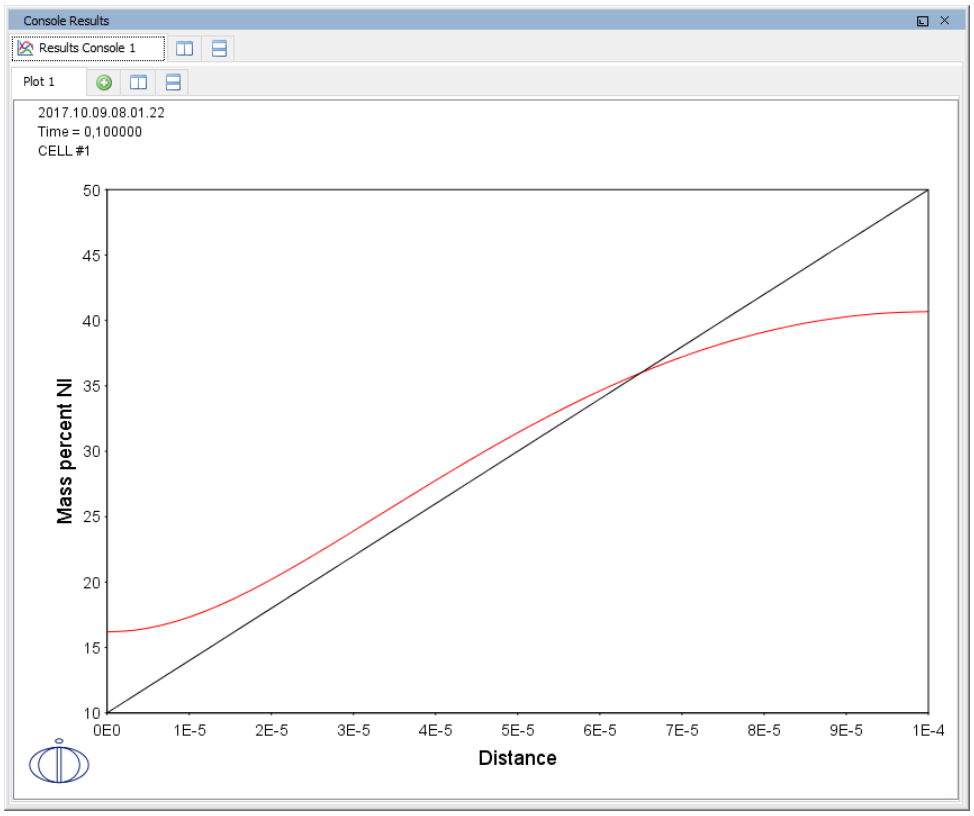
The flux expressions above are given in the so-called lattice-fixed frame of reference. In practical calculations it is more common to use a volume-fixed frame of reference. For a discussion of these concepts, see Andersson and Ågren (1992)[1.] .

1. Andersson, Jan-Olof, and John Ågren. 1992. "Models for Numerical Treatment of Multicomponent Diffusion in Simple Phases." Journal of Applied Physics 72 (4): 1350–55.

Running the Single Phase Simulation

For the single phase simulation, you use an example macro file called `simplest_dictra.dcm`. Open this file in in Console Mode as described in Opening the Module and Macro Files.

The simulation should automatically be set up, executed and finished within a matter of seconds. Results are plotted in the **Console Results** plot window.

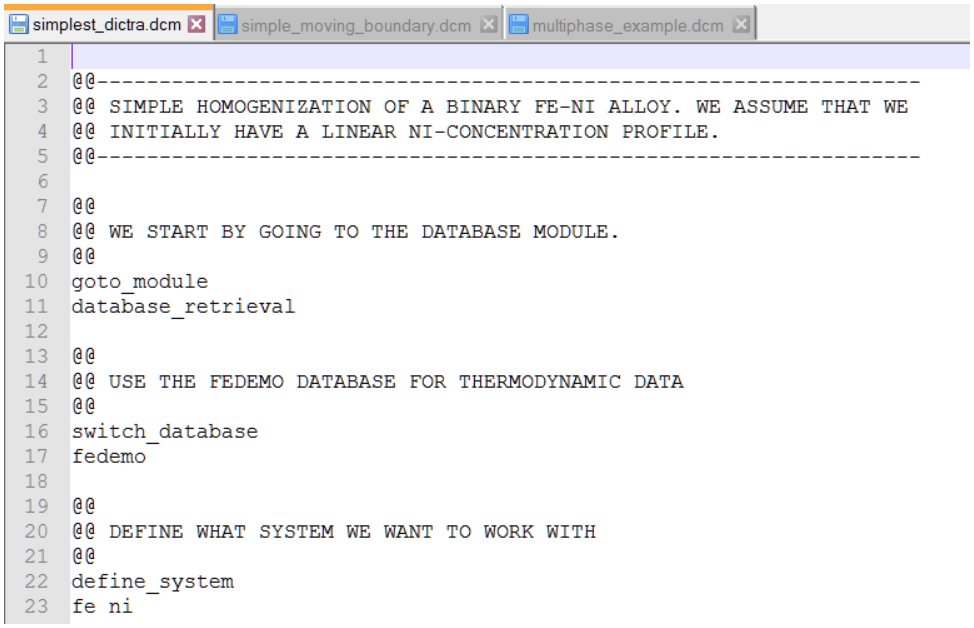


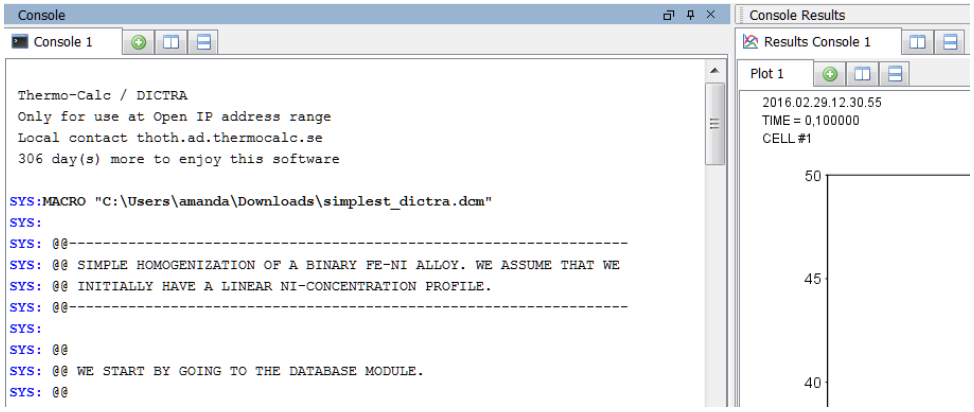
Output from the Single Phase example showing the initial and final Ni profile.

For the rest of the exercise, you will learn how to build this example step-by-step.

Single-Phase Command Details

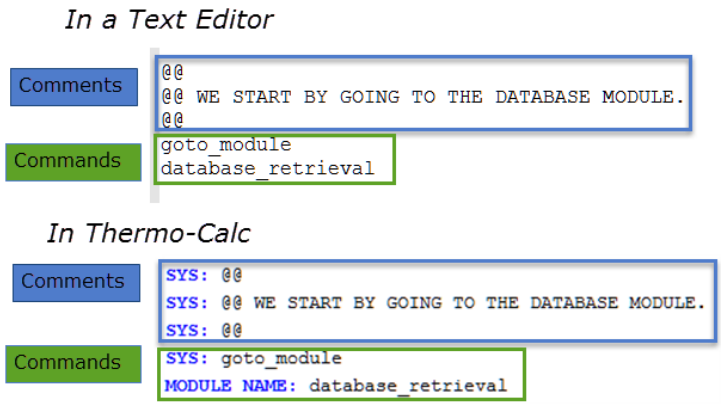
To examine the commands in the macro file, you can either open the file `simplest_dictra.dcm` in a text editor or scroll to the top of the **Console** window.





In the following sections, the commands are discussed in the order they are executed. The first time a command appears it is listed in its general form in UPPERCASE and then using `code font` to detail the specific form of the example. For subsequent examples, only the new commands are detailed. All commands may be abbreviated as long as they are unambiguous.

You can also review the comments included in the example files. The first command you will use is shown in the macro file as follows:



Single Phase - Specifying the Thermodynamic System

Thermo-Calc Console Mode has several modules used for different purposes. In order to define the thermodynamic system the DATABASE_RETRIEVAL module is used.

GOTO_MODULE <MODULE>

```
goto_module database_retrieval
```

There are many databases for different purposes and material types. In this example the *fedemo* database is used. This is the thermodynamic iron demonstration database.

SWITCH_DATABASE <DATABASE>

```
switch_database fedemo
```

Determine what elements to use in the simulation, in this case `Fe` and `Ni`.

DEFINE_SYSTEM <LIST OF ELEMENTS>

```
define_system fe,ni
```

Only the FCC_A1 phase takes part in this simulation and therefore all phases are initially rejected (the wildcard * means *all phases* in this context) and then, with the next command, the FCC_A1 phase is restored.

REJECT <ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM> <LIST OF THE RELEVANT TYPE>

```
reject phases *
```

RESTORE <ELEMENTS, SPECIES, PHASES OR CONSTITUENTS> <LIST OF THE RELEVANT TYPE>

```
restore phases fcc_a1
```

The thermodynamic system now consists of the elements `Fe` and `Ni` and the `fcc_a1` phase.

To actually read the data from file into computer memory the GET_DATA command must be executed.

GET_DATA

```
get_data
```

At this stage only the thermodynamic data is defined and read. The kinetic data (mobilities) are, in this case, stored in another database. This is normally the case though it is possible to have both thermodynamic and kinetic data in a single database.

To add data from a different database the APPEND_DATABASE command is used. The kinetic data in this example is stored in the *mfedemo* database. This is the kinetic iron demonstration database.

APPEND_DATABASE <DATABASE>

```
append_database mfedemo
```

The same sequence of commands used for thermodynamic data is used to read kinetic data from this database.

```
define_system fe,ni
reject phases *
restore phases fcc_a1
get_data
```

Setting up the Single-Phase Simulation

The simulation set-up is performed in the DICTRA_MONITOR module.

```
goto_module
dictra_monitor
```

In this example only one *global* condition is set, temperature. The other global condition that can be set is pressure, but that is rarely done as the default value (1 atm) is set automatically and usually accepted.

SET_CONDITION <GLOBAL OR BOUNDARY>

```
set_condition global
```

The SET_CONDITION command is immediately followed by these sub-prompts:

<T OR P>

```
T
```

The T is for temperature. Then follows a standard procedure for entering temporally piece-wise functions:

<LOW TIME LIMIT> <FUNCTION> <HIGH TIME LIMIT> <Y/N> <IF Y, THEN NEXT FUNCTION> <...>

```
0 1400; * N
```

These prompts start with the *low time limit*, here zero (`0`), then the *function* (here the constant value `1400`) closed by a semicolon (`;`), then the *high time limit* (here a wildcard `*` is entered), then a `Y` or a `N` depending on whether more functions will be entered (in this case `N` because only a single function is entered).

The wildcard * used for the upper time limit means that the entered function is valid for the whole simulation. What this means is that a constant temperature equal to 1400 K is used during the whole simulation.

In any simulation at least one *region* must be defined. This is a named container that designates a certain part of, in this case the whole, domain. The name of a region is arbitrary and specified by you.

ENTER_REGION <NAME OF REGION>

```
enter_region austenite
```



The use of regions becomes clearer in the context of so-called moving phase boundary simulations (see About the Moving Phase Boundary Simulation).

A region must contain a numerical *grid* specified by width and type.

ENTER_GRID_COORDINATES

<NAME OF REGION FOR WHICH GRID IS TO BE ENTERED>

<WIDTH OF REGION>

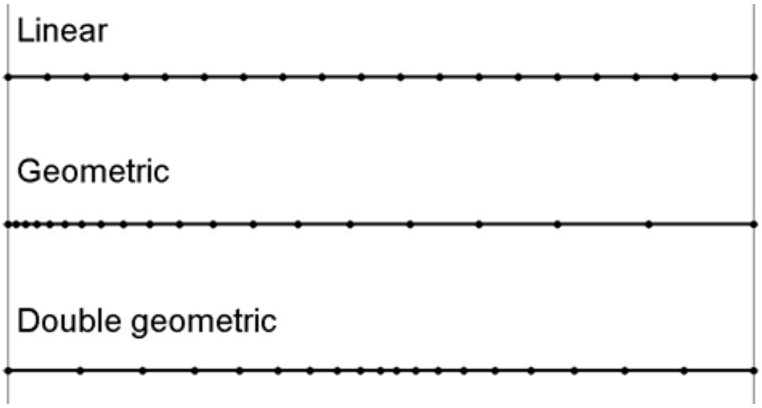
<TYPE OF GRID>

<NUMBER OF GRID POINTS>

```
enter_grid_coordinates
austenite
1e-4
linear
60
```

In the entries above, a 10^{-4} m wide (`1e-4`), `linear`, i.e. equidistant, grid is used with `60` grid points. There are many types of grids, see below for examples, and for other types than the linear there are additional sub-prompts.

These grid types are used in diffusion simulations: linear, geometric and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



A region must contain one *active* phase of type *matrix*. The meaning of active/inactive and phase type is explained in the next examples.

ENTER_PHASE_IN_REGION

<ACTIVE OR INACTIVE>

<NAME OF REGION>

<PHASE TYPE IN REGION>

<PHASE NAME>

```
enter_phase_in_region
active
austenite
matrix
fcc_a1
```

In this example only one phase participates, the `fcc_a1` phase, and it must therefore be `active` and of type `matrix`.

The initial composition profile must be specified for all phases that take part in a simulation. Since there are only two elements, Fe and Ni, in the present simulation the initial *composition profile* must only be given for one of them.

ENTER_COMPOSITIONS

<REGION NAME>

<PHASE NAME>

<DEPENDENT COMPONENT>

<COMPOSITION TYPE>

<COMPONENT NAME>

<TYPE OF COMPOSITION PROFILE>

<COMPOSITION PROFILE DEPENDENT INPUT>

```
enter_compositions
austenite
fcc_a1
fe
weight_percent
ni
linear
10
50
```

In the above entries, `Fe` is chosen as the dependent component and the initial profile for Ni is a `linear` variation going from `10` mass-% on the lower/left hand side of the system to `50` mass-% on the upper/right hand side of the system. The composition type can be chosen among a number of different types, e.g. `weight percent` or mole fraction. There are also many different ways of specifying the composition profile, e.g. an arbitrary position dependent function or reading it for each grid point from file. Here the simplest possible type is used a `linear` function.

Now you set the simulation time. If not specified the initial time is set to zero.

SET_SIMULATION_TIME

<SIMULATION END TIME>

<AUTOMATIC TIMESTEP CONTROL Y/N>

<MAXIMUM TIMESTEP>

<INITIAL SIZE OF TIMESTEP>

<SMALLEST ALLOWED TIMESTEP>

```
set_simulation_time
1E5
y
1E4
1E-7
1E-7
```

Here the simulation time is set to 10^5 [s] (`1E5`), the maximum timestep size to 10^4 (`1E4`) and the initial and smallest acceptable to 10^{-7} (both `1E-7`). The *automatic timestep control* should normally always be turned on, which it is by default (you answer `Y` above).

Now you save the workspace:

SAVE_WORKSPACES <FILENAME> <OVERWITE EXISTING FILE Y/N>

```
save_workspaces simplest_dictra y
```



The command name SAVE_WORKSPACES can be misleading. The meaning of this command is roughly set result file. The set-up is saved immediately, but all results during the simulation are also saved to the selected file.

Running and Plotting the Simulation

The following command starts the simulation.

SIMULATE_REACTION

```
simulate_reaction
```

In order to plot results it is necessary to enter the post processor sub-module (note that the GOTO_MODULE command is not used).

POST_PROCESSOR

```
post_processor
```

In most cases, either a specific position in the domain or one or more specific times must be specified with the SET_PLOT_CONDITION command, depending on whether time or spatial position is chosen as independent (x-axis) variable.

SET_PLOT_CONDITION <CONDITION WITH ARGUMENTS>

```
set_plot_condition time 0,1e5
```

Here, the composition profile of Ni at the initial and final time is plotted and thus `time` is chosen as plot condition.

In other cases distance can be given relative to, for example, a phase interface, hence the global specification in the following.

SET_DIAGRAM_AXIS <X OR Y> <AXIS QUANTITY>

```
set_diagram_axis x distance global
```

In this example the only meaningful measure of distance is relative to the domain as a whole, i.e. the leftmost position is zero and the rightmost position corresponds to the width of the region (10^{-4} m).

The dependent property to be plotted is mass-% Ni.

```
set_diagram_axis y weight_percent ni
```

Then plot the diagram:

PLOT_DIAGRAM

```
plot_diagram
```

In the **Console Results** plot window, graphs of the initial and final Ni profile display.

Finally, the SET_INTERACTIVE_MODE command is executed to return control to the user. If the command is absent in a macro the program terminates when the end of the macro file is reached.

SET_INTERACTIVE_MODE

```
set_interactive_mode
```

Moving Phase Boundary Simulations

In this section:

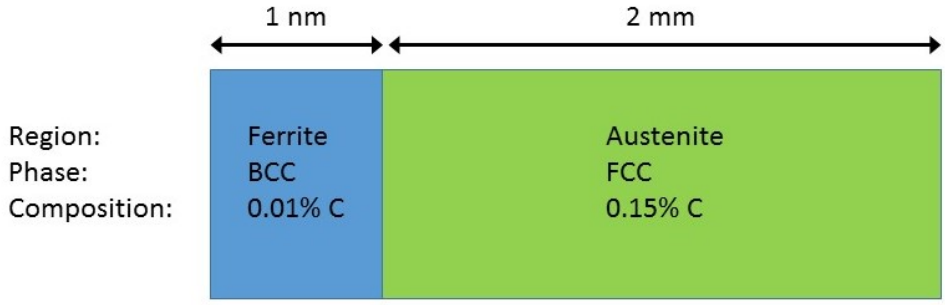
About the Moving Phase Boundary Simulation 27

Theory for the Moving Phase Boundary Simulation 29

Run the Macro File and Learn the Commands 30

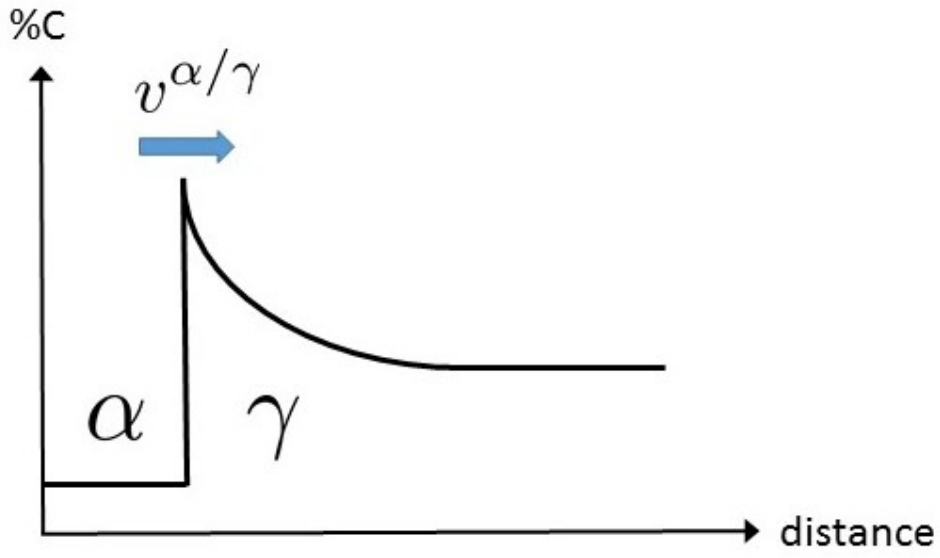
About the Moving Phase Boundary Simulation

The growth of ferrite (bcc) into austenite (fcc) is simulated in this example. The austenite is assumed to be initially homogeneous with the composition Fe - 0.15 mass-% C and the transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation. The initial state is as below.



The set-up of the Moving Boundary example. There are two regions, Ferrite and Austenite, consisting of bcc and fcc, respectively.

A schematic graph of the carbon profile during the transformation is shown in the image below. Crusius et al. (1992)[1.] is recommended as further reading.



1. Crusius, Sabine, Lars Höglund, Ursula Knoop, Gerhard Inden, and John Ågren. 1992. “On the Growth of Ferrite Allotriomorphs in Fe-C Alloys.” Zeitschrift Fur Metallkunde 83 (10): 729–38.

Schematic view of the carbon profile during the transformation from austenite (γ) to ferrite (α) in the Moving Boundary example.

Theory for the Moving Phase Boundary Simulation

It is assumed that local equilibrium holds at the phase interface, i.e. the chemical potentials of all elements are continuous across the boundary, but the chemical potential gradients are in general discontinuous.

In order to maintain mass balance a set of flux balance equations must be satisfied at the phase interface:

$$v^{\alpha/\gamma}(c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma \qquad k = 1, \ldots, n-1$$

where v is the interfacial velocity. The concentrations and the fluxes c and J are those at the interface on the α and γ sides, respectively.

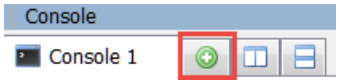
In the present case there are no degrees of freedom at the interface and the concentrations can be taken directly from a phase diagram. There is only one flux balance equation and the interface velocity can be evaluated once the fluxes at the interface are known. However, for ternary and higher systems the state at the interface must be found by some iterative procedure.

For more information on moving phase boundary problems, see, for example, Ågren (1982)[1.] ,Crusius et al. (1992)[2.] and Höglund (1997)[3.] .

1. Ågren (1982) "Numerical Treatment of Diffusional Reactions in Multicomponent Alloys," *J. Phys. Chem. Solids*, 43 (4), pp. 385–391.
2. Crusius, Sabine, Gerhard Inden, Ursula Knoop, Lars Höglund, and John Ågren. 1992. "On the Numerical Treatment of Moving Boundary Problems." Zeitschrift Fur Metallkunde 83 (9): 673–78.
3. Höglund (1997).*Computer simulation of diffusion controlled transformations in multicomponent alloys*, PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden.

Run the Macro File and Learn the Commands

If the single phase example has just been run, then either restart the software program or open another Console window by clicking the green button with the plus sign.



At the SYS prompt, type `macro` (short for the MACRO_FILE_OPEN command) and press <Enter>. Locate and select the macro file called `simple_moving_boundary.dcm` as described in Opening the Module and Macro Files. The commands in the macro file set up, run and plot the simulation in the Console Results window.

In the macro file some abbreviations of the commands are used. You can shorten command names in an arbitrary manner as long as the abbreviations are unambiguous.

In the macro file most commands are first given as comments with the full name and then abbreviated. Commands that were not used in the single-phase simulation, or are used differently, are explained in more detail.

Comments in the macro file can be entered after two `@@` symbols. In most cases the arguments of a command can be entered on the same line as the command itself.

Single-Phase Command Details

Moving Phase - Specifying the Thermodynamic System

This set of commands is the same as in the single-phase simulation example. Thermodynamic and kinetic data is read for Fe and C and the bcc and fcc phases.

```
@@ goto_module database_retrieval
go da
@@ switch_database fedemo
sw fedemo
@@ define_system fe,c
def-sys fe c
@@ reject phase *
rej ph *
@@ restore phase fcc_a1,bcc_a2
rest ph fcc,bcc
@@ get_data
```

```
get
@@ append_database mfedemo
app mfedemo
@@ define_system fe,c
def-sys fe c
@@ reject phase *
rej ph *
@@ restore phase fcc_a1,bcc_a2
rest ph fcc,bcc
@@ get_data
Get
```

Setting Up the Moving Phase Boundary Simulation

The first region to be entered is entered in the same way as in the single-phase simulation.

```
@@ goto_module dictra_monitor
go d-m
@@ set_condition global T 0 1050; * N
set-cond glob T 0 1050; * N
```

A constant temperature equal to `1050`K is used in this simulation.

```
@@ enter_region ferrite
ent-reg ferrite
```

The phase interface between ferrite and austenite is created by introducing a region called austenite that is attached to the ferrite region. Regions are always separated by phase interfaces and must therefore always contain different *matrix* type phases.

ENTER_REGION

<NAME OF REGION>

<NAME OF EXISTING REGION TO ATTACH TO>

<ATTACH TO THE RIGHT OF EXISTING REGION Y/N>

```
enter_region
austenite
ferrite
y
```

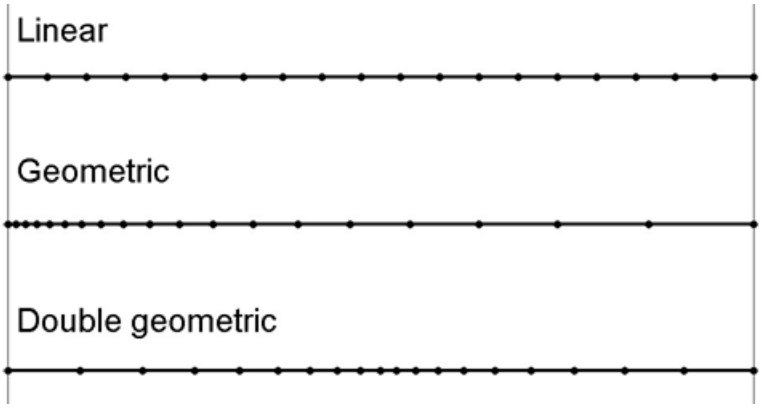
The domain now consists of two regions: `ferrite` and `austenite`.

As in the single-phase simulation example, the regions must contain both grids and one *active* phase of type *matrix*. These are entered separately for both regions.

```
enter-grid
ferrite
1e-9
linear
10
enter-grid
austenite
2e-3
geometric
50
1.05
```

In the above entries, the grid type for the `ferrite` region is the same as in the single-phase simulation example, i.e. equidistant. For the `austenite` region the grid type is called `geometric` and for these grids the grid point spacing changes by a constant factor between every grid point. In this case the spacing increases by 5%, i.e. a factor `1.05`, from the lower/left side for each grid point.

These grid types are used in diffusion simulations: linear, geometric and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Now the initial composition of both phases is entered. In this case Fe is automatically chosen to be the dependent component.

```
enter-phase
active
ferrite
```

```
matrix
bcc
enter-phase
active
austenite
matrix
fcc
```

Both phases are assumed to be initially homogeneous, the bcc phase having `0.01` mass-% C and the fcc phase `0.15` mass-% C, as shown in the following:

```
enter-composition
ferrite
bcc
w-p
C
linear
0.01
0.01
enter-composition
austenite
fcc
w-p
C
linear
0.15
0.15
```

Set the simulation time and other parameters related to the time-step size.

```
set-simulation-time
1e5
y
1e4
1E-7
1E-7
```

Finally, save the simulation set-up to file.

```
save simple_moving_boundary yes
```

Running and Plotting the Moving Phase Simulation

These commands are the same as in the single-phase example.

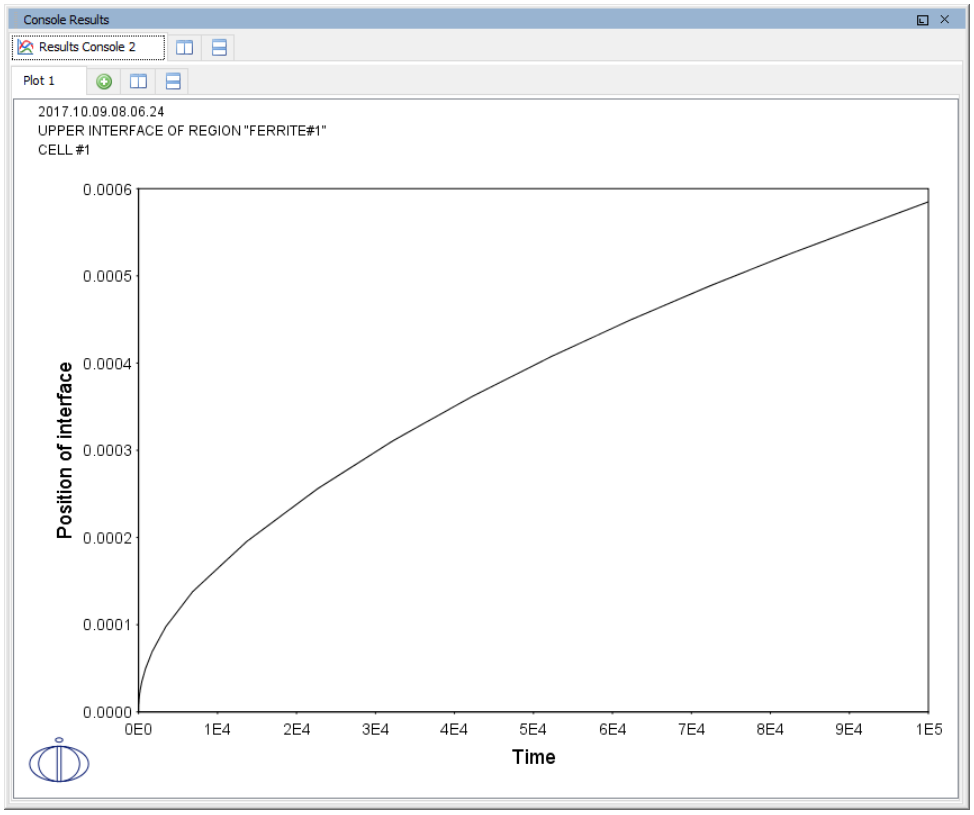
```
@@simulate_reaction

sim

@@ post_processor

post
```

The ferrite/austenite phase interface position as a function of time is plotted.



Output from the example simple_moving_boundary showing the phase interface position as a function of time.

As mentioned in the single phase example, in general either a specific spatial position or a specific time must be set as a plot condition. Here the phase `interface` is set as plot condition and it can be referenced as the lower interface of the austenite region or as the `upper` interface of the `ferrite` region.

```
SET_PLOT_CONDITION

<TYPE OF PLOT CONDITION>

<FOR INTERFACE CONDITION, SPECIFY REGION>
```

<LOWER OR UPPER INTERFACE OF REGION>

```
set-plot-condition
interface
ferrite
upper
```

Set time as x-axis variable

```
@@set-diagram-axis x time
s-d-a x time
```

Now set the interface position as y-axis variable

```
s-d-a y
```

POSITION_OF_INTERFACE

<SPECIFY REGION>

<LOWER OR UPPER INTERFACE OF REGION>

```
pos-of-int ferrite upper
@@ plot_diagram
plot
```

The plot has the parabolic appearance characteristic for many types of diffusion simulations.

Multiphase Simulations

In this section:

About the Multiphase Simulation 37

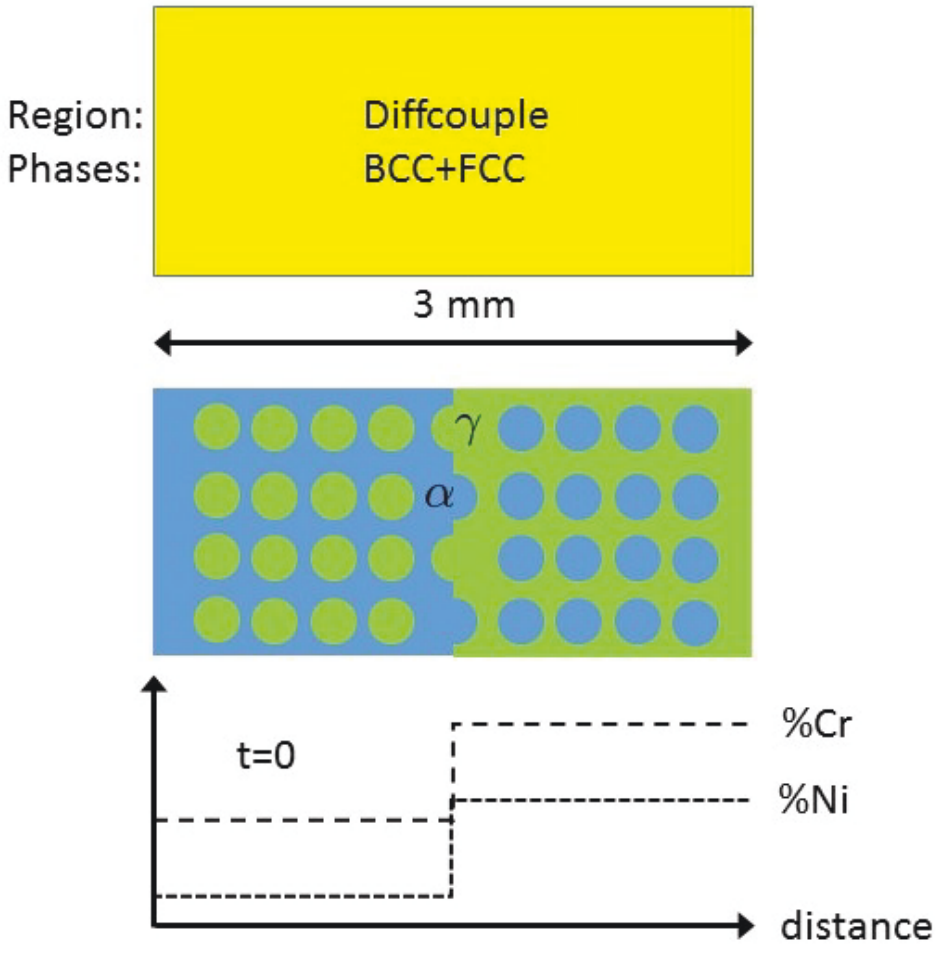
Theory for the Multiphase Simulation 38

Run the Macro File and Learn the Commands 39

About the Multiphase Simulation

This example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.



Schematic view of the initial state of the Multiphase example. Two ternary Fe-Cr-Ni alloys form a diffusion couple. There is a single region (diffcouple) where both the bcc and fcc phases are entered. Both alloys are duplex bcc+fcc, but the majority phase is bcc (α) in the left-hand side alloy and fcc (γ) in the right.

Theory for the Multiphase Simulation

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström (2006)[1.] and Larsson and Höglund (2009)[2.]. As mentioned in the description of this simulation, it is assumed that the material is locally fully equilibrated and that the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition. From a numerical point of view the homogenization model treats the multiphase material as a single phase having the "average", or "effective", properties of the local phase mixture.

When estimating the effective kinetics of a multiphase mixture the product of solubility and mobility in each phase is considered. It is therefore convenient to define

$$\Gamma_k^\phi = M_k^\phi c_k^\phi$$

for each phase ϕ. The effective kinetics of the multiphase mixture is denoted and in this example it was evaluated using the lower Hashin-Shtrikman bound. The default method is a simple rule of mixtures

$$\Gamma^\star = \sum_\phi f^\phi \Gamma_k^\phi$$

where f^ϕ is the volume fraction of ϕ. The flux is obtained as

$$J_k = -\Gamma_k^\star \frac{\partial \mu_k}{\partial z}$$

which replaces the single-phase equation

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

for multiphase simulations.

1. Larsson, Henrik, and Anders Engström. 2006. "A Homogenization Approach to Diffusion Simulations Applied to α + γ Fe–Cr–Ni Diffusion Couples." Acta Materialia 54 (9): 2431–39.
2. Larsson, Henrik, and Lars Höglund. 2009. "Multiphase Diffusion Simulations in 1D Using the DICTRA Homogenization Model." Calphad 33 (3): 495–501.

Run the Macro File and Learn the Commands

At the `SYS` prompt, type `macro` and pres <Enter>. Locate and select the macro file called `multiphase_example.dcm` as described in Opening the Module and Macro Files. The commands in the macro file should set up the simulation, run it and then produce a graph in the Console Results window.

Most of the set-up is the same as the single phase and moving phase boundary examples. Detailed comments are only given for the new commands for this simulation.

- Single-Phase Command Details

Specifying the Multiphase Thermodynamic System

Data for Fe, Cr and Ni and the fcc and bcc phases are read from the *fedemo* (thermodynamics) and *mfedemo* (kinetics) databases.

```
go da
sw fedemo
def-sys fe cr ni
rej ph *
rest ph bcc,fcc
get
app mfedemo
def-sys fe cr ni
rej ph *
rest ph bcc,fcc
get
```

Setting Up the Multiphase Simulation

Set the temperature `T` during the simulation to 1100° C (`1373.15` K) and enter a region `diffcouple`.

```
go dictra-monitor
set-cond glob T 0 1373.15; * N
ent-reg diffcouple
ent-grid
diffcouple
3e-3
double
```

```
60
0.85
1.15
```

In the above example a so-called `double` geometric grid is used. This is similar to the geometric grid used in the moving phase boundary example, but instead two geometrical factors are entered, one for the lower and one for the upper half of the region. In the lower half of the region the distance between subsequent grid points decreases by 15 % (`0.85`) and in the upper half it increases by 15 % (`1.15`). The resulting grid has a much larger grid point density toward the middle of the domain.

As always, a region must contain exactly one `active` phase that is of type `matrix`. In this example it is arbitrary whether it is the bcc or the fcc phase that is entered as matrix.

```
enter-phase
active
diffcouple
matrix
fcc
```

The bcc phase is entered in the same manner as the fcc phase, except that the type is set as `spheroid`.

```
enter-phase
active
diffcouple
spheroid
bcc
```

The initial composition profile of the fcc phase is entered as a `function` of distance.

```
enter-composition
diffcouple
fcc
fe
m-f
cr
function
2.57e-1+(4.23e-1-2.57e-1)*hs(x-1.5e-3);
ni
function
6.47e-2+(2.75e-1-6.47e-2)*hs(x-1.5e-3);
```

In the above entries, the `hs` denotes the Heaviside step function that has the following properties:

$$hs(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases}$$

The resulting Cr profile is thus `0.257` on the left half of the domain and `0.423` on the right with a sharp step at the center.

- As shown in About the Multiphase Simulation.

The initial composition of the fcc phase is actually the initial overall composition. This is due to the choice of initial composition of the spheroid bcc phase.

ENTER_COMPOSITIONS

<REGION NAME>

<PHASE NAME>

<USE EQUILIBRIUM VALUE Y/N>

```
enter-comp
diffcouple
bcc
y
```

When entering the composition for a type spheroid phase it is possible to either, as here, let the composition of the matrix phase be the overall composition or manually enter a start composition and volume fraction.

The local kinetics of the multiphase mixture must be estimated by means of some function that may depend on the local phase fractions, phase compositions and the mobilities of the individual phases. The command for choosing the function to use is ENTER_HOMOGENIZATION_FUNCTION. There are many such homogenization functions to choose from. In this particular example the so-called lower Hashin–Shtrikman bound[1] is a good choice.

ENTER_HOMOGENIZATION_FUNCTION

<ENTER FUNCTION NUMBER>

```
enter-homo-fun
1
```

Finally, set simulation time (100 h) and select the name of the result file:

1. Z. Hashin and S. Shtrikman (1962), *J. Appl. Phys.*, 33 (10), pp. 3125–3131.

```
set-sim-time
3.6e5
yes
3.6e4
1e-7
1e-7
save multiphase_example y
```

Running and Plotting the Multiphase Simulation Results

Run the simulation.

```
simulate
```

Go to the post processor.

```
post
```

Plot the mole fraction fcc phase as a function of distance at the end of the heat treatment.

```
set-plot-condition time last
set-diagram-axis x distance global
set-diagram-axis y npm(fcc)
```

Instead of explicitly entering the final time it is possible to use the keyword `last`. The `np` of npm stands for *number of moles* of the phase argument and the `m` is the normalizing quantity (moles). The limits of an axis can be set with the SET_SCALING_STATUS command. You manually set the scaling of the axis and then restore automatic scaling:

SET_SCALING_STATUS

<X OR Y AXIS>

<USE AUTOMATIC SCALING Y/N>

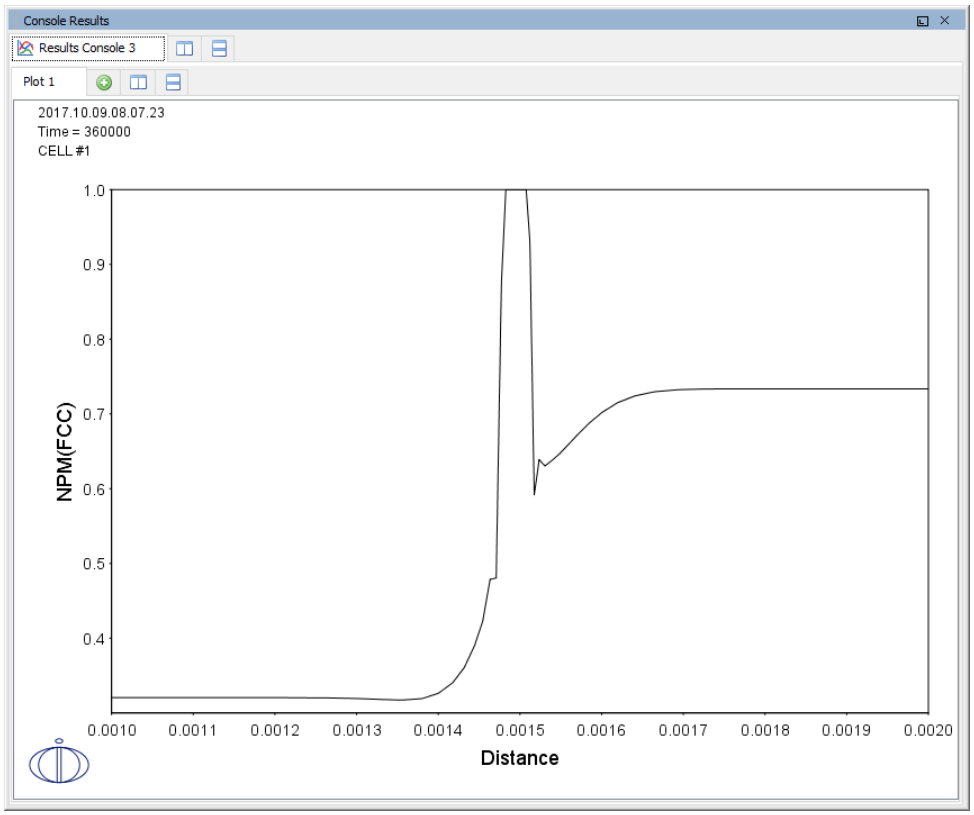
<IF MANUAL SCALING, ENTER LIMITS>

```
set-scaling-status x n 1e-3 2e-3
```

Plot the diagram.

```
plot
```

The plot below shows that a single phase fcc zone has formed and this was also observed experimentally, see A. Engström, 1995: "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24 (1), pp. 12–20.



Output from the multiphase_example showing the mole fraction fcc phase as a function of distance at the end of the heat treatment.

References

1. J.-O. Andersson, T. Helander, L. Höglund, P. Shi, and B. Sundman, "Thermo-Calc and DICTRA, computational tools for materials science," *Calphad*, vol. 26, no. 2, pp. 273–312, Jun. 2002.
2. A. Borgenstam, L. Höglund, J. Ågren, and A. Engström, "DICTRA, a tool for simulation of diffusional transformations in alloys," *J. Phase Equilibria*, vol. 21, no. 3, pp. 269–280, May 2000.
3. J.-O. Andersson and J. Ågren, "Models for numerical treatment of multicomponent diffusion in simple phases," *J. Appl. Phys.*, vol. 72, no. 4, pp. 1350–1355, Aug. 1992.
4. S. Crusius, L. Höglund, U. Knoop, G. Inden, and J. Ågren, "On the growth of ferrite allotriomorphs in fe-c alloys," *Zeitschrift für Met.*, vol. 83, no. 10, pp. 729–738, 1992.
5. J. Ågren, "Numerical Treatment of Diffusional Reactions in Multicomponent Alloys," *J. Phys. Chem. Solids*, vol. 43, no. 4, pp. 385–391, 1982.
6. S. Crusius, G. Inden, U. Knoop, L. Höglund, and J. Ågren, "On the numerical treatment of moving boundary problems," *Zeitschrift für Met.*, vol. 83, no. 9, pp. 673–678, 1992.
7. L. Höglund, *Computer simulation of diffusion controlled transformations in multicomponent alloys*, PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden, 1997.
8. Z. Hashin and S. Shtrikman, "A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials," *J. Appl. Phys.*, vol. 33, no. 10, pp. 3125–3131, 1962.
9. A. Engström, "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples," *Scand. J. Metall.*, vol. 24, no. 1, pp. 12–20, 1995.
10. H. Larsson and A. Engström, "A homogenization approach to diffusion simulations applied to α + γ Fe–Cr–Ni diffusion couples," *Acta Mater.*, vol. 54, no. 9, pp. 2431–2439, May 2006.
11. H. Larsson and L. Höglund, "Multiphase diffusion simulations in 1D using the DICTRA homogenization model," *Calphad Comput. Coupling Phase Diagrams Thermochem.*, vol. 33, no. 3, pp. 495–501, 2009.

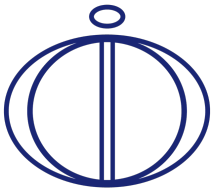
Next Steps

Below are suggestions for you to learn more about using the Diffusion (DICTRA) Module.

- Browse the Online Help (Help → Online Help) or open one of the available PDFs that is included with your installation (Help → Manuals Folder).
- You have been working with in Console Mode. You might also want to try the *Diffusion Module Graphical Mode Quick Start Guide* (Help → Manuals Folder).
- Run other Console Mode examples (Help → Examples Files), which contain many simulation types and advanced functionality. It is a good starting point when you are thinking of creating a new simulation. When you are setting up a new simulation there are two recommended ways to proceed:
    - Copy and gradually adjust an existing macro file from the examples collection.
    - Enter the set-up directly while recording a log file. The command for recording a log file is SET_LOG_FILE and this should be done immediately when starting the program in the SYS module. The log file can then be directly used as a macro file (it has the file extension *.TCM).
- You can also go to the Thermo-Calc website to see if there are other options suited to you, such as a course or video tutorials. (Help → Video Tutorials and Help → Thermo-Calc Website).

Diffusion Module (DICTRA) Command Reference

Thermo-Calc Version 2021b



Thermo-Calc Software

About This Guide

The guide is for users already familiar with Console Mode and it includes all the commands applicable to the Diffusion Module (DICTRA). It is a supplement to the commands described for Thermo-Calc and which can be found by searching the online help.

How you proceed depends on your experience with the software as well as your level of expertise with diffusion problems. In addition to this guide, the following supplemental documentation and training resources can help you learn how to use the Diffusion Module (DICTRA) in Console Mode.

Documentation Resources

You can search or browse all the documentation available either from within Thermo-Calc (press F1 or go to **Help → Online Help**) or browse the PDFs included with your installation by going to **Help → Manuals Folder**).



You can also download *The Role of Diffusion in Materials - a Tutorial*available from our website.

Training and Video Tutorials

Some of the Graphical Mode examples have video tutorials available both on our website or our YouTube channel. Watching those videos may help you with your simulation in Console Mode. You may also decide to enroll in a training course or if you have several people interested in on-site training.



Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.

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General Commands

These commands are universal in Console Mode.

Command/Syntax	Description and Prompts
BACK	Return to the previous module. From the POST-processor you go back to the DICTRA-MONITOR module.
EXIT	Terminates the program and returns to the operating system. Unless a SAVE_ WORKSPACES command has been given before all data entered is lost.
GOTO_MODULE	`Module name` Select and go to another module. The name of the module must be given. In order to obtain a list of available modules give a return.
HELP ?	Enter HELP or ? to either a list of all commands or specific help for a command by giving the command (abbreviated) `Command` The command for which a description is wanted should be given. If the abbreviation is not unique a list of all matching commands are given.

ADVANCED_HOMOGENIZATION_OPTIONS

UTILITIES_HOMOGENIZATION

Use this command and its subcommands with the HOMOGENIZATION_MODEL. Go to each command listed below for details.

Syntax	SPECIAL_HOMOGENIZATION_OPTIONS
Prompts	`Which option?` Enter ? to list the available commands as below. • BC_FOR_DEPENDENT_ELEMENT • SOLVE_IN_LATTICE_FIXED_FRAME • DEPENDENT_ELEM_BALANCE_FLUXES • USE_TWO_TYPES_OF_BOUNDARY_CON • CHECK_PHASE_SET

AMEND_CELL_DISTRIBUTION

Use this to amend the cell distribution factor of the currently selected cell.

Syntax	AMEND_CELL_DISTRIBUTION
Prompt	`Cell distribution factor /4.446590813-323/` A parameter that determines the weight of the cell, it can be used to simulate a distribution of different cell sizes.

AMEND_MOBILITY_DATA

Use this command to change an existing parameter.



Also see ENTER_MOBILITY_DATA for information about the parameter names and prompts.

Syntax	AMEND_MOBILITY_DATA
Prompt	`Parameter name <Identifier> (<Phase>, <Component array>; <Digit>)` Enter `?` to get an overview

BC_FOR_DEPENDENT_ELEMENT

Use this command to allow an "active" boundary condition (BC) for a dependent element. It is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.

The command enables you to enter a “fix flux” or an “activity-/potential-flux function” type of boundary condition for the dependent substitutional element if such a boundary condition is already entered for the independent elements.

Use of this command automatically ensures that the flux of the dependent element is not used to balance the independent fluxes, i.e. the feature “dependent element balance fluxes” is set to `No`.

Syntax	BC_FOR_DEPENDENT_ELEMENT
Prompts	`Enter BC for dependent element on lower boundary /NO/` If `YES` is entered, the subsequent prompts are the same as when the boundary condition was entered for the independent elements on the lower boundary; it is a prerequisite that such a boundary condition is already entered. This feature is only allowed with a “fix flux” or an “activity/potential flux function” type of boundary condition.
	`Enter BC for dependent element on upper boundary /NO/` If `YES` is entered, the subsequent prompts are the same as when the boundary condition was entered for the independent elements on the upper boundary; it is a prerequisite that such a boundary condition is already entered. This feature is only allowed with a “fix flux” or an “activity/potential flux function” type of boundary condition.

CHECK_DIFFUSION_MATRIX

Display the diffusion coefficient matrix for a phase at a given composition, pressure and temperature.

Syntax	CHECK_DIFFUSION_MATRIX
Prompts	`Output to screen or file /Screen/`
	`Phase name` Name of the phase for which the diffusion coefficient matrix is to be displayed.
	`Concentration of` Concentration of the component in U-fraction for which the diffusion coefficient matrix is to be displayed.
	`Pressure` Pressure for which the diffusion coefficient matrix is to be displayed.
	`Temperature` Temperature at which diffusion coefficient matrix is to be displayed. Use one or several of the options: • `D`: reduced diffusion matrix • `L:L` matrix (diagonal) • `P:L'` matrix • `B:L"` matrix • `M:MU(k)` array • `X:dMU(k)/dCj` matrix • `0`: unreduced diffusion matrix • `E`: Eigen values of matrix

CHECK_PHASE_SET

This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.



This command is only available with single region simulations.

One difficulty with single region multiphase simulations is to choose which phases should take part in the simulation, i.e. which phases should be entered in the region; what phases are stable, or become stable, is often a part of the question and the diffusion path is not known *a priori*. With this command it may be checked which, if any, phases read from the database but not entered in the region have become stable. The interval at which checks are made can be set to some extent. Whether a simulation should be terminated when a non-entered phase become stable can also be set. Finally, it can also be set whether some phases should be excluded from the check, if for example a phase has been read only to be used to define a reference state.

Syntax	CHECK_PHASE_SET
Prompt	CHECK SET OF PHASES ENTERED INTO SIMULATION (Y/N): USE THIS FEATURE WITH DEFAULT SETTINGS? (Y/N): if NO, the following settings can be made: OPTIONS FOR CHECK INTERVAL: 1. BEGINNING AND END OF SIMULATION 2. EVERY TIME RESULTS ARE SAVED 3. AS #2, BUT TERMINATE SIMULATION IF NON-ENTERED PHASE BECOME STABLE CHOOSE OPTION 1-3: PERFORM CHECK USING GLOBAL MINIMIZATION? (Y/N): SHOULD ANY PHASE BE EXCLUDED FROM THE CHECK? (Y/N): if YES, then those phases are prompted for.

COARSENING_MODEL

About the Coarsening Model in the *Diffusion Module User Guide*

The model allows you to perform coarsening simulations. Use this command to explicitly set the DICTRA module to use this model.

Enable or disable the use of the simplified model for calculating Ostwald-ripening in multicomponent systems. This also must be used together with the SET_SURFACE_TENSION command.

To use this mode, configure the calculation as follows:

- Have one cell only, with a single particle that is 1.5 times larger than the average particle size.
- The matrix phase should be in contact with the maximum size particle on the left/lower side, and then the model specifies a local equilibrium with an average sized particle on the right/upper side.
- The surface energy then results in growth of both the maximum size particle and the matrix phase. Use SET_SURFACE_TENSION to enter the surface energy to enable coarsening.

Syntax	COARSENING_MODEL
Prompt	`Enable coarsening model /N/` By default the coarsening model is not used. Enter Y to enable the use of this model.

CREATE_NEW_CELL

Create a new cell and attach it to the list of current existing cells.

Syntax	CREATE_NEW_CELL
Prompt	`Cell distribution factor` A parameter that determines the weight of the cell, this parameter can be used in order to simulate a distribution of different cell sizes.

DEBUGGING

Determines the debugging level. Depending on the value given, different amounts of information are written onto the output device. This can be used to determine what causes the program to crash during a simulation.

Syntax	DEBUGGING
Prompt	`Debug level (Yes, No, 0, 1, 2, 3, 4) /N/` The level of debugging information to be displayed.

DELETE_REGION

Delete a region and all its associated data from the current cell.

Syntax	DELETE_REGION
Prompt	`Region name` The region name to delete.

DEPENDENT_ELEM_BALANCE_FLUXES

Use this command to set whether the dependent element should balance fluxes at the boundaries. This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.

For most boundary conditions (the notable exception being the “gas” type of boundary condition) the default behavior is that the boundary flux of the dependent substitutional element balances the fluxes of all other substitutional elements such that the size of the domain is preserved. This generally means that the flux of the dependent element equals minus the sum of all other substitutional elements.

This feature allow the balancing of boundary fluxes to be turned off and consequently the domain may change its size as a result of the boundary condition.

The input for this feature is `Yes` or `No`, where `No` mean that the balancing of boundary fluxes is turned off.

Syntax	DEPENDENT_ELEM_BALANCE_FLUXES
Prompt	`Dependent element balance the fluxes /Yes/:`

ENTER_COMPOSITIONS

Enter the composition into the phases in a region.



The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the Thermo-Calc User Guide. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	ENTER_COMPOSITIONS
Prompts	`Region name` Name of the region into which the compositions are to be entered.
	`Phase name` Name of the phase in a region into which the compositions are to be entered.
	`Use equilibrium value` This is only for spheroid phases in simulations with dispersed phases. If this option is used the program automatically calculates the equilibrium fractions of the spheroid phase and its constitution at the start of the simulation.
	`Dependent substitutional species` A dependent substitutional species is required in order to be able to determine which species are independent. The program only queries for the compositions of the independent species.  Sometimes the dependent species is chosen by the program and thus this question is never given. This may be due to stoichiometric constraints or to the fact that it has been set already in the kinetics database due to the model selected for the diffusion.
	`Dependent interstitial species` A dependent interstitial species is required in order to be able to determine which species are independent. The program only queries for the compositions of the independent species.  Vacancies are always regarded as dependent and therefore if vacancies are present in the phase then this question is never given.
	`Composition type` Type of composition used for the constitution of the phase. Options are: SITE_FRACTION, MOLE_FRACTION, MOLE_PERCENT, WEIGHT_FRACTION, WEIGHT_PERCENT and U_FRACTION.
	`Type` Type of composition profile to be entered, options are: LINEAR, READ_POINT_BY_POINT, FUNCTION, and GEOMETRIC.

Syntax	ENTER_COMPOSITIONS
	• If READ_POINT_BY_POINT is chosen note the following. When compositions are read from a file it may often be the case that both grid coordinates and the composition at the grid points are given on the same line, e.g. the grid coordinates in the first column, the mole fraction of the first element at that grid point in the second column and so on. The column that contain the composition of a given element can then be specified in a macro file by, for example, having a line "read_point_by_point foo.dat 2". The "2" mean that the grid coordinates are in the 2nd column in the file foo.dat. In a corresponding manner the column that contain the grid point coordinates can be specified (see ENTER_GRID_COORDINATES). • If FUNCTION is chosen the composition profile can be given as a function of the global distance denoted X. Some useful functions are the error function denoted `erf(X)` and the Heaviside step-function denoted `hs(X)`. For example the function `3+2hs(x-1e-4)` provides a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at 1e-4m=100µm.
	`Value of first point` Composition in the first gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.
	`Value of last point` Composition for the last gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.
	`Input file` The input source from which to read the points when entering values point by point, default is TERMINAL.
	`Value of point` The value of the point when entering values point by point.
	`Value of R in the geometrical serie` Use the same geometrical factor as for the geometrical grid.
	`Volume fraction of` Initial volume fraction of a spheroid phase.

ENTER_ENHANCEMENT_FACTOR

Change the mobility of a specific element in a specific phase. The mobility of the element in the phase is multiplied by a factor which is specified as an argument to the command.

Syntax	ENTER_ENHANCEMENT_FACTOR
Prompt	`Mobility enhancement factor for phase`

ENTER_GEOMETRICAL_EXPONENT



The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the Thermo-Calc User Guide. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Enter the geometrical exponent which defines the geometry of the system. The program handles one-dimensional geometries defined by the geometrical exponent. These geometries are:

- **Planar**. This corresponds to an infinitely wide plate of a certain thickness.
- **Cylindrical**. This corresponds to an infinitely long cylinder of a certain radius.
- **Spherical**. Sphere with a certain radius.

Syntax	ENTER_GEOMETRICAL_EXPONENT
Prompt	`Geometrical exponent` Enter an integer value between 0 and 2.

ENTER_GRID_COORDINATES

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the Thermo-Calc User Guide. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Enter the size and gridpoint distribution of the grid in each region separately. The size of the region is specified in the units that the diffusion data is entered in. The grid in a specific region may also be subdivided into several parts, where the type of each part is chosen independently, by first entering SUB_REGION as the overall grid type.

Syntax	ENTER_GRID_COORDINATES
Prompts	`Region name` Name of the region into which a grid is to be entered.
	`Width of region /1/` The actual size of the region is entered. The size of the region is specified in units compatible with those of the diffusion data.
Options	**Description**
`TYPE` of grid	`Type /Linear/` Type of grid to entered, options are: • `LINEAR`: For an equally spaced grid. • `READ_POINT_BY_POINT`: Can be done either from the keyboard or from a predefined file. When grid coordinates are read from a file it may often be the case that both grid coordinates and the composition at the grid points are given on the same line, e.g. the grid coordinates in the first column, the mole fraction of the first component at that grid point in the second column and so on. The column that contain the grid coordinates can then be specified in a macro file by, for example, having a line "read_point_by_point 30 foo.dat 1". The "1" mean that the grid coordinates are in the 1st column in the file foo.dat (and "30" is the total number of grid points). In a corresponding manner the column that contain the composition of a specific component can be specified (see ENTER_COMPOSITIONS). • `GEOMETRIC`: Yields a higher number of gridpoints at the lower end of the region if a geometrical factor larger than one is given and a higher number of gridpoints at the upper end of the region if the factor is smaller than one. • `DOUBLE_GEOMETRIC`: Divides the region in two halves and generates a separate geometrical grid in each half. It gives a high number of gridpoints in the middle or at both ends of a region, two geometrical factors should be entered. • `AUTOMATIC`: Use this for automatic grid point distribution. An appropriate grid is

Syntax	ENTER_GRID_COORDINATES
	generated at the start of the simulation where the grid points are automatically distributed according to the entered composition profile and boundary conditions.
`Sub_region`	If `SUB_REGION` is entered when you are prompted to enter the grid type, then the next prompt is `End coordinate in Sub-Region /1/` Enter a value equal to or less than the total width of the region. You are then prompted for the number of grid points and the grid type to be used between the left-hand side of the region and the end coordinate. As long as the end coordinate is less than the total width of the region you are prompted for an end coordinate and the grid to be used in the sub region starting at the end of the former sub region. Thus, progressively higher end coordinates must be entered and the final end coordinate must be equal to the total width of the region.
	`Number of points /50/` The number of points present in the region. Please consider the interspacing of the grid when determining the number of points.
	`Input file` The input source from which to read the points when entering values point by point, default is TERMINAL.
	`Value of point` The value of the point when entering values point by point.
	`Value of R in the geometrical series` Value in the geometrical factor in the series determining the distribution of the grid points. A geometrical factor larger than one yields a higher density of gridpoints at the lower end of the region and a factor is smaller than one yields a higher density of gridpoints at the upper end of the region.
	`Value of R in the geometrical serie for lower part of region` The geometrical factor in the series for the lower (left) part of a region in a double geometrical grid
	`Value of R in the geometrical serie for upper part of region` The geometrical factor in the series for the upper (right) part of a region in a double geometrical grid.

ENTER_HEAT_TRANSFER_PARAMETER

A model for thermos-migration simulates the thermal induced diffusion in temperature gradients. This model requires that the temperature depends on the length coordinate in the system and that the quantity `heat of transport` (`Q*`), is entered.

Syntax	ENTER_HEAT_TRANSFER_PARAMETER
Prompt	`Heat transfer parameter for phase` The phase for which the parameter is to be entered. This parameter is entered separately for each component in each phase.
	 The implementation and functionality of this model is described in Höglund and Ågren (2010)[1].

1. Höglund, Lars and John Ågren(2010)."Simulation of Carbon Diffusion in Steel Driven by a Temperature Gradient", *J. Phase Equilibria Diffus.* 31, 212–215.

ENTER_HOMOGENIZATION_FUN

Use this with the homogenization model for multiphase simulations. The homogenization model is based on the assumption of local equilibrium at each node point, which yields the local chemical potentials at each node point from which the local chemical potential gradients may be estimated. The chemical potential gradients are the driving forces for diffusion. The local kinetics must also be evaluated by some averaging procedure, the choice of which is determined by this command. The local kinetics is evaluated by considering the product of mobility times u-fraction for each component in each phase and the volume fraction of each phase.



The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the Thermo-Calc User Guide. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	ENTER_HOMOGENIZATION_FUN
Prompt	`Enter homogenization function # /5/` Enter a digit between 1 and 14 (default is 5). The options corresponding to the numbers are listed below.

Homogenization Functions

Enter a digit between 1 and 14 (default is #5) to assign the homogenization function then follow the prompts. The homogenization functions are:

No.	Function name
1	General lower Hashin-Shtrikman bound*
2	General upper Hashin-Shtrikman bound*
3	Hashin-Shtrikman bound with prescribed matrix phase*
4	Hashin-Shtrikman bound with majority phase as matrix phase*
5	Rule of mixtures (upper Wiener bound)
6	Inverse rule of mixtures (lower Wiener bound)
7	Labyrinth factor f with prescribed matrix phase
8	Labyrinth factor f**2 with prescribed matrix phase

No.	Function name
9	General lower Hashin-Shtrikman bound with excluded phase(s) *
10	General upper Hashin-Shtrikman bound with excluded phase(s) *
11	Hashin-Shtrikman bound with prescribed matrix phase with excluded phase(s) *
12	Hashin-Shtrikman bound with majority phase as matrix phase with excluded phase(s) *
13	Rule of mixtures (upper Wiener bound) with excluded phase(s)
14	Inverse rule of mixtures (lower Wiener bound) with excluded phase(s)



* For the Hashin-Shtrikman bounds, see Hashin, Z. & Shtrikman, S. “A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials”. *J. Appl. Phys.* 33, 3125–3131 (1962).

About the Homogenization Functions

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase. For the general lower Hashin-Shtrikman bound the outermost shell consists of the phase with the most sluggish kinetics and vice versa for the general upper bound. The geometrical interpretation of the Hashin-Shtrikman bounds suggest further varieties of the bounds, viz. *Hashin-Shtrikman bound with prescribed matrix phase* and *Hashin-Shtrikman bound with majority phase as matrix phase*, where the outermost shell consist of a prescribed phase or the phase with highest local volume fraction, respectively.

The geometrical interpretation of the Wiener bounds are continuous layers of each phase either parallel with (upper bound) or orthogonal to (lower bound) the direction of diffusion.



The labyrinth factor functions (described below) are available in Console Mode and when using TC-Python.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with either the volume fraction (*Labyrinth factor f with prescribed matrix phase*), or the volume fraction squared (*Labyrinth factor f**2 with prescribed matrix phase*), of the matrix phase.



The varieties with excluded phases (described below) are available in Console Mode and when using TC-Python.

The varieties with excluded phases are useful in several respects. First, if a phase is modeled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as excluded causes the mobility of all components in that phase to be set to zero. Second, often there are some major matrix solid solution phases and some minor precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it produces a kinetic coefficient of zero. However, using *General lower Hashin-Shtrikman bound with excluded phase(s)* the excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

ENTER_LABYRINTH_FUNCTION

Enters a constant value or a function of temperature, pressure, or the volume fraction of the phase where diffusion occurs. This function increase or reduces the diffusion coefficient matrix. This function is primarily used when spheroid phases have been entered into a region. It may also be used for increasing or decreasing all diffusion coefficients in a certain matrix phase by a constant factor.

Syntax	ENTER_LABYRINTH_FUNCTION
Prompt	`Region` `f(T,P,VOLFR,X)=`

ENTER_MOBILITY_DATA

Use this command to enter previously non-existing mobility parameters. If there is already a function is defined for the same parameter, it is deleted.

You can also use:

- ENTER_ENHANCEMENT_FACTOR to enter a factor by which element mobilities are multiplied with.
- ENTER_MOBILITY_ESTIMATE to enter a rough mobility estimate for elements in specific phases. This can be useful for phases where there is no data in the database.

A valid parameter should have the general form of:

```
<Identifier> ( <Phase name> , <Component array> ; <Digit> )
```

The `identifier` must be followed by an opening parenthesis, a phase name, a comma and a component array. Optionally, the component array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.

These identifiers are legal:

- `MQ` (activation energy for mobility)
- `MF` (frequency factor for mobility)
- `DQ` (activation energy for diffusivity)
- `DF` (frequency factor for diffusivity)
- `OQ` (activation energy for mobility, ordered part)
- `OF` (frequency factor for mobility, ordered part).

The `phase name` must be followed by an & and directly following that the name of the diffusing specie.

The `component array` consists of a list of constituent names. Interaction parameters have two or more constituents separated by a comma. If the phase has sublattices at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array a subindex `digit` can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the subindex depends on the excess model used for the phase. If no semicolon and digit is given the subindex value is assumed to be zero.

Syntax	ENTER_MOBILITY_DATA

Prompt	`Parameter: <Parameter name>`
	As explained above, specify a correct and complete parameter name, which should contain all the necessary parts of the general form:
	`<Identifier>(<Phase>,<Component array>;<Digit>)`
	If a parameter name is not acceptable or <Enter>, is pressed, the error message displays:
	`*** Error, please re-enter each part separately`
	Examples
	• `MQ(FCC&C,Fe:Va)` Mobility of C in fcc Fe with interstitials.
	• `MQ(FCC&C,Fe,Cr;0)` The regular parameter for Fe and Cr in fcc.
	• `MQ(FCC&C,Fe,Cr;1)` The subregular interaction parameter (Redlish-Kister model).

`Identifier`	`Identifier /MQ/ <MQ, MF, DQ, Df, OQ, OF>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`Phase Name`	`Phase name /FCC&C/` Each parameter is valid for a specific phase. The name of that phase must be supplied. The name must not be abbreviated. The phase name must be followed by an '&' and directly following that, the name of the diffusion specie.

ENTER_MOBILITY_ESTIMATE

Use this command to enter a function yielding a mobility estimate for a specific element in a specific phase.

- LIST_MOBILITY_ESTIMATES

Syntax	ENTER_MOBILITY_ESTIMATE
Prompt	`Mobility estimate for phase` Interactively enter a function yielding a mobility estimate for a specific element in a specific phase. This can be used to enter mobility estimates in phases for which there is no assessed data. Estimates entered here override database values.

ENTER_PHASE_IN_REGION

Enter a phase into a previously defined region.

Syntax	ENTER_PHASE_IN_REGION
Prompts	`Active or Inactive phase` Type of phase entered. An inactive phase is a phase which does not participate in the calculations until it is stable. This is done by regarding the driving force for precipitation of the phase in an equilibrium calculation. The program then automatically retransforms the inactive phase into an active one.
	`Region name` Name of the region into which the phase is to be entered.
	`Phase type` Type of phase entered. Legal types are: • MATRIX • LAMELLAR (see ENTER_PHASE_IN_REGION - Lamellar Prompts). • SPHEROID: requires that a MATRIX phase has been previously entered.
	`Phase name` Name of the phase that is to be entered. A #-sign and a digit may append the phase name in order to specify the composition set number, e.g. FCC#2.
	`Composition set` Number of the composition set. This is needed if the phase has been amended to have more than one composition set and the number was not given directly on the phase name, see above.
	`Attach to region named` Enter the name of the region onto which the inactive phase is to be attached.
	`Attached to the right of` Enter Y to attach the inactive phase on the right side of the region. Enter N to attach on the left side.
	`Required driving force for precipitation` The required driving force (evaluated as DGM (phase) in POLY-3) to be used for determining whether an inactive phase is stable.
	`Condition type` Boundary condition used if the inactive phase becomes stable.

ENTER_PHASE_IN_REGION - Lamellar Prompts

The following are the ENTER_PHASE_IN_REGION subprompts for Lamellar.

For a LAMELLAR type of phase, the pearlite calculation model is invoked. The following is displayed:

```
eutectoid reaction is "gamma" ==> "alpha" + "beta"
```

This is to clarify what is meant with GAMMA, ALPHA and BETA in the specific sub-prompts that display as follows.

Subprompts	LAMELLAR
	`Enter name of "alpha" phase` Enter the GES phase name for the ALPHA phase of the eutectic/eutectoid decomposition product.
	`Enter name of "beta" phase` Enter the GES phase name for the BETA phase of the eutectic/eutectoid decomposition product.
	`Enter name of "gamma" phase` Enter the GES phase name for the GAMMA matrix phase.
	`Enter "alpha"/"beta" surface tension:` Enter function for the surface tension between the ALPHA and BETA phases, $\sigma^{\alpha/\beta}$
	`Enter "alpha"/"gamma" surface tension:` Enter function for the surface tension between the ALPHA and GAMMA phases,$\sigma^{\alpha/\gamma}$
	`Enter "beta"/"gamma" surface tension:` Enter function for the surface tension between the BETA and GAMMA phases,$\sigma^{\beta/\gamma}$
	`Optimum growth condition factor /2/:` Enter the Optimum-growth-rate-factor. Due to Zener's maximum growth rate criteria this factor has a value of 2 for volume controlled growth and 3/2 for boundary controlled growth. Due to Kirkaldy's extreme in entropy production criteria the values are 3 and 2, respectively.
	`Name of dependent element` Enter the name of the substitutional element to consider as the dependent one.
	`Growth model (Volume/Boundary/Kirkaldy) for element x` Select growth model to be used for element X. Choose between: • `Volume` diffusion model • `Boundary` diffusion model • `Kirkaldy`'s mixed mode diffusion model. Implies MIXED, see below.
	`df(x) = /Value/Automatic/Mixed/TDB/`

Subprompts	LAMELLAR

	Either input a numerical value on the pre-exponential factor DF or select one of the keywords:
	• AUTOMATIC
	• MIXED
	• TDB
	AUTOMATIC is only available for element Carbon. It implies a mixed type of calculation where the volume diffusion part is calculated due to J. Ågren "A revised expression for the diffusivity of carbon in binary Fe-C austenite". *Scr. Metall.* 20, 1507–1510 (1986) (volume diffusion of C in Austenite) and the boundary diffusion part due to J. Ågren "Computer simulations of the austenite/ferrite diffusional transformations in low alloyed steels" *Acta Metall.* 30, 841–851 (1982) (boundary diffusion of C is assumed to be the same as C diffusion in Ferrite).
	The k' or k'', as appropriate, are given by B. Jönsson (1992)[1]. MIXED means a mixed mode calculation using an effective diffusion coefficient. Coefficient k' or k'' is asked for, see below. TDB means calculate the diffusion coefficient for volume diffusion for element X from the parameters stored in the database.
	`DQ(X)=`
	Input a numerical value on the activation energy DQ for element X.
	`k'=`
	`k''=`
	Input a numerical value on the k coefficient used to calculate the effective diffusion coefficient, use in MIXED mixed mode calculations, see B. Jönsson, 1992"On the Lamellar Growth of Eutectics and Eutectoids in Multicomponent Systems." Trita-Mac 478 (January): 27.

	`DF_boundary(x)=` Input a numerical value on DF for boundary diffusion of element X in a mixed mode calculation.
	`DQ_boundary(x)=` Input a numerical value on DQ for boundary diffusion of element X in a mixed mode calculation.
	`DF_volume(x)=` Input a numerical value on DF for volume diffusion of element X in a mixed mode calculation. N.B. key word TDB may also be used, see TDB above.
	`DQ_volume(x)=` Input a numerical value on DQ for volume diffusion of element X in a mixed mode calculation.
	`Automatic start values for the s0 determination /Y/:` Enter `Y` if you want automatic start values for the unknown parameters in the S0 determination else enter `N`. S0 is the critical lamellar spacing for which the growth rate is zero.
	`Critical thickness of "alpha" lamella:` If you answered `N` this prompt displays. The critical thickness of ALPHA is about 0.9 of S0, which in turn is about 1/3 to 1/2 of the observed lamellar spacing S. For binary Fe-C alloys the observed pearlite lamellar spacing is approximately given by

1. "On the Lamellar Growth of Eutectics and Eutectoids in Multicomponent Systems" *Trita-Mac* 478.

Subprompts	LAMELLAR
	$$S = 1.75 \cdot 10^{-5}(A_{1e} - T)^{-1}$$ The equation may be used as a start value approx. for alloyed steels. However, use the A_{1e} temperature of the steel.
	`Critical thickness of "beta" lamella:` The critical thickness of BETA is about 0.1 of S0, see above.
	`Automatic start values on potentials /Y/:` By default, automatic start values for the unknown potentials are used. Choose N to enter your own start values.
	`Give potentials for "alpha"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.
	`Give potentials for "beta"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.
	`Growth rate v:` Enter a start guess on the growth rate. As a hint on what value to choose we recognize that for binary Fe-C alloys the pearlite growth rate is approximately given by: $$v = 8 \cdot 10^{-9}(A_{1e} - T)^2$$ The equation may be used as a start value approx. for alloyed steels. However, use the A_{1e} of the steel.
	`Automatic start values on other variables /Y/:` By default there are automatic start values for the unknowns in the determination of the growth rate.
	`Fraction of "alpha" phase:` Enter a guess on the fraction of the ALPHA phase. For pearlite it is about 0.9.
	`Give potentials for "alpha"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.
	`Give potentials for "beta"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.

ENTER_REGION

Enter a region into the system. Enter this before entering a grid or any phases.

Syntax	ENTER_REGION
Prompts	`Region name` Name of a region to be entered. The name of the region can be arbitrarily chosen.
	`Attach to region named` Name of a region to which the new region should be attached.
	`Attached to the right of` Relative position of the new region. Enter Y to attach the inactive phase on the right side of the region. Enter N to attach on the left side.

GB_MODEL

Grain-boundary and dislocation assisted diffusion is implemented by assuming that these contributed to the diffusion by using the same frequency factor and a modified bulk activation energy. The grain-boundaries and the dislocations contribute to the total amount of diffusion according to the weighted fractions.

Syntax	GB_MODEL
	The parameters are entered separately for each region in order to different expression for different phases.
	The used expressions for the grain-boundary and dislocation contributions are: $$M^{gb} = M_0^{bulk} \cdot \exp(F_{redGB} \cdot Q^{bulk}/R/T)$$ $$M^{disl} = M_0^{bulk} \cdot \exp(F_{redDisl} \cdot Q^{bulk} R/T)$$ where • M_0^{bulk}: frequency-factor in the bulk • Q^{bulk}: activation energy in the bulk • F_{redGB}: bulk diffusion activation energy multiplier (typical value 0.5) • $F_{redDisl}$: bulk diffusion activation energy multiplier (typical value 0.8) The weighted calculated value for the mobility M^{new} is then evaluated from: $$M^{new} = \delta/d \cdot M^{gb} + \rho \cdot b^2 \cdot M^{disl} + (1 - \delta/d - \rho \cdot b^2) \cdot M^{bulk}$$ where • δ: grainboundary thickness (typical value $0.5 \cdot 10^{-9}$ or $0.5 \cdot 10^{-10}$) • d: grainsize as a function of time and temperature (typical value $25 \cdot 10^{-6}$) • ρ: dislocation density as a function of time and temperature • b: burgersvector (typical value $1 \cdot 10^{-10}$) • M^{bulk}: mobility in the bulk (δ/d being the fraction of grain boundaries in the bulk and $\rho \cdot b^2$ being the fraction of dislocations in the bulk)

HOMOGENIZATION_MODEL

- UTILITIES_HOMOGENIZATION
- ADVANCED_HOMOGENIZATION_OPTIONS

This command enables or disables the use of the homogenization model and its default settings. The homogenization model is used for multiphase simulations assuming that local equilibrium holds at each node point. When entering phases into a region one of them is entered as MATRIX phase and all other phases as SPHEROID, but it does not matter which one is entered as matrix phase and it does not affect simulations. Homogenization model simulations differs from all other DICTRA module simulations in that it is implemented using an implicit finite volume method in order to increase numerical stability (degree of implicity can be chosen using the SET_SIMULATION_CONDITION command). Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations.



The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the Thermo-Calc User Guide. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	HOMOGENIZATION_MODEL
Prompts	`Enable homogenization model:` Enter `Y` to enable the homogenization model. If it is already enabled, you can enter `N` to disable it.
	`Use default settings /Y/:` Press <Enter> to keep the default settings for the homogenization model. Otherwise enter N and follow the prompts.

	`Add ideal flux contribution /N/:`
	If you enter `Y` you are prompted as follows:
	`Fractional ideal contribution(0->1) /.01/:`
	Enter a number between zero and one. In multiphase regions the system loses degrees of freedom which may cause fluctuations in the composition profiles. This can be amended by adding a small ideal contribution to the fluxes. The ideal flux contribution should normally not be used.

	`Use interpolation scheme /Y/:`
	By default the interpolation scheme is used and it normally speeds up simulations. You are then prompted with the following:
	`Enter number of steps between XMin and XMax /10000/:`
	Enter the number of steps in composition space. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However,

Syntax	HOMOGENIZATION_MODEL

	excellent results can be obtained with a reasonable discretization.
	`Linear or logarithmic discretization /Log/:`
	The discretization can be either linear or logarithmic (the default). For the linear discretization the scheme is not used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where a good discretization is required for very low solute contents, the logarithmic discretization can be tried.
	`Fraction of free physical memory to be used /.1/:`
	Enter the fraction of free physical memory to be used by the interpolation scheme. If a value larger than one (1) is entered it is interpreted as the number of MB to be used for the interpolation scheme.

	`Use global minimization /N/:` By default global minimization is not used in equilibrium calculations. In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.
	`Refresh Jacobian every iteration /N/:` If there are convergence problems, enter Y to see if this solves the issue. This does increase computational demand for each iteration.
	`Default grid parameter values /Y/:` These settings only affect simulations where the grid changes during the simulation. If you enter N, you are prompted with the following.
	`Geometrical coefficient (0+ -> 1) /.98/:` The geometrical coefficient used in each region.
	`Fixed interface width (<0 DISABLES) /-1/:` A value larger than zero makes interface widths fixed to that value.
	`Grid fineness away from interface /1/:` A value other than one causes the grid away from the interface to be coarser (>1) or finer (<1) than what would be obtained just by the geometrical coefficient.
	`Interface width fraction (0+ -> 0.1) /.005/:` If the interface width is not fixed the program aims for a width equal to this factor times the cell width.
	`Consecutive critical time-steps (DT) to delete region /20/:` If the width of a region falls below a certain critical value and shrinks monotonically for this number of time-steps it is deleted.

INPUT_SCHEIL_PROFILE



As per normal procedure, and before entering the DICTRA monitor, you need to read thermodynamic and kinetic data to use this command.

This command takes a previously calculated Scheil segregation profile and performs most of the setup needed to use that profile in a simulation, for example a homogenizing heat treatment.

The command creates a region called SCHEIL_REGION. You then create a linear grid and enter the composition read from the file containing the segregation profile.

After issuing this command, you specify simulation time (SET_SIMULATION_TIME) and simulation temperature (SET_CONDITION, enter `GLOBAL` and variable `T`) to finalize setup.



In order to limit the computational effort, this feature cannot be combined with the fast diffusers option in the Scheil module.



Press F1 in Thermo-Calc to search the online help for detailed information about Scheil simulations.

Syntax	INPUT_SCHEIL_PROFILE
Prompts	`Enter file location of Scheil segregation profile` In interactive mode (the command line), a file dialogue window opens. Navigate to the file containing the Scheil profile. Alternately, if you are working from a macro file, the line should contain the name of the file.
	`Enter width of region` Enter the width of the region [m] that contains the Scheil profile. This typically corresponds to the secondary dendrite arm spacing.
	`Enter main solid solution phase` Enter the name of one of the main solid solution phases. In the next prompt you can enter other phases that enter the simulation.
	`Should more phases be entered in the region` Enter Y to enter more phases then enter the phase name as prompted next.
	`Enter phase name` Enter the name of another phase that should be entered into the region.

INTERFACE_SURFACE_TENSION

This command enters a distance- and velocity-dependent function that is added to the Gibbs energy of the phase at left side of a specified interface. This can then be used to emulate the effect of surface tension on the equilibrium between at the phase interface or limited phase mobility. This command is similar to the SET_SURFACE_TENSION command but more flexible because if there is more than one interface in a cell, the user can add different Gibbs energy expressions to different interfaces, each specified by the two neighboring phases.

Syntax	INTERFACE_SURFACE_TENSION

	`PHASE ON LEFT SIDE OF INTERFACE`
	The name of the phase on the left side of the specified interface.
	`PHASE ON RIGHT SIDE OF INTERFACE`
	The name of the phase on the right side of the specified interface.
	`Function F(X,V,TIME,T):`

Prompt	Enter a function which adds to the Gibbs energy expression for the phase located at the lower (left) side of the interface. The expression is multiplied with the volume per mole substitutional atoms (10-5m^3/mole). This command is also used to simulate a limited interfacial mobility control where the energy function is a function of the interface velocity. It is used to enter the surface energy to enable coarsening. However, it can also be used to simulate a case with a limited interfacial mobility. ▶ For detailed syntax for the function, see the SET_SURFACE_TENSION command.

LIST_CONDITIONS

Use the LIST_CONDITIONS command to lists the conditions defined with the SET_CONDITION command.

Syntax	LIST_CONDITIONS
Prompt	`Output file` File where the information is to be written.

LIST_MOBILITY_DATA



This command does not work for encrypted databases.

Lists the mobility data from the database or entered interactively by the ENTER_MOBILITY_DATA command.

Syntax	LIST_MOBILITY_DATA
Prompt	`Output file` File where the information is to be written.

LIST_MOBILITY_ESTIMATES

Use the LIST_MOBILITY_ESTIMATES command to list on screen the mobility estimate entered interactively using the ENTER_MOBILITY_ESTIMATE command.

LIST_PROFILES

Lists the concentration profiles and grid coordinates in the cell.

Syntax	LIST_PROFILES
Prompts	`Name of region` Name of region(s) in which the profiles are to be listed.
	`Output file` File where the information is to be written.
	`Composition type` Composition type in which the profiles are to be written. Legal composition types are: • SITE_FRACTION • MOLE_FRACTION • WEIGHT_FRACTION • U_FRACTION
	`Components` The output information may be limited to the specified components.
	`Constituents` The output information may be limited to the specified constituents.

LIST_REGION

List the names of the defined regions, active and inactive phases and the global coordinates of the interfaces.

Syntax	LIST_REGION
Prompt	`Output file` File where the information is to be written.

LIST_TIMESTEPS



This for the DICTRA module. Also see LIST_TIME_STEPS for the POST module.

Use the LIST_TIMESTEPS command to list the time steps in the workspace and those stored on file during a simulation.

MACRO_FILE_OPEN

Use this to predefine sequences of commands on a file and then execute them with the MACRO command. This is useful when the same calculation is made often with just small changes. One good case for applying this is when calculating diagrams from an assessment. With a macro file all commands can be stored on a file and you just type MACRO <filename>.

Syntax	MACRO_FILE_OPEN
Prompt	`Macro filename` Give the name of the file with the macro commands. Default extension is DCM.
	The macro file can contain any legal DICTRA module commands. The macro must be terminated with EXIT or in the SYS, DICTRA, POLY-3 or POST module with the command SET_INTERACTIVE_MODE.

PARA_EQUILIBRIUM_MODEL

Turns on the para-equilibrium model in the simulation. Using this model implies that the local equilibrium assumption is no longer valid and that substitutional components are regarded as one composite component.

The model is limited to treating only one single moving interface in one cell.



See the Diffusion Module (DICTRA) example EXH2, which is briefly described in Deviation from Local Equilibrium Examples

Syntax	PARA_EQUILIBRIUM_MODEL
Prompts	`Enable paraeq` Enables or disables the use of this model by using one of the key words YES or NO.
	`Auto` Choose this to set it to the value at the region's lower or upper boundary.
	`Value %` Enter a value followed by a percentage sign (%) to set it to a certain percentage from the moving boundary inside the region.
	`-Value` Enter a hyphen (-) followed by a value to set it to a fixed distance from the moving boundary.
	`Value` Enter a value to set the composition to that specific value,

POLY_COMMAND

This command sends a string to the POLY-3 module interpreter where it is then executed.



An example of the use of this command is as follows. There are some differences in the default settings for equilibrium calculations based on whether the equilibrium calculation is performed from the DICTRA module or POLY. The changes in the defaults are performed automatically every time the DICTRA module is entered. By using this command it is possible to override those changes.

Syntax	POLY_COMMAND
Prompt	`To POLY` Command line sent to the POLY-3 module.

POST_PROCESSOR

Use the POST_PROCESSOR command to "give control" to the post processor. Then you can start using the commands described in POST PROCESSOR Commands.

READ_WORKSPACES



Both GES6 and GES5 data are saved to/read from a dic-file. For information about GES versions, see About the Gibbs Energy System (GES) Module.

The DICTRA, POLY-3 and GES workspaces can be read from a file where they must be already saved with a SAVE command. This file is not printable.

Syntax	READ_WORKSPACES
Prompt	`File name` Name of the file where the workspaces shall be read from. The default file extension is `dic`.

SAVE_WORKSPACES



Both GES6 and GES5 data are saved to/read from a dic-file. For information about GES versions, see About the Gibbs Energy System (GES) Module.

The workspaces in DICTRA, POLY-3 and GES are saved in a file. Return to the state before the SAVE command by entering a READ command. The SAVE command should normally be given before starting a simulation with SIMULATE_REACTION.

Syntax	SAVE_WORKSPACES
Prompts	`File name` Name of the file where the workspaces shall be saved on. The default file extension is DIC.
	`Overwrite current file content`
	`Proceed with save` If there is already a file with this name and if you answer Y the previous content is overwritten. If you have results from SIMULATE_REACTION these are lost when SAVE is used. You may append several results by the SIMULATE_REACTION command without destroying the previous results but SAVE erases them all.

SELECT_CELL

Selects the current cell from the list of existing cells and enables you to enter and display data into that cell. This command is for the DICTRA.

- See also POST PROCESSOR prompt of the same name SELECT_CELL.

Syntax	SELECT_CELL
Prompt	`Number` Specify the cell number by giving an integer or one of the key words NEXT or PREVIOUS.

SELECT_TIMESTEP

Select a time step from those stored on file during a simulation. The profiles can be listed and simulation can be continued from this time step.

Syntax	SELECT_TIMESTEP
Prompt	`Timestep` The time step to be selected, legal syntax is: • `FIRST` • `LAST` • `time` • `#nnn` • `#?` When selecting a time no interpolation is performed but the time step closest to the time entered is selected. #nnn can be obtained from the number given by LIST_TIMESTEPS or by typing `#?`.
	`Delete all other timesteps` Clears the current workspace from all other time steps except the one selected. This is necessary if the simulation is to be continued from this time step.

SET_ACCURACY

Enter the accuracy requirements to use in the determination of the time step when using the automatic time step procedure. It may also be necessary to modify the parameters to control the removal of grid points and set manual starting values for velocities and potentials at the phase interfaces.



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Syntax	SET_ACCURACY
Prompts	`Max relative error` The maximum allowed relative error of the profile during one time step integration.
	`Max absolute error` Maximum allowed absolute error of the profile during one time step integration. This parameter must be chosen with some relation to the smallest concentration in the profiles.

SET_ALL_START_VALUES

Enter starting values for various quantities, such as velocities and potentials.

Syntax	SET_ALL_START_VALUES
Prompts	`Start value for velocity of interface` A starting value for velocity at the named interface is required.
	`Start value for potential` A starting value for a potential at the named interface is required. If an AUTOMATIC value is specified the program attempts to determine a starting value and also selects a suitable component for which the potential is varied.
	`Varying species in interface` The species which potential is treated as unknown.
	`Automatic starting values for phase compositions` Compositions used as starting values in the equilibrium calculations using POLY-3. When using automatic starting values the compositions are taken from the entered profiles.

SET_CONDITION

Define conditions to reduce the degrees of freedom at equilibrium or defines the boundary conditions at the outer rims of the system. Use it to set the temperature, pressure or heat extracted from the system.

Conditions can be a function of time and different time-dependent functions can be specified at different time intervals. The syntax for this is approximately the same as used in the GES to specify temperature ranges for thermodynamic parameters.

DICTRA uses a constant molar volume, which is included in the flux, i.e. the unit of flux as entered in boundary conditions is:

$$\texttt{flux*molar volume} = \texttt{mol*m}^{-2}\texttt{*s}^{-1}\texttt{*m}^{3}\texttt{*mol}^{-1} = \texttt{m*s}^{-1}$$

State, Integral and Auxiliary Variables

Syntax	SET_CONDITION
Prompts	`Global or Boundary Condition /Global/` Type of condition to be specified. A global condition is either pressure (P), temperature (T) or heat content removal (P) and may be specified as a function of time. Boundary conditions determine how the cell interacts with the world outside the cell.

	`Variable`
	Legal variables are pressure (P), temperature (T) or heat extracted (Q) as a function of time (TIME), or time-temperature-pairs (T-T-P) that specifies temperature at a specific time and lets the program calculate the cooling or heating rate. For Q the amount of extracted heat per time unit is normalized and the size of the system is normalized to 1 mole of atoms.
	For example, if you enter T-T-P at the Variable prompt then at the next prompt:
	`TIME,TEMPERATURE`
	Specify temperature and time pairwise such as e.g.:
	`0 1400`
	`60 1200`
	`* 1200`
	Where entering an asterisk(*)" is required in order to indicate the end time of a simulation.

	`Boundary` Defines on which side of the system the boundary conditions are to be specified. Options are UPPER (the rightmost side of the system) and LOWER (the leftmost side of the system).
	`Condition type` Defines the type of boundary condition to be specified. The options may in most cases be functions of both TIME, T (temperature) and P (pressure). The default is CLOSED_SYSTEM which is equivalent to setting the fluxes of all components to zero at the boundary. Options are:

Syntax	SET_CONDITION
	• FIX_FLUX_VALUE: Enter functions that yield the flux times the molar volume for the independent components. May be a function of time, temperature and pressure. • STATE_VARIABLE_VALUE: A legal expression in POLY-3 syntax that reduces the degrees of freedom. This type of boundary condition should be used with the uttermost care as no checks are done if it is a legal expression in advance. • POTENTIAL_FLUX_FUNCTION and ACTIVITY_FLUX_FUNCTION: These types of boundary conditions are used to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $$J_k = f_k(T,P,TIME)^* \left[ACTIVITY_k^N - g_k(T,P,TIME) \right]$$ or $$J_k = f_k(T,P,TIME)^* \left[POTENTIAL_k^N - g_k(T,P,TIME) \right]$$ where *f* and *g* may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.  The activities are those with user defined reference states. The function f_k is the mass transfer coefficient, g_k is the activity of the corresponding species in the gas and *N* is a stoichiometric coefficient.  For more details see L. Sproge and J. Ågren, "Experimental and theoretical studies of gas consumption in the gas carburizing process" *J. Heat Treat*. 6, 9–19 (1988). • ITERATIVE_ACTIVITY_FLUX_FUNCTION: Same as activity flux function above. However, an iterative scheme is used to determine the flux. This method may be used instead of activity flux function when the latter has problems. • CLOSED_SYSTEM: Corresponds to a fix flux value, which is set to zero at all times. • MIXED_ZERO_FLUX_AND_ACTIVITY: The flux of selected components is set to zero and the activity of others may be set to a prescribed value. • GAS: The flux of selected components is set to zero and the activity of others may be set to a prescribed value. This option is used for treating an expanding system, e.g. the growth of an external oxide scale.
	`Low time limit` The lower time limit to be used when entering a time dependent function.
	`High time limit` The upper time limit to be used when entering a time dependent function. An asterisk * indicates the high limit as infinity.
	`Any more ranges` To specify whether any additional time dependent functions exists or not.

Syntax	SET_CONDITION
	`Type of condition for component` The type of condition when setting a boundary condition of the type MIXED. Options are ZERO_ FLUX and ACTIVITY.

SET_FIRST_INTERFACE

Set the coordinate of the first interface in the cell, when a value other than zero is required, for instance when simulating diffusion through a tube wall or a hollow sphere. The default value is zero.

Syntax	SET_FIRST_INTERFACE
Prompt	`Coordinate for first interface` The coordinate to which the first interface is to be set.

SET_INITIAL_TEMPERATURE

This command is only used when the heat removal rate from the system is specified. It yields the initial temperature of the system. How the temperature then varies during the simulation is a result of the heat removed from the system.

Syntax	SET_INITIAL_TEMPERATURE
Prompt	`Initial temperature /2000/`

SET_LOG_LEVEL

Use the SET_LOG_LEVEL command to choose the amount of output to the logs during a homogenization model simulation. The default (2) keeps the log output to a minimum and thus limits the possibility of slowing down a calculation.

Syntax	SET_LOG_LEVEL
Prompt	`HOMOGENIZATION MODEL LOG LEVEL(1=NORMAL, 2=MINIMAL): /2/:`
	Choose 1 to set the amount of logging to normal and 2 to set it to a minimal amount (the default).

SET_NUMERICAL_LIMITS

Set parameters to control the integration, the solution of the flux balance equations, diffusion equations and the equilibrium calculation during the simulation.



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Syntax	SET_NUMERICAL_LIMITS
Prompts	`Required sum of squares in NS01A` Required accuracy during the solution of the flux-balance equations.
	`Max number of calls to Calfun of NS01A` The maximum number of iterations when solving the flux-balance equations. This number acts as a *safety valve*, a moderate choice is 10*(number_of_interfaces *(number_of_components - 1)) but use a larger value if necessary.
	`Step used by NS01A` A user supplied parameter which is used to calculate the estimates of the partial derivatives numerically when solving the flux-balance equations.
	`Max step used by NS01A` A parameter which must be set to a generous estimate of the 'distance' between the initial approximation and the required solution of the flux-balance equations.
	`Max number of equidistant points in a region` The number of equidistant parts in which a region is divided into that is required to describe the profile. This parameter is used by the procedure that removes unnecessary gridpoints from the profile during the simulation; the number of gridpoints is normally not allowed to be less than this number if a linear grid is used.
	`Fraction of region assigned to the interface` Fraction of a region at the region border that is to be regarded as part of the interface. This parameter is used by the procedure that removes unnecessary gridpoints from the profile during the simulation.
	`Smallest number used in scaling flux equations` The flux-balance equations are scaled by the velocities calculated in the previous time step. This number may however decrease to such a small value so that convergence may be affected. The scaling factor is therefore not allowed to decrease below this value.
	`Default driving force for inactive phases` Sets the necessary driving force needed before an inactive phase is allowed to start to precipitate.

SET_REFERENCE_STATE

The reference state for a component is important when using activities, chemical potentials and enthalpies and it is determined by the data. For each component the data must be referred to a selected phase, temperature and pressure the *reference state*. All data in all phases where this component dissolves must use the same reference state. However, different datasets may use different reference states for the same element. Thus one must mix data from different databases with caution.

By default activities etc. are computed relative to the reference state used by the database and this may thus differ depending on the database. You can select the reference state of a component if the reference state in the database is not suitable.

Syntax	SET_REFERENCE_STATE
Prompts	`Component` The name of the component must be given.
	`Reference state` The name of a phase that must be either entered or dormant must be given. The component must be a constituent of this phase of course. A subtle problem is if the component exists in several species in the phase, for example oxygen as O, O2 and O3 in a gas. Normally one would like to have the most stable species as reference state of oxygen, i.e. O2 in this case. Therefore the program calculates the Gibbs energy of all possible states with the phase with the pure component at the current temperature and selects the most stable one.
	`Temperature` Select the temperature for the reference state. The value * means the temperature used for the calculation.
	`Pressure` Select the pressure for the reference state.

SET_SIMULATION_CONDITION

Set parameters used to control output and certain parameters during the simulation.



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Syntax	SET_SIMULATION_CONDITION
Prompts	`NS01A print control` Determines whether data should be printed about the iterative procedure to solve flux-balance equations. This parameter is normally set to 0 but can be set to 1 when difficulties with convergence occur. NS01A prints out the values used in the iterations and the residuals.
	`Flux correction factor` This parameter controls if the flux correction scheme should be used in the calculations. The value should normally always be 1.
	`Number of delta timesteps in calling MULDIF` This parameter specifies the number of equally large time steps that one time step should be subdivided into.
	`Check interface position` This parameter determines whether the time step is to be controlled by the phase interface displacement during the simulation. The default is `Auto`.
	`Vary potentials or activities or LNAC` Determines whether the program should use the potential or the activity of a component in order to find the correct tie-line at the phase interface. The potential or the activity is varied by the program and is set in order to reduce the degrees of freedom at the local equilibrium. The default is `Activities`.
	`Allow automatic switching of varying element` Determines whether the program is allowed to itself switch the component that is used to reduce the degrees of freedom at the local equilibrium. The scheme used is that of choosing the components which activities or potentials varied most during the previous time step. The default is `Yes`.
	`Save workspace on file` This parameter determines whether the workspaces are to be saved to file during the course of the simulation. Options are `Yes` (the default) to always save to file, `No` to never save to file, or `##` to save every n^{th} time to file where ## is a integer value ranging from 0 to 99.
	`Degree of implicity when integrating PDEs` The default is `Auto` where the default degree of implicity corresponds to trapezoidal (0.5) for classic and Euler Backward (1.0) for the homogenization model. If large fluctuations occur in the profiles it may be necessary to use the value 1.0 (Euler backwards).

Syntax	SET_SIMULATION_CONDITION
	• `Auto` • `0.0` Euler forwards • `0.5` Trapezoidal rule • `1.0` Euler backwards
	`Max timestep change per timestep` Factor specifying the maximum increase in the time step taken from one time step to another. For example, if the default, `2` is used the maximum time step is twice as long as the previous time step taken.
	`Use forced starting values in equilibrium calculation` This concerns the calculation of the equilibrium when using the disperse model where the equilibrium calculations sometimes fail due the abrupt changes in the composition over the region. The default `Auto` means it always sets forced starting values for composition and phase amounts before preforming the equilibrium calculation.
	`Always calculate stiffness matrix in MULDIF` This determines how often the diffusion coefficient matrix is calculated when solving the partial differential equations (PDE) of diffusion problem. The default setting `Yes` calculates the diffusion coefficient matrix, yielding the stiffness matrix, at each iteration. However, when setting this parameter to `No`, it is only calculated at the first iteration and a constant stiffness matrix is used to obtain the solution to the PDEs. This then leads to an implicit solution and therefore the degree of implicitly is automatically set to 1.
	`Calculate residual for dependent component /No/` Keep the default.

SET_SIMULATION_TIME

Enter the time specific conditions for a simulation.



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Syntax	SET_SIMULATION_TIME
Prompts	`Eend time for integration` The time up to which the simulation is to be carried out.
	`Automatic timestep control` Determines whether the time step should be controlled by an automatic procedure or not. If you answer `N` you are prompted for the fixed time step to use during the simulation. The time step determined by the automatic time step control procedure is controlled by the parameters set by the command SET_ACCURACY.
	`Max timestep during integration` The maximum time step allowed during the simulation. This is required when using the automatic procedure to determine the time step.
	`Timtestep during integration` Fixed time step used when the automatic time step procedure is disabled.
	`Initial timestep` Time step used as the initial time step.
	`Smallest acceptable timestep` The smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step.

SET_SURFACE_TENSION

This command enters a distance- and velocity-dependent function which is added to the Gibbs energy of the phase at left side of each phase interface. This can then be used to emulate the effect of surface tension on the equilibrium between at the phase interface or limited phase mobility.

Syntax	SET_SURFACE_TENSION
Prompt	`Function` Enter a surface energy function which adds to the Gibbs Energy expression for the phase located at the lower (left) side of the interface. The expression is multiplied with the volume per mole substitional atoms. This command is also used to simulate a limited interfacial mobility control where the energy function is a function of the interface velocity. It is used to enter the surface energy to enable coarsening. However, it can also be used to simulate a case with a limited interfacial mobility.

	 This function should only be used in spherical geometries if the function is solely dependent of the interface position.
	
	Function describing how the (surface) energy function varies with the particle radius and/or the interface velocity.
	
	The classical expression for the surface energy contribution has the form of $\frac{2\sigma V_m}{r}$.
	
	The molar volume should be given relative to the molar volume used by default in DICTRA, 1 x 10^{-5} (m^3/mole). The volume should also be given per mole of substitutional atoms. For a precipitate of type M_xC_y this means multiplying with a factor (y+x)/x. If we use M_6C as an example with surface tension 0.5 (J/m^2) and molar volume of 0.71 x 10^{-5} (m^3/mole), the entered function should be 2*0.5*0.71*(7/6)/X;
	
	Commonly the surface tension function is defined as:
	
	`delta-G = 2 * SIGMA * Vm / R`
	
	The function to be entered will then be:
	
	`2*SIGMA/X;`
	
	A limited interface mobility can be expressed as:
	
	`delta-G = v * Vm /const`
	
	The function to be entered is then:
	
	`v/"const";`
	
	  The expression is multiplied by the partial molar volume of the substitutional components.

SIMULATE_REACTION

This command starts the simulation. If given without any argument, you are prompted for certain values during simulations where phases appear or disappear.

Syntax	SIMULATE_REACTION
Prompt	The command can also be given with the argument YES typed on the same line: `Simulate_Reaction Yes` With the YES argument, default values are used during simulation and no user input can be given. This is especially useful when using batch mode.

SOLVE_IN_LATTICE_FIXED_FRAME

Use this command to solve a diffusion problem in the lattice-fixed frame of reference. This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.

Syntax	SOLVE_IN_LATTICE_FIXED_FRAME
Prompts	`Solve in the lattice-fixed frame of reference /NO/` Enter `Yes` to enable this feature.

By default, DICTRA solves diffusion problems in a volume-fixed frame of reference under the assumption that the partial molar volume of all substitutional elements is constant and equal and that the partial molar volume of interstitial elements is zero. When you enable this command, the diffusion problem will instead be solved in a lattice fixed frame of reference. In addition, this option forces the use of the assessed molar volumes read from the current thermodynamic database.



Simulations with moving boundaries as well as cell simulations are currently not available with this feature.

For all geometries the leftmost/lower coordinate is fixed during a simulation (by default it is zero). This command also enforces some constraints for planar and cylindrical geometry. For a planar geometry the size of the domain in the plane orthogonal to the direction of diffusion is fixed. For a cylindrical geometry the length of the cylinder is fixed. For all geometries there may be changes in the size of the domain as a result of the diffusion process, even with closed boundaries, since the assessed molar volumes of the thermodynamic database is used.

All elements are set as substitutional. Though the notion of substitutional/interstitial elements has no meaning when running a simulation with this feature turned on, it does have implications in the POST processor.



The DICTRA POST processor does not use assessed molar volumes, which means that certain plots will be erroneous. There may for example be changes in the total domain size even for a single phase simulation with a closed system due to changes in the molar volume. A plot of the total number of moles in the domain would then, erroneously, show a change over time. Other axis quantities that in general will be incorrect are, for example, IV(*) and VP(*).

Further, when solving in the lattice-fixed frame of reference the unit of the flux is $mol*m^{-2}s^{-1}$, which differs from the default unit wherein the assumed constant substitutional molar volume (10^{-5} m^3*mol^{-1}) is included in the flux. This must be taken into account for certain types of boundary conditions, that is, the conditions of type

- FIX_FLUX_VALUE
- POTENTIAL_FLUX_FUNCTION
- ACTIVITY_FLUX_FUNCTION
- ITERATIVE_ACTIVITY_FLUX_FUNCTION

See SET_CONDITION for details about the above commands.

In order to roughly get the same result for these boundary conditions the evaluated flux must be a factor 10^5 higher when solving in the lattice-fixed frame of reference compared to simulations with the default setting.

STORE_HOMOGENIZATION_DATA

Read/write the interpolation scheme data to file. The interpolation scheme is an option of the homogenization model that is used to speed up simulations. Use if this option can speed up simulations further.

Syntax	STORE_HOMOGENIZATION_DATA
Prompt	`Store/Read homogenization model interpolation data <Y/N>` Answering `Y` or `N` enables/disables read/write of interpolation scheme data to file.

SWITCH_MODEL

Use the SWITCH_MODEL command to use the HOMOGENIZATION_MODEL to solve a problem if the classic model fails.

There are two solvers for moving phase boundary problems. The classic computationally efficient model and the more robust, but computationally more demanding, homogenization model. By default, the classic solver is tried first. If this fails, then the new solver is tried for a few time-steps before switching back to the classic solver, and so on.



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Syntax	SWITCH_MODEL
Prompts	`Enable automatic switch of model (Y/N)` Determine if automatic switching from the classic solver to the homogenization model is allowed.

USE_INTERPOLATION_FOR_D



In Graphical Mode, `Complex` is the default and cannot be changed.

An interpolation scheme can be used to calculate the chemical diffusivities of complex phases. If this is enabled, the performance gain from this ranges in orders of magnitude. This is ON by default for complex phases and can be set to OFF with this command.

Syntax	USE_INTERPOLATION_FOR_D

Prompts	`The following phases will be affected if complex is selected:`
	When there are phases in the system that will be affected, these are listed. The phases are based on the thermodynamic model.
	`Interpolate diffusivities in /None/Complex/All phases /Complex/`
	The default is `Complex`. A complex phase means that an equilibrium calculation is needed in order to determine the site-fractions in a phase with converting from *u*-fraction (or any other type of composition variable).

	`Enter number of steps between Xmin and Xmax /10000/:` Enter what is essentially the number of steps in each dimension in composition-P-T space for each equilibrium condition (Nk, P, T). In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization.
	`Linear or Logarithmic discretisation /Log/:` The discretization can be either linear or logarithmic. For the linear discretization the scheme will not be used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where composition span many orders of magnitude, the logarithmic discretisation can be tried.

	The system confirms the discretization setting and displays the amount of free memory available for the calculation. You are prompted to enter how much of this memory to use for the simulation.
	`Discretisation set as Logarithmic (or Linear)`
	`Free physical memory (mb): 8535`
	`Fraction of free physical memory to be used /.1/:`
	The fraction of free physical memory to be allocated for the interpolation scheme.

USE_TWO_TYPES_OF_BOUNDARY_CON

This command enables you to use two types of boundary conditions (BC). This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS. During the simulation one arbitrary boundary will be closed, but for the other open boundary and for each element, you can select which of the two entered boundary conditions should apply.

Syntax	USE_TWO_TYPES_OF_BOUNDARY_CON
Prompts	`Use two types of boundary conditions /NO/` Enter `Yes` to define the boundary conditions further.
	`Close the upper boundary /YES/` Select whether the upper or lower boundary should be closed during the simulation.
	`For <element>, use lower boundary BC: /YES/` You are prompted for each element whether the boundary condition entered for the lower or the upper boundary should apply.

UTILITIES_HOMOGENIZATION

ADVANCED_HOMOGENIZATION_OPTIONS

Use this with the HOMOGENIZATION_MODEL for the available utilities.

Syntax	UTILITIES_HOMOGENIZATION
Prompts	`Set temperature according to solidus temperature /N/:` Set the global temperature such that it goes to a certain value T_{target}=T_{sol}-X, where X is an entered value. Also enter the rate by which the temperature approaches T_{target}. The solidus temperature is determined with a +/- 1 K accuracy. Input guesses of the minimum and maximum temperature to occur during the simulation. This utility can be useful to optimize homogenization heat treatments.  The liquid phase must be entered into the system.
	`Dump results to text files /N/:` Enter `Y` to save simulation results to various text files. The names of these files are fixed and are saved to the current working directory.
	`Read initial composition from text file /N/:` Enter `Y` to read initial composition from a text file `XF.TXT` that must be present in the working directory. The file should contain the mole fractions of all elements, in alphabetical order, starting from the first grid point, in the first region, in the first cell.
	`Enter ghost phase /N/:` Enter `Y` to force the so-called ghost phase to be created. This phase has full solubility of all components and zero diffusivity. The Gibbs energy surface of the ghost phase is set above all other phases. The name of this phase is ZZDICTRA_GHOST. It can be used for numerical reasons. It is created automatically if there is a phase that lack solubility range of one or more components and then used internally by the program.
	`Enter inactive phases into one region /N/:` Enter `Y` to make all inactive phases at a given interface to be entered into a single multiphase region when any one of the phases becomes stable.
	`Explicitly set substitutional/interstitial /N/:` Enter `Y` to explicitly select for each element whether it should be substitutional or interstitial. There must be at least one substitutional element in each region. These settings only have effect for the homogenization model and results viewed in the post processor must be interpreted with care; use `DUMP RESULTS TO TEXT FILES` to get results corresponding to the settings entered here.
	`Save average finite volume composition /N/:` Save the average finite volume composition instead of a converted piece-wise linear composition.
	`Set constant phase addition /N/:` Add constant Gibbs energy contributions to phases (in J/mol formula unit).
	`Use element mobility prefactor /N/:`

Syntax	UTILITIES_HOMOGENIZATION
	Enter constant factors which the mobilities of elements are multiplied with in all phases.
	`Enter element mobility constant value /N/:` Interactively enter a constant mobility estimate for specific elements in specific phases. This can be used to enter mobility estimates in phases for which there is no assessed data. Estimates entered here override database values.
	`Enter minimum save interval /Y/:` Enter a minimum time interval (in seconds) that must pass between subsequent saved time-steps. This is useful in cases where a large number of small time-steps may occur in order to keep down the size of the result file.
	`Simplified evaluation of activity boundary condition /N/:` Enter `Y` to evaluate the fluxes on boundaries directly from the activity gradient, i.e. without taking into account the change of state on the boundary caused by the prescribed boundary activities.
	`Enter explicit limits on composition /N/:` Use this setting with caution to explicitly enter upper and lower limits on composition for all components (in mole fraction).
	`Enter chemical potential contribution /N/:` Enter a function (in valid POLY-3 syntax) that is evaluated separately at all grid points and added to the chemical potential of all elements. The contribution affects the flux between grid points.
	`Do not balance external boundary fluxes /N/:` For all boundary conditions except type GAS, the flux of substitutional elements into the domain is balanced with the flux of the dependent substitutional elements such that the size of the domain is preserved. Enabling this setting disables the balancing of the substitutional fluxes.  This feature is now available under the ADVANCED_HOMOGENIZATION_OPTIONS command. The use of this feature under the command UTILITIES HOMOGENIZATION is deprecated.
	`Fix external boundary flux of dependent component /N/:`  This feature is disabled. A more general version is available under the ADVANCED_HOMOGENIZATION_OPTIONS command. It is still visible for backwards compatibility reasons.
	`Modified kinetics on boundary /N/:` Use this to modify the kinetics on the boundary and enter a factor. If the factor is greater/smaller than one, the mobilities of all elements on the boundary is set equal to the maximum/minimum mobility of all elements times the factor. This can be useful in order to quickly saturate an outermost finite volume.

POST PROCESSOR Commands

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Purpose and Methodology

The purpose of the POST PROCESSOR is to read and process data from the internal data structure of the DICTRA module in order to present the result of a simulation in either* GRAPHICAL (command PLOT_DIAGRAM) or* TABULAR FORM (command MAKE_EXPERIMENTAL_DATAFILE).

Before plotting/printing, you have to specify what variables should be plotted on the diagram axis or printed in the table columns. For this purpose there is a command SET_DIAGRAM_AXIS. After having SET both X- and Y-axis variables, you have to SET also plot condition and independent variable. It is also possible to specify a Z-axis. Its values appear as tick marks on the XY-curve.

Plot Condition and Independent Variable

There are two free variables after a simulation is done by the DICTRA module. One is the simulation TIME, the other is a DISTANCE in the system.

In general, when plotting a diagram you MUST set either type as fixed, i.e. the *plot condition*, use command SET_PLOT_CONDITION. The plot condition chosen is printed on a separate line above the diagram.

The other variable is then the independent variable, use command SET_INDEPENDENT_VARIABLE. The independent variable is used as stepping variable. It varies along the calculated curve.

Legal Plot Conditions

- TIME: Integration time
- DISTANCE: Distance in the system. It can be a GLOBAL distance counted from the rightmost interface of the system. A LOCAL distance is counted from the LOWER interface of the specific region prompted for.
- INTERFACE: At a certain interface. An interface is identified by the NAME of the adjacent region, with the addition that you will be prompted to specify if the interface is at the upper or lower end of the region.
- INTEGRAL: Is automatically SET when using an INTEGRAL VARIABLE as axis variable.
- TIE_LINE: At a certain interface. Allows you to plot a certain quantity from both sides of an interface. The typical application is for plotting tie-lines.

Legal Independent Variables

- TIME: Integration time. Is automatically SET when using an INTEGRAL VARIABLE' or TIME as axis variable.
- DISTANCE: Space coordinate. It may be GLOBAL. It is then counted from the rightmost interface of the system. Alternatively, it may be LOCAL. The distance is then counted from the LOWER interface of the specific region prompted for.

APPEND_EXPERIMENTAL_DATA

Add experimental data and text on a calculated diagram. The experimental data and text are added to a file prepared according to the syntax of the DATAPLOT graphical language. The picture generated from the data is superimposed on the ordinary graphical output from the POST PROCESSOR. The experimental data file can be created with an ordinary text editor. Another use of the APPEND_EXPERIMENTAL_DATA command is to superimpose plots from several independent calculations. For this purpose, there is a command MAKE_EXPERIMENTAL_DATAFILE which dumps a calculated diagram on a file according to the DATAPLOT syntax. With the aid of a basic text editor many such files may be merged. Remember to have only one prologue section on the file (see below).

▶ About DATAPLOT Files

Syntax	APPEND_EXPERIMENTAL_DATA
Prompts	`Use experimental data (Y or N) /N/:` By default, no experimental data is plotted.
	`Experimental datafile` Specify the name of the file with the experimental data. Default file extension is exp.
	`Prologue number` Select which prologue to use. In a prologue one may e.g. give the scaling of an axis, the axis texts, and so on. -1 gives a list of all prologues on the file. Read more about prologues below.
	`Dataset number(s)` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. -1 gives a list of all datasets on the file.

DETERMINE_KIRK_PLANE

To use this command a certain time must be set as plot condition. You are prompted for the position of a plane at time zero. The position of the plane at the plot condition time is then calculated. The difference in position is equal to the Kirkendall shift, i.e. how much an inert marker would drift in the material due to a net flux of vacancies.

Syntax	DETERMINE_KIRK_PLANE
Prompt	`Initial zero plane /-1/`

DIFFERENTIATE_VALUES

Use the DIFFERENTIATE_VALUES command to determine differences between values in a plotted curve.

DUMP_DIAGRAM

An alternative way to create plots. Supported graphical formats are PNG, BMP, PDF, JPEG and TIFF. The plot is saved to a file.

Syntax	DUMP_DIAGRAM
Prompt	`Output format (PNG,BMP,PDF,JPEG,TIFF)` Specifies which graphical format to use.
	`Resolution (Low, Medium, High)` Specifies the resolution of the plot.

ENTER_SYMBOL

The information about this command is specific to the Diffusion Module (DICTRA) Console Mode. The ENTER_SYMBOL command is also available in the GIBBS, POLY3 and POST modules in Thermo-Calc.

Define a symbolic name to represent either a table or an 'arbitrary' function. Legal variables in functions and columns in tables are described in the sections state variables, auxiliary variables, integral variables or can be previously defined functions. Functions are a useful feature of the POST PROCESSOR to define quantities.

Syntax	ENTER_SYMBOL
Prompts	`Function or table /Function/` Select what kind of symbol to enter.
	`Name` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. If one wishes to enter the name and the value on the same line they must be separated with an equal sign =.

	`Function`
	Functions are evaluated from an expression of state variables, auxiliary variables, integral variables or previously defined functions. The expression is a Fortran-like expression and operators +, -, *, / and ** can be used (** only with integer powers). Unary functions like LOG, LOG10, EXP, SIN, COS, ABS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon or an empty line.
	Examples
	`POI(CEM,U)-POI(CEM,L);`
	The thickness of the region named CEMENTITE
	`AC(CR)/X(FCC,CR);`
	The activity coefficient for Cr in phase FCC
	`SQRT(TIME);`
	The square root of the simulation time
	`&`
	The ampersand & sub-prompt displays if the function was not terminated by a semicolon. It allows a user to continue to write the function on the new line if one line is not enough for the function. If one has finished the function just press return again.

	`Variable(s)` When entering a table, specify what variables are to be in the various columns. Separate the variables with commas or space characters. At present a maximum of 15 columns are allowed. The independent variable is always printed in the first column.

Syntax	ENTER_SYMBOL
	Auxiliary Variables, Integral Variables, and State Variables for details and examples of the short names (mnemonics).

INFORMATION

Some general information about the POST PROCESSOR module is given.

Syntax	INFORMATION
Prompt	`Which subject` Select which subject you want additional information about. Type ? to get a list of topics. • PURPOSE • STATE VARIABLES • INTEGRAL VARIABLES • AUXILIARY VARIABLES • PLOT CONDITION AND INDEPENDENT VARIABLE • BASIC METHODOLOGY

INTEGRATE_VALUES

Use the INTEGRATE_VALUES command to mathematically integrate the plotted curve.

LABEL_CURVES

Create labels. Each label is explained with to the right of the diagram.

Syntax	LABEL_CURVES
Prompt	`Label curves` Enter Y or N. For example: *1. X: X(CR); Y: TIME; PC:3* is read as *1 is a curve with X(CR) on the x-axis, TIME on the y-axis and plot condition PC according to value 3 specified on the plot condition line printed above the diagram*.

LIST_PLOT_SETTINGS

Use the LIST_PLOT_SETTINGS command to list on screen the present values of most parameters specifying the type of diagram to be plotted.

LIST_REGION_NAMES



All region names have a #-sign and the cell number appended.

Use the LIST_REGION_NAMES command to list all region names that are defined.

LIST_SYMBOLS

Use the LIST_SYMBOLS command to list a specific symbol or enter an asterisk (*) to list all defined symbols.

Syntax	LIST_SYMBOLS
Prompt	`Name` Give the name of a symbol or an asterisk * to list all defined symbols.

LIST_TIME_STEPS



This for the POST PROCESSOR module.

Use the LIST_TIME_STEPS command to list all integration time steps.

MAKE_EXPERIMENTAL_DATAFILE

Save graphical information in a file with the DATAPLOT format. To merge two or more diagrams from separate calculations, use the MAKE_EXPERIMENTAL_DATAFILE command to export it and add them together with a normal text editor.

- APPEND_EXPERIMENTAL_DATA and About DATAPLOT Files

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	`Output file` File where the graphical information is written. Default file extension is `exp`

PLOT_DIAGRAM

Plot graphical information on the specified device using the plot format set by SET_PLOT_FORMAT.

Syntax	PLOT_DIAGRAM
Prompt	`Plot file` The name of the file or graphical device.

PRINT_DIAGRAM



This command is only available for Windows operating systems.

Use the PRINT_DIAGRAM command to print a plot or diagram using the printers defined in Windows.

QUICK_EXPERIMENTAL_PLOT

Use the QUICK_EXPERIMENTAL_PLOT command to define a pair of axes, sets the axis labels to X and Y, and scale both x- and y-axis between 0.0 and 1.0 unless a prologue is read from the data file. It is similar to the APPEND_EXPERIMENTAL_DATA command but can be used when there is no graphical information to be plotted in the DICTRA module workspace.

- See APPEND_EXPERIMENTAL_DATA about the format of the data file.

REINITIATE_PLOT_SETTINGS

Use the REINITIATE_PLOT_SETTINGS command to give all parameters describing the diagram as default values.

SELECT_CELL

Select the cell data to be processed. You can only plot data from one cell at a time. Type ? to get a list of valid cell numbers. This command is for the POST PROCESSOR.

Also see the DICTRA module prompt of the same name SELECT_CELL.

The current cell number is displayed as a part of the POST PROCESSOR prompt.

Syntax	SELECT_CELL
Prompt	`Number` Number of the cell to be selected. Specify cell number by giving an integer or one of the key words NEXT or PREVIOUS.
	`Tabulate` Tabulate a named table. The independent variable is always printed in the first column.
	`Name` Give the symbolic name of the table.
	`Output file /Screen/` Select output device/file. Press Enter to get output on the screen.

SET_AXIS_LENGTH

Change the relative length of an axis, i.e. the number of tic-marks on the axis. The default number of tic-marks on an axis is 10 when the relative length is 1. The number of units per tic-mark must be a multiple of 1, 2, or 5 to obtain a reasonable scaling of an axis.

Syntax	SET_AXIS_LENGTH
Prompts	`Axis` Specify the axis to set the axis length.
	`Axis length` Specify the relative axis length. The relative length 1 corresponds to 10 tic-marks on the axis.

SET_AXIS_PLOT_STATUS

Specify to plot a diagram axis. Use it to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default to plot the axes.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	`Axis plot` `Y` or `N` to plot axis.

SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to another text.

Syntax	SET_AXIS_TEXT_STATUS
Prompts	`Axis (X, Y or Z)` Specify which axis text status to change (if the axis type is INVERSE, X2 or Y2 may be used to set the corresponding opposite linear axis text).
	`Automatic axis text (Y or N)` Specify if automatic axis text is to be used or not.
	`Axis text` Enter axis text.

SET_AXIS_TYPE

Select a linear, logarithmic or inverse axis.

Syntax	SET_AXIS_TYPE
Prompts	`Axis (X, Y or Z)` Specify which axis to change the axis type.
	`Axis type` Specify which axis type to set. Select `LIN`ear (default), `LOG`arithmic or `INV`erse. Only the three first characters are needed.

SET_COLOR

On devices that support colors/(line types), select different colors/(line types).

Syntax	SET_COLOR
Prompt	• Text and axis Color • Diagram Color • DATAPLOT Color

SET_DIAGRAM_AXIS

Specify the axis variables of a plot. At least two axis variables (x and y) must be specified.



Also see Auxiliary Variables, Integral Variables, and State Variables for lists of variables including its abbreviated name (i.e. the mnemonic) as well of the names of these variables.

Syntax	SET_DIAGRAM_AXIS
Prompts	`Axis (X,Y or Z)` Specifies the axis to set a variable.
	`Variable` Specifies the variable to plot along this axis. A variable is specified by its mnemonic (i.e. its abbreviated name) or by name. The variable types are None, Integral Variables, Functions, Auxiliary Variables or State Variables. • `NONE`: Use this variable to clear an axis setting. • `INTEGRAL VARIABLES`: A quantity obtained by integration in space over the whole system or over a specific region. In a planar geometry values are given per unit area, in a cylindrical geometry they are given per unit length, and in a spherical geometry they are absolute values. See Integral Variables for examples. • `FUNCTIONS`: These are identified by a name which is entered with the ENTER_FUNCTION command. Use the LIST_SYMBOLS command to get a list of valid function names. • `AUXILIARY VARIABLES`: As a complement to state variables and integral variables the auxiliary variables are defined. The variables can be called by their mnemonic names, which are shown in the rightmost column. These are useful in user-defined functions. See Auxiliary Variables for examples. • `STATE VARIABLES`: State variables in the DICTRA POST module are similar to those defined in POLY-3. Examples of state variables are temperature, mole fraction, enthalpy, etc. In POLY-3 a general notation method based on character mnemonics is designed for a predefined set of state variables. See State Variables for examples. Depending on the axis variable some sub-prompts may be available.
	`For component` When an activity, flux, mole-, weight- or U-fraction or percent is plotted the name of the component must be supplied.
	`In region` When the lamellar spacing, e.g. for pearlite, is plotted the name of the region must be supplied.
	`For phase` When the lamellar thickness, e.g. for ferrite in pearlite, is plotted the name of the phase must be supplied.

Syntax	SET_DIAGRAM_AXIS
	`Interface` When the velocity or the position of an interface is plotted the name of the interface must be given. An interface is identified by the name of the region on its upper side.
	`Type` When choosing distance as variable one has additionally to specify what type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you are prompted for.
	`Region name` Name of the region wherein the local distance is measured.

SET_DIAGRAM_TYPE

Set the diagram to a square (the default) or triangular plot (Gibbs triangle).

Syntax	SET_DIAGRAM_TYPE
Prompts	`Triangular diagram` Select `Y` for a triangular plot.
	`Plot 3rd Axis` For triangular plots is selected specify if a 3:rd axis, connecting the end points of the x- and y-axis is plotted.
	`Clip along the 3rd axis` Remove all lines outside the region limited by a line joining the end points of the X- and Y-axis.

SET_FONT

Select the font to use for labels and numbers when plotting the diagram. For some devices (e.g. PostScript) there may be other fonts available and these are selected by the SET_PLOT_FORMAT command.

Syntax	SET_FONT
Prompts	`Select Font number` Give the number for the font to select. Type ? to get an online list of the available fonts.
	`Font size` A value of 0.3 is recommended.

SET_INDEPENDENT_VARIABLE

There are two free variables after a simulation is done in theDiffusion Module (DICTRA). One is the simulation TIME, the other is a DISTANCE in the system. When plotting a diagram you must choose either one to vary along the curve, i.e. the independent variable, the other one is then the plot condition.



When plotting integral quantities TIME should be the independent variable.

Syntax	SET_INDEPENDENT_VARIABLE
Prompts	`Variable` Select which variable TIME (integration time) or DISTANCE (space coordinate) to treat as the independent variable.
	`Type` When choosing distance as independent variable specify the type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you are prompted for.
	`Name of region` For a LOCAL distance supply the name of the region within which the distance is measured. Type a ?, to get a list of valid region names.

SET_PLOT_CONDITION

There are two free variables after a simulation is done in theDICTRA module. One is the simulation TIME, the other one is a DISTANCE in the system. In general, when plotting a diagram you must choose either type as fixed (i.e. the plot condition), the other one is then the independent variable. However, when plotting integral quantities, plot condition is automatically set to INTEGRAL and TIME is chosen as independent variable. N.B. You cannot mix different kinds of plot conditions. However, for TIME and DISTANCE you may supply up to 15 different condition values, see sub-prompt VALUE(S) below. The plot condition chosen is printed on a separate line above the diagram.

Syntax	SET_PLOT_CONDITION
Prompts	`Condition` Specify the type of condition to set. Valid conditions are: • `NONE`: Condition not set. • `TIME`: Integration time. • `DISTANCE`: Distance in system. • `INTERFACE`: At a certain interface. • `INTEGRAL`: Value is integrated over the phase/region/system volume • `TIE_LINE`: Pair of values from both sides of certain interface. Depending on the condition some or none of these sub-prompts may display.
	`Interface` Specify at which interface the condition should be set. FIRST and LAST refer to the leftmost and the rightmost interface of the system, respectively. Type ? to get a full list of relevant region names.
	`Type` When distance is chosen as plot condition specify the type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you are prompted for.
	`Name of region` Give the name of the region within which the distance is measured.
	`At upper interface of region` Give the name of the region which upper interface is specified for the TIE_LINE plotting. This plot-condition allows you to plot a certain quantity from both sides of an interface. The typical application is for plotting tie-lines.
	`Upper or lower interface of region` Specify if the condition is at the LOWER or UPPER interface of a region. The LOWER interface is placed on the left side of a region and the UPPER interface on its right side.
	`Value(s)` Supply up to 15 numerical values separated by commas or spaces for the condition set. If plot

Syntax	SET_PLOT_CONDITION
	condition TIME was chosen FIRST, LAST or #n (where n is an integer number) may be specified. #? provides a list of time steps.

SET_PLOT_FORMAT

Adjust the format of the graphical output to another graphical device. This default can be changed with the SET_PLOT_ENVIRONMENT command in the SYSTEM MONITOR.

Syntax	SET_PLOT_FORMAT
Prompt	`Graphic device number /#/: <Number of the device>` Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark `?`. For some formats there can be additional sub-prompts (Y or N) about the available fonts being used for the chosen format. Also enter Y for further specifications, e.g. font type and size.

SET_PLOT_OPTIONS

Toggle on/off the plotting options on the diagram.

Syntax	SET_PLOT_OPTIONS
Prompts	`Plot header` Toggle the plot of the text above the diagram.
	`Plot logo` Toggle the plot of the logo at lower-left corner of the diagram.
	`Plot footer` Toggle the plot of the footer identifier text (only on postscript devices).
	`White contoured PS CHARS` Toggle the option of having a thin white contour around postscript characters (only on postscript devices).
	`Plot remote exponents` Toggle the plot of the remote exponents on the axis.
	`Plot cell #` Toggle the plot of the cell number text at the upper-right corner of the diagram.
	`Plot condition status` Toggle the plot of the plot-condition status line above the diagram.

SET_PLOT_SIZE

Specify a relative scale factor to change the size of the diagram. The default value of the scaling factor depends on what output device is chosen by the SET_PLOT_FORMAT command. The default plot size is adjusted to the chosen device.

Syntax	SET_PLOT_SIZE
Prompt	`Relative plot size` Enter the relative scaling factor.

SET_PREFIX_SCALING

When prefix scaling is enabled the remote exponent for an axis is automatically chosen to have a value which is a multiple of three, i.e. ..., -6, -3, 0, 3, 6,…

Syntax	SET_PREFIX_SCALING
Prompts	`Axis (X or Y)` Specify `X`- or `Y`- axis.
	`Use prefix scaling` Enables or disables prefix scaling, `Y` or `N`. Give an integer value to select a prefix power of your own.

SET_RASTER_STATUS

Set to have a raster plotted in the diagram. Default is no raster plotted.

Syntax	SET_RASTER_STATUS
Prompt	`Raster plot (Y or N) /Y/` Enables (`Y`) or disables (`N`) the raster plot.

SET_SCALING_STATUS

Choose between manual or automatic scaling on a specified axis. If manual scaling is chosen specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram. When an axis variable is selected by the SET_DIAGRAM_AXIS command the scaling status for the axis is always set to automatic scaling.

Syntax	SET_SCALING_STATUS
Prompts	`Axis (X, Y or Z)` Specify what axis to set the scaling status.
	`Automatic scaling (Y or N)` Automatic (`Y`) and manual (`N`) scaling.
	`Min value` For manual scaling specify the value of the starting point of the specified axis.
	`Max value` For manual scaling specify the value of the end point of the specified axis.

SET_TIC_TYPE

Change the size of the tic marks and the placement either inside or outside of the axis.

Syntax	SET_TIC_TYPE
Prompt	`TIC type` Place on either the inside or the outside of the diagram axis. The absolute value of TIC TYPE determines the length. • `TIC TYPE > 0` (outside the axis) • `TIC TYPE < 0` (inside the axis)

SET_TITLE

Specify a title that displays on all listings and diagrams from the POST PROCESSOR.

Syntax	SET_TITLE
Prompt	`Title` Enter the title to include on all output. There is a maximum length of about 60 characters.

SET_TRUE_MANUAL_SCALING

Use the SET_TRUE_MANUAL_SCALING command to turn manual scaling on and off. The default is where the tic marks on the axis are placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this.

Syntax	SET_TRUE_MANUAL_SCALING
Prompt	`Axis (X or Y)` Specify the axis you want to toggle between automatic adjustment or avoiding the adjustment of the given maximum and minimum values.

DATPLOT Files

In this section:

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About DATAPLOT Files

A DATAPLOT file can be divided into two sections. The prologue, which contains directives for manipulating the default settings on the diagram layout, and the dataset, which contains the actual data and any text to be plotted in the diagram. The sections may contain multiple PROLOGUE and DATASET statements, respectively.

DATPLOT User Guide included with this documentation set.

- All prologues must be placed before the first DATASET statement. See Keywords for Prologues and Keywords for Datasets.
- The syntax must be used for the DATAPLOT file.
- In general, each line in a DATAPLOT file must consist of a legal keyword plus its parameters or an XY coordinate pair.
- An XY coordinate pair is two real numbers and an optional graphical operation code (GOC). See Available Graphical Operation Codes (GOCs).

Example

```
700 2.54
50 1.91 WRDS
1.1 0.9 NS3
100 20'This is a text
BLOCK GOC=C3,MWAS; X=C1+273.15; Y=C2*4.184;
600 -1400 S1'text
700 -1500
BLOCKEND
```

Keywords for Prologues

Keyword	Parameters
PROLOGUE	inumb text
XSCALE	min max
YSCALE	min max
XTEXT	text
YTEXT	text
XTYPE	LIN, LOG or INV
YTYPE	LIN, LOG or INV
XLENGTH	rnumb
YLENGTH	rnumb
DIAGRAM_TYPE	TRIANGULAR or SQUARE
TIC_TYPE	rnumb
TITLE	text

Keywords for Datasets

Keyword	Parameters
DATASET	inumb text
FONT	inumb
CHARSIZE	rnumb
COLOR	inumb
GLOBALSIZE	rnumb
LFSIZE	rnumb
LINETYPE	inumb
BLOCK GOC=C3,DEFGOC; X=C1+273.15; Y=LOG10(C2);	Select one X and one Y variable
BLOCK GOC=C3,DWR; X1=C1+273.15; X2=C1; Y=C1+C2*4.184;	or multiple X and one Y variable
BLOCK GOC=C4,MWAS; X=C1+273.15; Y1=C2*4.184; Y2=C3;	or one X and multiple Y variables
BLOCK GOC=C5,DWA; X1=C1; X2=C4; Y1=C2*4.184; Y2=C3;	or multiple XY pairs
BLOCKEND	
DRAWLINE	x,y x,y
TEXT	text or ~name (of a string, see below)
ATTRIBUTE	TOP, CENTER or BOTTOM
STRING	name text The text string may contain text formatting codes namely: ^S# to set font size, ^G for Greek font, ^F# to set font type, ^U# for positioning the text upwards, ^D# for positioning the text downwards, ^R#for positioning the text to the right, ^L# for positioning the text to the left, and finally ^N for printing without updating current position to the end of the character. These text formatting codes only work for soft fonts not hardcopy postscript fonts.
INCLUDE	filename
CLIP	ON or OFF

Keyword	Parameters
SYMBOLSIZE	rnumb
FUNCTION Y=203 (X); or X=203 (Y);	<start end steps GOC> The < > denotes an optional parameter.
PAINT	<code> <video> <mode> The <> denotes optional parameters. Paint the area enclosed by the current path in the current pattern. The current path starts at the last 'moveto' given and includes all subsequent 'draws'. Also see PCFUNCTION below. Default is <code>=0, <video>=NORMAL and <mode>=TRANSPARENT. To set a new current pattern supply any or all of the optional parameters. <code> is a single letter 0-9, A-Z or a-t (if <code>=t supply also a number in the range 0.00 - 1.00, e.g. PAINT t 0.25.) <video> is a string reading NORMAL or INVERSE. <mode> is a string reading TRANSPARENT or OPAQUE.
PCFUNCTION Y=203 (X); or X=203 (Y);	<start end steps GOC> The <> denotes an optional parameter. May be used to add a function to the current path.

Available Graphical Operation Codes (GOCs)

These are the available GOCs:

- `W`: World coordinates (* DEFAULT)
- `V`: Virtual coordinates
- `N`: Normalized plot box coordinates (NPC)
- `M`: Move to this XY (*)
- `D`: Draw to this XY
- `A`: XY is absolute values (*)
- `R`: XY are relative values
- `S`: Plot current symbol at XY
- `B`: Apply soft spines on the drawn curve (use only on BLOCK data)
- `S2`: Change current symbol to 2 and plot at XY
- `'`: Plot the following text at XY

State, Integral and Auxiliary Variables

In this section:

State Variables 130
Integral Variables 135
Auxiliary Variables 137

State Variables

Also see SET_DIAGRAM_AXIS and ENTER_SYMBOL in the DICTRA POST module.

State variables in the DICTRA POST module are similar to those defined in Thermo-Calc POLY-3 module. Examples of state variables are temperature, mole fraction, enthalpy, etc. In POLY-3 a general notation method based on character mnemonics is designed for a predefined set of state variables.

The numerical values of some state variables, e.g. activity, chemical potential, and the energetic extensive properties, are given relative to some reference state which has been defined in the thermodynamic database file. Sometimes you may have specified a reference state using SET_REFERENCE_STATE. To get numerical values relative to the user-defined reference state, append an R to the mnemonic names as defined.

Intensive Properties

Mnemonic	Description
T	temperature
P	pressure
AC(component)	activity
MU(component)	chemical potential

Extensive Properties

NORMALIZATION of extensive properties: For all extensive properties a suffix can be added to the mnemonic name to indicate a normalized extensive property. The following tables describe each mnemonic .

Extensive Property `Z at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z at each grid point.
ZM	Extensive property `Z per moles of atoms.

Mnemonic	Description
ZW	Extensive property `Z per mass (gram).
ZV	Extensive property `Z per volume (m^3).

Extensive Property `Z for a Phase at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z for the current amount of the phase.
ZM	Extensive property `Z per mole of atoms of the phase.
ZW	Extensive property `Z per mass (gram) of the phase.
ZV	Extensive property `Z per volume (m^3) of the phase.
ZF	Extensive property `Z per mole formula unit of the phase.

Energetic Extensive Properties



Suffixes M, W, V and F can be applied.

Mnemonic	Description
S	entropy
S(phase)	entropy of a phase
V	volume
V(phase)	volume of a phase
G	Gibbs energy
G(phase)	Gibbs energy of a phase

Mnemonic	Description
H	enthalpy
H(phase)	enthalpy of a phase
A	Helmholtz energy
A(phase)	Helmholtz energy of a phase

Amount of Components

Suffixes M, W and V can be applied.

Mnemonic	Description
N(component)	Number of moles of a component.
N(phase,component)	Number of moles of a component in a phase.
B(component)	Mass of a component.
B(phase,component)	Mass of a component in a phase.

Total Amount

Suffixes M, W and V can be applied.

Mnemonic	Description
N	Number of moles
B	Mass The legal combination BW is not very interesting as it will always be unity. BV is the density

Amount of a Phase

Suffixes M, W and V can be applied.

The normalizing properties are calculated at each grid point.

Mnemonic	Description
NP(phase)	Number of moles of a phase.
BP(phase)	Mass of a phase.
VP(phase)	Volume of a phase.
Y(phase,species#sublattice)	site fraction  This quantity is dependent upon the model chosen for the phase.

Constitution

 This quantity is dependent upon the model chosen for the phase.

Mnemonic	Description
Y(phase,species#sublattice)	site fraction

Integral Variables

An integral variable is a quantity that has been obtained by integration in space over the whole system or over a specific region. In a planar geometry values are given per unit area, in a cylindrical geometry they are given per unit length, and in a spherical geometry they are absolute values.

- SET_DIAGRAM_AXIS and ENTER_SYMBOL commands in the DICTRA POST module.

The variable mnemonics are constructed in the following way.

- The first letter is always I for INTEGRAL VARIABLE.
- The second letter specifies quantity.
- The third letter is OPTIONAL and specifies the normalizing quantity.

First and Second Letter

Class	Quantity	Description
I	N	for number of moles
I	W	for mass
I	V	for volume
I	U	for number of moles of volume-contributing elements
II	S	for entropy
II	H	for enthalpy
II	G	for Gibbs energy
II	A	for Helmholtz energy

Class I

Integral quantities of CLASS=I may take 0-3 arguments.

The arguments MUST be given in 'falling' order of significance.

1. Region name
2. Phase name
3. Component name

Class II

Integral quantities of CLASS=II may take 0-2 arguments.

The arguments MUST be given in 'falling' order of significance.

1. Region name
2. Phase name

Third Letter - Normalizing Quantity

Quantity	Description
N	for total number of moles in system
W	for total mass of system
V	for total volume of system
U	for total number of moles of volume-contributing elements in system

Examples

- IW(PEARLITE,BCC,CR) is the mass of CR in the BCC phase in region PEARLITE.
- IW(PEARLITE,BCC) is the mass of BCC phase in region PEARLITE. IW is the total mass in the system.
- IVV(Austenite) is the volume fraction of Austenite in a single cell calculation.
- IVV(2, Austenite) is the volume fraction of Austenite in Cell 2 for a multi cell calculation.

Auxiliary Variables

The following table lists auxiliary variables that are associated with both names and mnemonics.

- SET_DIAGRAM_AXIS and ENTER_SYMBOL in the DICTRA POST module.

Interface names are the same as the region names with the addition that you also have to specify if the interface is at the U(pper) or L(ower) end of the regions.

Name and Mnemonic Auxiliary Variables

Name	Mnemonic	Argument
ACTIVITY	AC(component)	component
DISTANCE		
FLUX	JV(component)	component
LAMELLAR-SPACING	LS(name)	region name
LAMELLAR-THICKNESS	LT(name)	phase name
MOLE-FRACTION	X(component)	component
MOLE-PERCENT		component
POSITION-OF-INTERFACE	POI(name,U/L)up*)	interface name
TEMPERATURE-KELVIN	T	
TEMPERATURE-CELSIUS	-	
U-FRACTION	UF(component)	component
VELOCITY-OF-INTERFACE	VOI(name,U/L)up*)	interface name
WEIGHT-FRACTION	W(component)	component
WEIGHT-PERCENT		component

Mnemonic Auxiliary Variables

There are also auxiliary variables that are only associated with a mnemonic.

Mnemonic	Description
GD	global distance
LD	local distance

Mnemonic	Description
M(phase,J)	mobility coefficient where J=diffusing specie
LOGM(phase,J)	^{10}log of the mobility coefficient
DT(phase,J)	tracer diffusion coefficient where J=diffusing specie
LOGDT(phase,J)	10log of the tracer diffusion coefficient
DC(phase,J,K,N)	chemical diffusion coefficient where K=gradient specie, and N=reference specie
LOGDC(phase,J,K,N)	^{10}log of chemical diffusion coefficient
DI(phase,J,K,N)	intrinsic diffusion coefficient
LOGDI(phase,J,K,N)	^{10}log of intrinsic diffusion coefficient
JV(phase and/or specie)	flux in volume fixed frame of reference
JL(phase and/or specie)	flux in lattice fixed frame of reference
QC(phase,J,K,N)	Q=R(ln (DC{T1}) - ln (DC{ T1+e}))/(1/(T1+e) - 1/ T1)
QT(phase,J)	Q=R(ln (DT{T1}) - ln (DT{T1+e}))/(1/(T1+e) - 1/ T1)
QI(phase,J,K,N)	Q=R(ln (DI{T1}) - ln (DI{T1+e}))/(1/(T1+e) - 1/T1)
FC(phase,J,K,N)	D0=exp(ln (DC{T1})+Q/R/ T1)
FT(phase,J)	D0=exp(ln (DT{T1})+Q/R/T1)
FI(phase,J,K,N)	D0=exp(ln (DI{T1})+Q/R/T1)

The Thermo-Calc Documentation Set

Thermo-Calc Version 2021b



About the Thermo-Calc Software

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The Thermo-Calc Software

The Thermo-Calc software is a sophisticated database and programming interface package used to perform thermodynamic calculations. It can calculate complex homogeneous and heterogeneous phase equilibria, and then plot the results as property diagrams and phase diagrams.

The Thermo-Calc software (also referred to as the *Thermo-Calc program* or *the software* to distinguish it from the company name) fully supports stoichiometric and non-ideal solution models and databases. These models and databases can be used to make calculations on a large variety of materials such as steels, alloys, slags, salts, ceramics, solders, polymers, subcritical aqueous solutions, supercritical electrolyte solutions, non-ideal gases and hydrothermal fluids or organic substances. The calculations take into account a wide range of temperature, pressure and compositions conditions.

About the Thermo-Calc Add-on Modules

The Thermo-Calc program also includes Add-on Modules as briefly described below and at the links to our website.

- The Diffusion Module (DICTRA) is used to simulate diffusion controlled transformations in multicomponent systems. You can find more on our website.
- The Precipitation Module (TC-PRISMA) is used to simulate diffusion controlled multi-particle precipitation process in multicomponent and multiphase alloy systems. You can find more on our website.
- The Process Metallurgy Module is used to set up calculations used in steel making and other metallurgical industries. You can find more on our website.

Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to Thermo-Calc. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulation calculations are both time- and space-dependent. The Diffusion Module (DICTRA) is available in both Graphical Mode (as the *Diffusion Calculator*) and Console Mode (as the *DICTRA module*).

The Diffusion Module (DICTRA), which is often just referred to as DICTRA, is ideally suited to solve diffusion simulations that include a moving boundary (*Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. Simulations are one-dimensional and three different geometries can be performed: planar, cylindrical, and spherical.

Examples of cases that have been simulated using the Diffusion Module (DICTRA) include:

- Microsegregation during solidification
- Homogenization of alloys
- Growth/dissolution of carbides, nitrides and intermetallic phases
- Coarsening of precipitate phases
- Interdiffusion in compounds, e.g. coating systems
- Austenite to ferrite transformations in steel
- Carburization, nitriding and carbonitriding of high-temperature alloys and steels
- Post weld heat treatment
- Sintering of cemented-carbides

Precipitation Module (TC-PRISMA)

The Precipitation Module, or TC-PRISMA, is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Precipitation Calculator*.

The Module treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multi-component and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach. It is a general computational tool for simulating kinetics of diffusion controlled multi-particle precipitation processes in multicomponent and multiphase alloy systems.

You can use the Precipitation Module for:

- Concurrent nucleation, growth/dissolution and coarsening of precipitates
- Temporal evolution of particle size distribution
- Average particle radius and number density
- Volume fraction and composition of precipitate
- Nucleation rate and coarsening rate
- Time-Temperature-Precipitation (TTP) diagrams
- Continuous-Cooling-Transformation (CCT) diagrams
- Estimation of multi-component interfacial energy
- Estimation of yield stress using the Yield Strength Property Model

Process Metallurgy Module



The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

The Process Metallurgy Module is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Process Metallurgy Calculator*. The Add-on Module is designed to model reactions that occur in metallurgical processes. Although primarily used in steelmaking and steel refining processes—such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy, and so forth—applications are not limited to steelmaking.

There are two main branches of calculations possible: **Equilibrium** and **Process simulation**. Equilibrium calculations do not consider any kinetics, the process simulation includes reaction kinetics.

In general, for both types, the main difference compared to using a standard Equilibrium Calculator is that it is easy to handle the different materials present in a metallurgical process. The materials used in the process can be pre-defined, saved and used for the equilibrium calculations. Metallic materials can be defined in element weight percent, oxide materials in weight percent of oxide components, the gas phase in volume percent of gas components and its amount can be defined in normal cubic meters, and so forth. In principle this can be done in a standard Equilibrium Calculator. However, it is much easier when using the Process Metallurgy Calculator as this is designed for this specific purpose.

When using the **Equilibrium** branch of calculations, both isothermal and adiabatic calculations are possible. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction, meaning that the temperature changes as a result of exothermal or endothermal reactions taking place.

For a **Process simulation** branch of calculation, the reaction kinetics of the process are considered. This is done by dividing the system into zones. Typically one would have one steel zone containing liquid metal and a slag zone containing liquid oxide (slag). The kinetic model assumes that only a fraction of the steel zone reacts with a fraction of the slag zone per time step. This reacting fraction of the whole system is termed the reaction zone (in literature it has become known as Effective Equilibrium Reaction Zone or EERZ).

You can use the Process Metallurgy Module to calculate the following:

- The equilibrium between custom-defined steels, slags, and gasses.
- The equilibrium between other metallic and non-metallic phases.
- Desulfurization, dephosphorization, and decarburization.
- Any partition coefficient, for example the partitioning of sulfur between the liquid steel and slag phase.
- Slag characteristics, such as slag basicity or sulfur capacity.
- The fraction of liquid and solid in the slag.
- The temperature change in an adiabatic process.
- Kinetics of the reaction between phases. Typically this is the reaction between a liquid metal and slag phase, but it could also be the reaction between a solid oxide and slag (simulation of refractory wear) or between a solid metal and liquid metal (simulation of dissolution of alloy), etc.

Graphical Mode vs Console Mode

There are two interfaces available in Thermo-Calc: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface. Thermo-Calc and the Diffusion Module (DICTRA) are available in both modes, and the Precipitation Module (TC-PRISMA) and Process Metallurgy Module are only available in Graphical Mode.

If you are a new user, Graphical Mode is a good way to learn how to work with Thermo-Calc. Depending on what you want to simulate, Console Mode can have more functionality but until you are comfortable with the concepts, it is recommended you start in Graphical Mode.



In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a Wizard available to guide you through the process of defining the project.

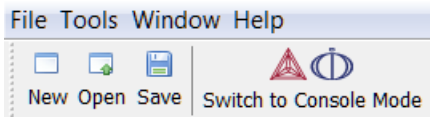


In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, ask you a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations and plotting the results.

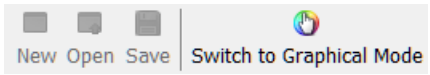
How to Switch Between Modes

The first time you open Thermo-Calc, it defaults to Graphical Mode. For any future instance it defaults to the last mode used.

Along the top of the GUI is the **GRAPHICAL MODE TOOLBAR** where you switch between modes.



In Console Mode, except for the **SWITCH TO GRAPHICAL MODE** button, the toolbar is not used.





See Menu, Toolbar and Keyboard Shortcuts for information about the **Tools**, **Window** and **Help** menus, which are available in both modes.

File Extensions

The file extensions are different based on the mode you are in (Graphical vs. Console). In Console Mode the extensions are also based on whether you are working with Thermo-Calc or the Diffusion Module (DICTRA).



In Graphical Mode, the Thermo-Calc project files have the extension *.`tcu`. This includes the examples for the add-on Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA).



In Console Mode, Thermo-Calc macro files have a *.`TCM` extension and the Diffusion Module (DICTRA) file extension is *.`DCM`. In addition to macro files in Console Mode the are also *Log* files and *Workspace* files, which also differ.

Modes Run Simultaneously

The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings. See Global Settings: Graphical and Console Mode Plotting.

Data Optimization and Thermodynamic / Kinetic Assessments



Although many calculations can be done in either mode, data optimization and thermodynamic or kinetic assessments are only available in Console Mode.

Graphical Mode Activities vs Console Mode Modules

- Graphical Mode: About the Activity Nodes
- Console Mode Modules

Although many calculations can be done in either Graphical Mode (GM) or Console Mode (CM), only data optimization and thermodynamic or kinetic assessments are available in Console Mode. Conversely, only the Property Model, Precipitation and Process Metallurgy Calculators are available in Graphical Mode.

Graphical Mode (GM) versus Console Mode (CM)

GM Activity	CM module (Short Name)	Primary Functions
Binary Calculator	BIN	Calculate binary phase diagrams. Access to specific databases designed for BIN, such as TCBIN, is required.
System Definer	DATA	Select appropriate databases, define chemical systems and retrieve the data required for calculations.
Diffusion Calculator	DICTRA	Run simulations of diffusion controlled transformations in Thermo-Calc using the Diffusion Module (DICTRA). An additional license is required for this feature.
–	DIC_PARROT	This is to do data optimization for the Diffusion Module (DICTRA). It allows you to assess experimental data and use such data to optimize calculations. An additional license is required for this feature.
–	ED_EXP	Part of the PARROT submodule, use it to edit experimental data points to make reliable optimizations.
This is the calculation engine	GIBBS or GES	Handles thermodynamic models and quantities. Generally you do not need to use this, but you can get information about models, and list, add or amend the thermodynamic parameters in use.
–	PARROT	Used for data optimization to assess experimental data and use the data to optimize calculations.
Precipitation Calculator	–	Set the conditions for, and perform, a precipitation calculation.
Property Model Calculator	–	Predict and optimize material properties based on their chemical composition and temperature. There are preconfigured **General Models** and **Steel Models** available.

GM Activity	CM module (Short Name)	Primary Functions
Equilibrium Calculator	POLY	Equilibrium calculation command module. Specify conditions and make calculations.
Plot Renderer	POST	This is a submodule to POLY and is for post-processing and plotting of calculation results. Modify property and phase diagrams, add labels, change the diagram colors and so forth.
Ternary Calculator	POTENTIAL	Calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes.
–	POURBAIX	Calculate and plot pH-Eh diagrams (Pourbaix diagrams) and property diagrams for heterogeneous interaction systems involving aqueous solutions.
Process Metallurgy Calculator	–	Use this to model reactions that occur in metallurgical processes. Although primarily used in steelmaking and steel refining processes (such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy and so forth), applications are not limited to steelmaking.
–	REACTOR	Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.
Scheil Calculator	SCHEIL	Simulate and plot Scheil-Gulliver solidification processes with no diffusion in the solid phases and with/without consideration of back diffusion of interstitial components (such as C, N, O, S).
–	SYS	In Console Mode, interact with the operating system and change environmental settings. Create and execute macro files.
–	TAB	Tabulate properties of chemical reactions and substances (stoichiometric or solution phases).
Ternary Calculator	TERN	Calculate ternary phase diagrams.

Graphical Mode vs Console Mode: Calculation Types

- The Calculation Types in Graphical Mode
- Calculations

When you are using Thermo-Calc and the Add-on Modules, you generally first set up a system, select the databases to use, and then define various parameters related to the simulation you want to conduct. Once this is set up you decide what calculation type to perform, choose a plot type (or a table for single equilibrium, for example) to use and then eventually get a result.

How Thermo-Calc handles the calculation behind the scenes is the same whether you use Graphical Mode or Console Mode. However, there are differences with the workflow and for historical reasons some calculation types are named differently based on whether you are in one mode or another. In addition, the plot types (diagrams) you choose to output the information are also different based on whether you are in Graphical or Console Mode. These plot types are often based on the type of calculation being done, where in some cases you can only do it in one mode and not the other. For example, precipitation calculations are only available with the Precipitation Calculator, which is only available in Graphical Mode, but you can do diffusion calculations in both Graphical and Console Mode.

Comparison of Calculation Types in Graphical Mode vs Console Mode

The table lists most of the calculation types that you will want to perform based on whether it is in Graphical Mode or Console Mode. The first column is primarily based on the calculation types you can select when working in Graphical Mode and when using the various calculators as indicated in the second column. The third column is the module or command in Console Mode that you would use to perform the same, or similar, type of calculation.

Calculation Type	Graphical	Console	Definition
Equilibrium calculations	Equilibrium Calculator	POLY3 module	An equilibrium defines the amount(s) and composition(s) of one or several phases that have the minimum Gibbs energy at a given temperature and pressure. A prerequisite for a successful equilibrium calculation is that the number of degrees of freedom according to Gibb's phase rule must be zero. This means that the right number of independent conditions must be set in order to successfully be able to calculate an equilibrium.

Calculation Type	Graphical	Console	Definition
Single equilibrium	Property Model Calculator (Equilibrium model) and Equilibrium Calculator	POLY3 module	To calculate a single equilibrium. The results from this calculation are displayed as follows: • Graphical Mode: In the Results window for a Table Renderer or in the Event Log window (for the Property Model Calculator) • Console Mode: With the LIST_ EQUILIBRIUM command.
Single (no axes)	Property Model Calculator and Process Metallurgy Calculator	POLY3 module	To calculate a single point. The results from this calculation are displayed as follows: • Graphical Mode: In the Results window for a Table Renderer or in the Event Log window. • Console Mode: With the LIST_ EQUILIBRIUM command.
One axis	Property Model Calculator, Equilibrium Calculator and Process Metallurgy Calculator	POLY3 module	To vary a quantity on the X-axis.
Property diagrams	One axis: available with Equilibrium Calculator or Property Model Calculator	POLY3 module, *STEP* command	A property diagram is calculated by stepping one of the conditions that were defined for the equilibrium calculation and plotting some other property against this variable. For example stepping through temperature and plotting equilibrium composition of a certain phase, or stepping through composition and plotting equilibrium phase fractions, and so forth.
Phase diagrams	Equilibrium Calculator, Binary Calculator, and Ternary Calculator	POLY3 module, *MAP* command, BINARY module, and TERNARY module	A phase diagram is mapped within a specific space constructed by two (or more) independent mapping variables. These are mostly temperature and composition, but can be many other, such as temperature and pressure, activity of oxygen and activity of sulfur, and so forth.
Scheil calculations	Scheil Calculator	Scheil module	Simulate a non-equilibrium transformation or partial-equilibrium transformation, also called a Scheil-Gulliver solidification.
Gibbs energy curves	Binary Calculator	BINARY module	To calculate at a constant temperature over the whole composition range.

Calculation Type	Graphical	Console	Definition
Activity curves	Binary Calculator	BINARY module	To calculate at a constant temperature over the whole composition range.
Phase fractions	Binary Calculator	BINARY module	To calculate as a function of temperature at a constant composition.
Isothermal section	Ternary Calculator	TERNARY module	To calculate the ternary system for the whole composition range at a constant temperature.
Monovariant lines	Ternary Calculator	TERNARY module	To calculate the variation of the liquid compositions with temperature.
Liquidus projection	Ternary Calculator	TERNARY module	The projection liquid surface and the monovariant lines are calculated over the given temperature range.
Potential diagrams	not available	Potential Diagram module and POLY3 module	A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. For example, use this for a metal-oxide/sulphide-gas interaction system to calculate a diagram based on a specific temperature and pressure .
T0 temperature simulations	not available	POLY3 module	The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition for a certain alloy composition.
Paraequilibrium	not available	POLY3 module	A paraequilibrium is a partial equilibrium where one interstitial component, such as carbon (C) and nitrogen (N), in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements).
Grid	Property Model Calculator, Equilibrium Calculator, and Process Metallurgy Calculator	not available	With the Equilibrium Calculator, it computes the equilibrium of each grid point in a two-dimensional grid. With the Property Model Calculator, it evaluates two axis variables of the selected quantities in the specified range and number of steps.
Min/Max	Property Model Calculator	not available	Evaluates the Property Model(s) for all variations of the selected quantities at the given limits.
Uncertainty	Property Model Calculator	not available	Evaluates the Property Model(s) where

Calculation Type	Graphical	Console	Definition
	and Process Metallurgy Calculator		the values of the quantities are sampled from Gaussian distributions.
Aqueous solutions, Pourbaix diagram	Equilibrium Calculator	Pourbaix Diagram module, POLY module	A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential).
Tabulation reaction	not available	TAB module	To tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction.
Diffusion simulation	Diffusion Calculator	DICTRA monitor	Detailed simulation of diffusion controlled reactions in multicomponent systems.
Isothermal	See below	POLY3, DICTRA monitor	Isothermal calculations in general can be done in all Console Mode modules, for example an Isothermal diffusion in DICTRA monitor and an isothermal calculation in POLY3 using the STEP command.
Isothermal and non-isothermal	Precipitation Calculator	See above	You can calculate nucleation, growth/dissolution and coarsening of particles size classes under these conditions: isothermic (precipitation simulation at constant temperature) or non-isothermic (precipitation simulation with user-defined temperature profile).
TTT and CCT	Precipitation Calculator	not available	The TTT (Time-Temperature-Transformation) and CCT (Continuous Cooling Transformation) diagram can be simulated for one or more particles.

About the File Types and Formats

The file formats (and the file extensions / suffixes) are based on whether you are working in Graphical or Console Mode, and in Console Mode, whether you are working with Thermo-Calc and/or the Diffusion Module (DICTRA).

Graphical Mode

In Graphical Mode you work with one file type, a *project* file, which has a `*.tcu` file extension. This is applicable to Thermo-Calc and the add-on Diffusion Module (DICTRA)Precipitation Module (TC-PRISMA) and Process Metallurgy Module.

Console Mode

In Thermo-Calc Console Mode there are file *types*—**macro** (including log files) and **workspace**—and *extensions* —`*.TCM`, `*.POLY3`, `*.GES5`, `*.PAR`, `*.POP`, and `*.EXP`.



A reminder that Linux and macOS are case sensitive; when applicable ensure you enter file extensions with capital letters.



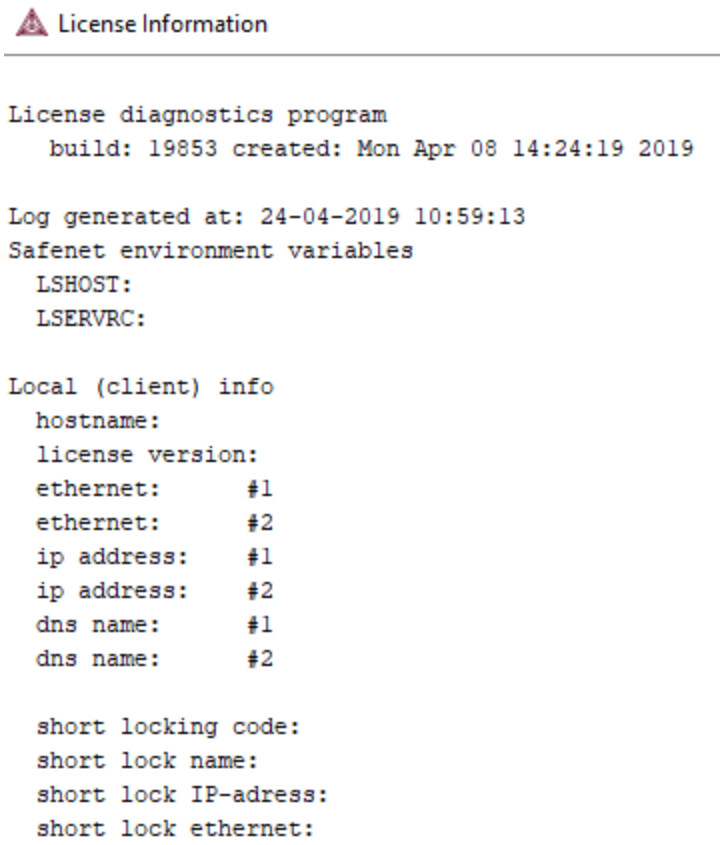
Workspace files are not currently available with GES6.

- Working with the Console Mode File Types

Displaying Thermo-Calc License Information

You can start (and install) the software without a valid Thermo-Calc license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.

This is an example of part of a License Information window for a network installation. It only shows the fields you would expect to see as the details are unique for each installation.



Network Licenses

For a *network* license, under each license type with instances checked out, there is a list of who checked out each license.



In Graphical Mode, an instance is checked out when an Equilibrium Calculator activity is created, and checked back in when that Equilibrium Calculator is removed. For the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Process Metallurgy Modules this also applies to the Diffusion Calculator and the Precipitation Calculator.



In Console Mode, an instance is checked out when you enter the POLY module and is checked back in when you exit the POLY module.

- The **Features** column is a list of the specific software, databases and API licenses purchases.
- The **Version** is an internal version number for the feature.
- The **number of licenses** column is how many instances of each license type available to be checked out simultaneously.
- The **in use** column shows how many license instances are checked out.

Console Mode License Restrictions

- If you start Thermo-Calc without a valid Thermo-Calc license you cannot leave the SYS module.
- If all the licenses are checked out for a network client installation of Thermo-Calc, you may not be able to enter the POLY or DICTRA modules until a license is available.
- To enter the DICTRA and the DIC_PARROT modules, you need a valid Diffusion Module (DICTRA) license key.
- If you enter and use either the DIC_PARROT module or the PARROT module, then you cannot enter the other module in the same session. You must close down Thermo-Calc and launch the program again to enter the other data optimization module.

Network Computer License Restriction

If you have a network computer installation of Thermo-Calc, then you may not be able to do any calculations even if you have access to a valid network license file. This is because others who are part of your network installation may have checked out all allowed instances of the software.

If you are running a network installation of Thermo-Calc, you can see how many instances of the client licenses are currently checked out and how many of them are left. You can also see which client computers have checked out the licenses.

About the Documentation and Examples

In this section:

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Examples, Manuals, and Materials Folders

There are several ways to access the examples, manuals (containing PDF documentation), and materials data folders.

Item	Main Menu	System Definer	From the Windows Start Menu	On your Computer	Website
Manuals (PDF documentation, DATAPLOT EXP files, TC-Python and TC-Toolbox for MATLAB® HTML help)	x	-	x	x	x
Software Development Kits (SDKs) (TC-Python, TC-Toolbox for MATLAB®, TQ-Interface, and TC-API)*	x	-	-	x	x
Examples (project and macro files)*	x	-	x	x	x
Materials	-	x	x	x	x
Property Models	-	-	-	x	-
Process Metallurgy Materials**	-	-	-	x	-

* The SDK folder is installed during installation and available when you have a license for the applicable SDK. There are also differences based on the API as to where examples are installed.

** The Process Metallurgy Module user-defined material compositions are saved from the Process Metallurgy Calculator and managed from the **Tools** → **Options** menu.

From the Main Menu

Once your Thermo-Calc software is installed you can open the Examples and PDF documentation (*Manuals*) from the main menu:

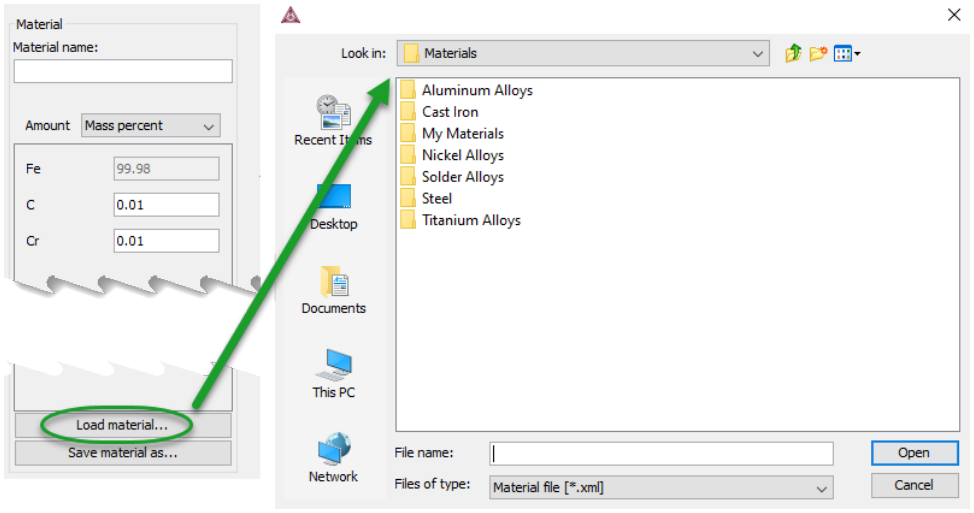
- To open the Manuals folder select **Help → Manuals Folder**. Note for Linux openSUSE users: This link is not functional. To access the folder, navigate to the default location based on your installation type
- To open the Examples based on whether you are in Console Mode or Graphical Mode, select **File → Examples Files** or **Help → Examples Files**.

From the System Definer (Materials Only)

When you are working with the System Definer you can open the default **Materials** folder included with your installation.

At the bottom of the window under **Material**, click **Load material** to navigate to a material file.

There is a separate folder for materials saved using the Process Metallurgy Calculator. See Installation Default Directory: Process Metallurgy Materials.



The default directory where these files are stored is based on operating system:

Operating System	Materials Installation Directory
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2021b\Materials`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2021b/Materials`
macOS	`/Users/Shared/Thermo-Calc/2021b/Materials`

Start Menu (Windows Only)

On Windows, once Thermo-Calc is installed, you can locate the Examples and Materials folders, plus all the Manuals. Go to **Start → All Programs** or **All Apps → Thermo-Calc** and search as needed. You can also uninstall from this menu and access all installed versions of Thermo-Calc.

On Your Computer (All Operating Systems)

The PDFs, example files and materials xml files are included with your installation in a folder location based on the operating system.

In the table, *<user>* stands for the username and *<version>* for the version of Thermo-Calc, for example 2021b.

Windows File Paths

User Type	Default Directory
Administrator	**Software** Program Files\Thermo-Calc\<*version*> **Examples, Manuals, Materials, Property Models, Process Metallurgy Materials and SDK folders:** Users\Documents\Thermo- Calc\<*version*>

macOS File Paths

User Type	Default Directory
Administrator (user name and password required)	**Examples, Manuals, Materials, Property Models, Process Metallurgy Materials and SDK folders:** /Users/Shared/Thermo-Calc/<*version*> To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.

Linux File Paths

User Type	Default Directory
Non root user	home/<*user*>/Thermo-Calc/<*version*>
Root user	usr/local/Thermo-Calc/<*version*>

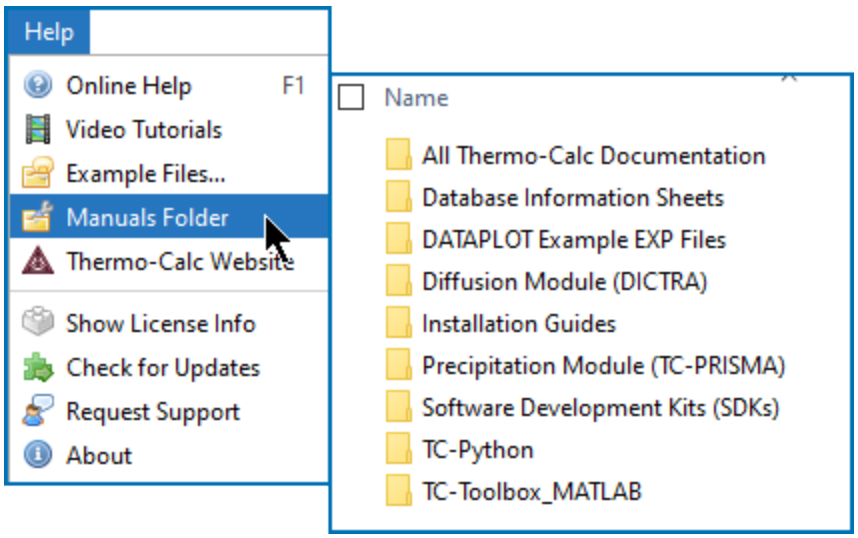
Website

Many resources are available from our website. On the Support > Documentation page you can download the current and archived PDF documentation and examples, or navigate to the TC-Python and TC-Toolbox for MATLAB® help and diagnostics tools. For current technical information and examples collections for the databases, you can access these by database starting on the Products > Databases page.

About the Manuals (Documentation) Folder

It is recommended you search the help (press F1 in Thermo-Calc) if you cannot find what you are looking for in a particular folder or PDF.

There is documentation available in PDF format from the **Manuals** folder as part of your installation. Except for two of the SDKs, this is the same information as that contained in the Thermo-Calc online help, just in a different format. The contents of each folder are described below.



A *Documentation Set* contains a variety of user guides packaged together in one PDF.

Process Metallurgy Module and Steel Model Library (Property Models): For these specialized products, all the content is contained in the *Thermo-Calc Documentation Set* or online help.

All Thermo-Calc Documentation

The *Thermo-Calc Documentation Set* is one large PDF that includes the information needed to work with the Thermo-Calc software. By having all content in one PDF it enables you to search the content just like you would when in the online help (with some exceptions). For example, this PDF does not include specific database or other specialized content that can require additional licenses.

The Thermo-Calc Documentation Set includes the following.

Thermo-Calc Installation Guides

Includes all installation instructions for all platforms and license types.

Graphical Mode User Guide

Includes details about all features and calculators included with Graphical Mode. For example, it includes details about calculators available with add-on products such as the Diffusion Calculator, Precipitation Calculator, Process Metallurgy Calculator, and all the Steel Model Library Property Model content. For the Add-on Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), additional information is included in the separate documentation.

Console Mode User Guide

Includes details about the functionality and features available with the Console Mode version of Thermo-Calc.

For example, the following is only in Console Mode and the associated documentation is included in the respective documentation.

- The PARROT module optimization content is described in the *Data Optimization User Guide*.
- If you develop your own custom databases, this is described in the *Database Manager User Guide*. There is some other generally related documentation that is found under General Reference.
- If you use the old DATAPLOT functionality for plotting, this is included in the *DATAPLOT User Guide*.
- The POURBAIX module is only in Console Mode and there is the *Pourbaix Diagrams*

Educational Material guide included.

- A separate *Thermo-Calc Console Mode Example Macros* PDF is available in the folder but NOT included in the Documentation Set due to its file size and page length.

Thermo-Calc General Reference

This is content that spans some of the general topics applicable to multiple applications within Thermo-Calc, i.e. it might be for both Console Mode and Graphical Mode, or needed for a specific database calculation in Thermo-Calc (i.e. model information, variables, and functions for thermophysical properties).

- **Parameters, Functions, and Variables**: Information applicable to both Console Mode and Graphical Mode with respect to understanding the format these are to be written in for Thermo-Calc to use the parameter, function, or variable. However, many of the sections are specific to Console Mode where the explicit use of these terms is more often used.
- **Thermophysical Properties Data**: This includes the model descriptions and data parameters you would need in combination with a database that has the relevant thermophysical property.
- **Database Files and Database Checker**: Information about the database initialization file, differences between Thermo-Calc encrypted and user-defined unencrypted databases, about cached database files, and more. Some content is more specific to those developing their own databases, other information is intended for advanced users, for example, the Database Checker information is a supplement to the *Database Manager User Guide*.
- **Global Settings**: In the **Options** window (select **Tools → Options**) you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

Database Information Sheets

The *Technical Info* content available as a PDF is also included in the online help system and contains details such as the elements, systems, phases, and properties available with a specific database. It includes the revision history for the database.



Starting with Thermo-Calc 2020b, databases are transitioning from the *Extended Info* PDF, which can include examples, to individual *Examples Collections*. The *Examples Collections* are only available on the website or in the help.

All *Technical Info* and *Examples Collection* PDFs for the current version of the database are available for download from the Thermo-Calc website.

DATAPLOT Example EXP Files

The examples are available as supplementary information as described in the *DATAPLOT User Guide*, which you can find in either the online help, *Thermo-Calc Documentation Set* or *Diffusion Module (DICTRA) Documentation Set*.

Diffusion Module (DICTRA)

The *Diffusion Module Documentation Set* is one large PDF that includes the information needed to work with the Add-on Diffusion Module (DICTRA) and Thermo-Calc software in Graphical Mode and Console Mode. By having all content in one PDF it enables you to search the content just like you would when in the online help (with some exceptions). For example, this PDF does not include specific database or other specialized content that can require additional licenses.

The Documentation Set includes:

- All the content available in the *Thermo-Calc Documentation Set* and described above.
- Diffusion Module (DICTRA) *Quick Start Guide - Graphical Mode* and *Quick Start Guide -Console Mode*.
- *Diffusion Module (DICTRA) Command Reference* (for Console Mode only)

Also available separately in this folder:

- *Diffusion Module Quick Guide - Console Mode*
- *Diffusion Module Quick Guide - Graphical Mode*
- The *Diffusion Module (DICTRA) Console Mode Example Macros* PDF is available in the folder but NOT included in the Documentation Set due to its file size and page length.

Installation Guides

Includes the *Quick Install* guides for Standalone (SUNLL) Windows and macOS systems, instructions for TC-Python and TC-Toolbox for MATLAB®, with the full installation instructions for all platforms and license types.



For convenience, the *TC-Python Installation Guide* is also included as a separate PDF in this folder.

Precipitation Module (TC-PRISMA)

There is a User Guide in this folder, which includes examples, Precipitation Calculator settings, references, and details about the theoretical models and numerical methods. Use the *Thermo-Calc Documentation Set* or online help for all other content.

Software Development Kits (SDKs)



Separate TC-Python and TC-Toolbox for MATLAB® HTML documentation is stored in its own folder and each available from our website. This folder has the PDF version of this content.

- **TC-Python API Programmer Guide**: This guide is the PDF format of the HTML help described below.
- **TQ-Interface Programmer Guide**
- **TC Toolbox for MATLAB® Programmer Guide**: This guide is the PDF format of the HTML help described below and only for the new *TC-Toolbox*.
- **TC-API Programmer Guide**: This is the Thermo-Calc API. Note that TC-Python is a more robust alternative to this API and is recommended instead.

TC-Python

This folder contains the TC-Python HTML files. Double-click `Index.html` file to open it. This help is also available on our website. TC-Python includes details about working with custom property models (the Property Model Framework).

TC Toolbox_MATLAB

This folder contains the TC Toolbox for MATLAB® HTML files. Double-click `Index.html` file to open it. This help is also available via our website and is only for the new version of TC-Toolbox.

About the Examples

To learn more about how to use the software you can open and run the example projects (Graphical Mode) and macro files (Console Mode).

Graphical Mode Examples

Graphical Mode examples are available for Thermo-Calc and the Add-on Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), and Process Metallurgy Module. There are also examples for the Property Models, including the Steel Model Library and more. These are in the format of project files (*.tcu).

Console Mode Examples

Console Mode examples are available for Thermo-Calc and the Diffusion Module (DICTRA). The *macro* files are in the format of *.TCM and *.DCM, respectively.



There are other file types when you are working in Console Mode. Search the Help for *About the File Formats* or *About the DICTRA File Formats*.

Watch the Video Tutorials



Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.

Examples by Product

Thermo-Calc Examples

A description of the Thermo-Calc examples, and how to access them, is based on whether you are using Graphical Mode or Console Mode.



Graphical Mode Examples



Thermo-Calc Console Mode Examples

Diffusion Module (DICTRA) Examples

A description of Diffusion Module (DICTRA) examples, which are available for both Graphical Mode and Console Mode, is included in both the Thermo-Calc and Diffusion Module (DICTRA) documentation.



For Graphical Mode, see Diffusion Module (DICTRA) Graphical Mode Examples

For Console Mode, search the help or go to the Diffusion Module (DICTRA) documentation set.



All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

Precipitation Module (TC-PRISMA)

A description of examples using the Precipitation Calculator, which is only available in Graphical Mode, is included in both the Thermo-Calc and Precipitation Module (TC-PRISMA) documentation.

Precipitation Module (TC-PRISMA) Graphical Mode Examples

Process Metallurgy Module Examples

A description of examples using the Process Metallurgy Calculator, which is only available in Graphical Mode, is included in the Thermo-Calc documentation.

Process Metallurgy Module Examples Collection

Property Models and Steel Model Library Examples

A description of examples using the Property Model Calculator, which is only available in Graphical Mode, is included in the Thermo-Calc documentation. These examples include both General and the Steel Model Library models.

Thermo-Calc General Property Model Examples Collection

TC-Python Examples

There are examples for TC-Python available after installing the SDK. A brief description of the TC-Python SDK examples, and how to access these, is available in the Help.

TQ-Interface Examples

There are examples for the TQ-Interface available. You can also find information by searching the online help.

TC-Toolbox for MATLAB® Examples

There are examples for TC-Toolbox for MATLAB® available in MATLAB® after installing the SDK. See Installation Default Directory: TC-Toolbox and the Examples to learn where these are located.

Help Resources

'Online' Help: No Internet Required

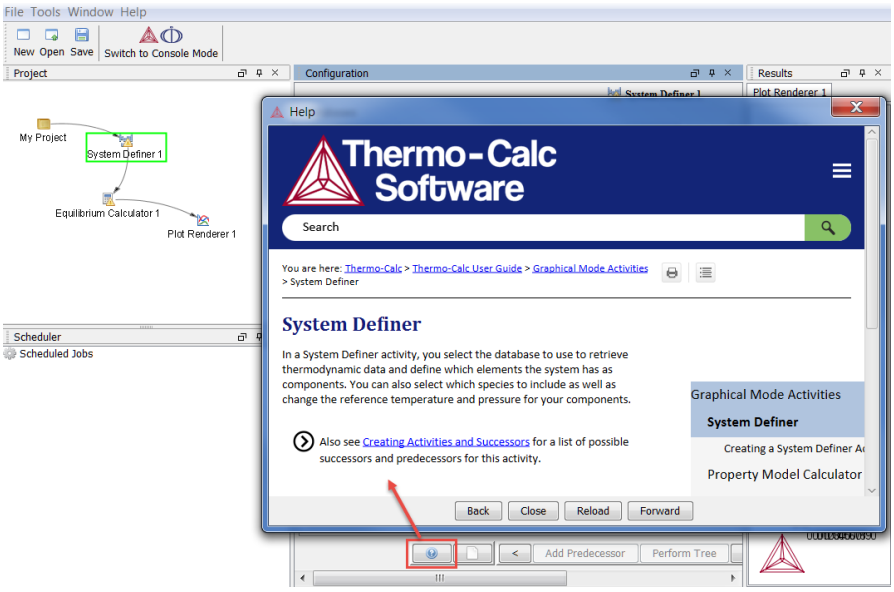
To access online help in a browser, open Thermo-Calc and press <F1> on the keyboard, or select **Help → Online Help**.

The content opens in a browser but uses local content so you don't need an Internet connection except for links to external websites.

Context Help (Graphical Mode Only)

When you are in Graphical Mode, you can access feature help (also called *topic-sensitive* or *context help*) for the activity nodes in the tree.

1. In the **Project** window, click a node. For example, **System Definer**.
2. In the lower left corner of the **Configuration** window, click the help button .
3. The **Help** window opens to the relevant topic.



The window that opens has the same content as the help you access in the browser. There are these extra navigation buttons in this view.

4. Use the buttons on the bottom of the window, 

, to navigate **Back** and **Forward** (these are only active once you have started using the help to load pages and create a history), to **Close** the window, and **Reload** the original content.

Console Mode Help



Console Mode is for Thermo-Calc and the Diffusion Module (DICTRA).

In Console Mode at the command line prompt, you can access help in these ways:

- For a list of all the available commands in the current module, at the prompt type a question mark (`?`) and press <Enter>.
- For a description of a specific command, type `Help` followed by the name of the command. You can only get online help about a command related to the current module you are in.
- For general system information type `Information`. Specify the subject or type `?` and the available subjects are listed. This subject list is specific to the current module.

Typographical Conventions

The following typographical conventions are used throughout the documentation, both online and in the PDF documents.

Text

Convention	Definition
Forward arrow symbol →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **Tools → Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **Tools→Options**, or to click **Save**.
Italic font	An *italic* font in the body of the text indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	For features in Thermo-Calc that use Console Mode (i.e. the command line), this font and all capital letters indicates that this is a Console Mode COMMAND. Examples of how you can use a command are written with code font. For example: Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`).
HELP	Text in blue and underline and a page number is a link to another topic in the current or referenced guide. Command names are often also topics. Clicking the link takes you to more detail about a particular command or subject in the PDF or documentation set.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return) or to use a series of keys such as <Ctrl + S>.
`code` and **`code bold`**	A `code` font shows a programming code or code example. The **`code bold`** font highlights the entry. It is also used for file names or paths to help distinguish it from other text. e.g. • For Windows users, the documents, materials, examples and other folders that sometimes require additional licenses are installed in C:\Users\Public\Public Documents\Thermo-Calc\<*version*>."
click vs press	In general, you *click* with the mouse to perform an action on the screen (e.g. click **Save**) and you *press* keys on a keyboard to enter a set of commands (e.g. press Ctrl+S).  When working in Console Mode, you can use keyboard shortcuts. Sometimes a window opens where you have the option to **Save**, **Cancel** or **Open** a file, for example. In these cases the instructions might say *click* Save, whereas you would need to *press* the applicable keys to perform the action.

Icons

Convention	Definition
Important	 Provides important information. It is recommended that you read the text or follow the link.
Note	 The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Also see	 Go to the link or guide to see more general information about the topic being discussed. Usually includes both text and a link.  The small blue arrow is used when there is one (sometimes two) cross reference and no text describing the link. Often used in settings pages to link you to accompanying theory or extra detail.
Tip	 This is general information that can be of use but is not required knowledge.
Examples	 Go to the example collection to learn more.
Console Mode	 This note relates specifically to something in Console Mode.
Video	 Indicates there is a video tutorial on our website, usually in relation to an example.
Graphical Mode	 This note relates specifically to something in Graphical Mode.
Diffusion Module (DICTRA)	 This indicates that the information relates to the add-on Diffusion Module (DICTRA).
Precipitation Module (TC-PRISMA)	 This indicates that the information relates to the add-on Precipitation Module (TC-PRISMA).

Convention	Definition
Process Metallurgy Module	 This indicates that the information relates to the add-on Process Metallurgy Module.

Installation Guide

Windows®, macOS®, and Linux Operating Systems

Thermo-Calc Version 2021b

Including the TC-Python and TC-Toolbox for MATLAB® Installation Guides



Installing Thermo-Calc

In this section:

Key to Using this Guide 3
Installation Terminology 5
About the Thermo-Calc Components Being Installed 7
System Requirements 9
Platforms Tested and SDK Availability 10

Key to Using this Guide

This guide is available in PDF format: (1) On the website or (2) when in Thermo-Calc go to **Help → Manuals Folder → Installation**.

This installation guide is for all Thermo-Calc installations running on Windows, macOS, or Linux operating systems. It is also applicable to previously installed versions of Thermo-Calc (the new version is installed next to the old version).

This guide includes information about:

- The types of licenses and installations available.
- Installing the Thermo-Calc software and its components on standalone computers, servers, and client computers.
- Installing the license management software for network installations.
- Retrieving and installing license files.
- Details about the specific instructions needed to install two of the SDKs, *TC-Python* and *TC-Toolbox for MATLAB®*.
- Troubleshooting to solve common installation problems.

Icons in this Guide

Name	Description
Information	Provides important information and indicates that more detail is located in the linked or named topic.
Note	The information can be of use to you. It is recommended that you read the text or follow the link.
Operating system	The operating system is indicated when the information is specific to a *Windows*, *macOS*, or *Linux* operating system.
License file	The Thermo-Calc license file, which contains the license keys and is installed on either a standalone computer or a network server.

Name	Description
 Thermo-Calc	The Thermo-Calc software and its components (including databases and SDKs) to be installed.

Typographical Conventions

Convention	Definition
Forward arrow →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **Tools → Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **Tools → Options**, or to click **Save**.
Italic font	An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
`code` and **`code bold`**	A `code` font indicates you are to make a keyboard entry. It also shows a programming code or code examples. The **`code bold`** font highlights the entry.

Installation Terminology

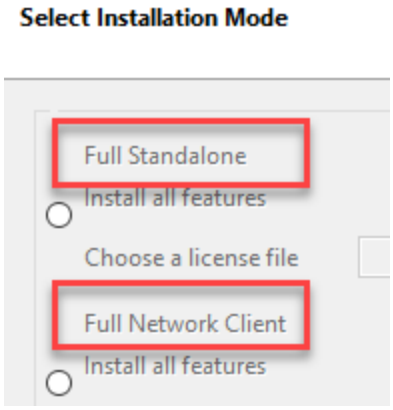
Term	Definition
client	A computer without a license file of its own but connected through the network to a computer with the license information. The client receives a license token from the computer where the license management software is installed.
consolidated network	A type of network installation where the Thermo-Calc software and a Thermo-Calc licensing software are installed on a single server computer. This allows all computers in the network to access both the software and a license on the server via a client installation.
distributed network	A type of network installation where the Thermo-Calc software is installed on one server computer in a network and the Thermo-Calc licensing software is installed on a different computer. After a thin client installation, all computers in the network can access both the software and the network license key via the server.
host ID	The MAC address on the computer that a license is locked to.
legacy TC-Toolbox for MATLAB®	The old version of the TC-Toolbox for MATLAB® SDK, which is replaced by TC-Toolbox. This API is supported until Thermo-Calc version 2023a.
license file	The file (called *lservrc*) that contains all the purchased license keys. It is issued by Thermo-Calc Software, usually by email.
license key	The information contained in the license file that represents the products purchased and which is then authorised for installation.
license management software (see Sentinel RMS License Software)	The Thermo-Calc license management software. When working in Windows it is called *License Manager* (full name is Sentinel RMS License Manager by SafeNet) and on Linux it is called *License Server* (full name is Sentinel License Sever by Safenet).
license server	The use of the term *license server* (lower case letters) is reserved for use for scripts and option files (for example, in an Unattended Network Client Installations). For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the license management program. See *Sentinel RMS Software* below.
Network License (NWL)	The license type used with the licensing software. The NWL can only be used on one specific computer that hosts the licensing software. This restricts license usage to a certain subnet or subnets. The software may be used on the number of sites you have paid for and by the number of persons you have paid for on any number of network connected computers
Sentinel RMS License Software	The Thermo-Calc license management software that supplies the client computers in your network with license tokens when it runs the Thermo-Calc software. This is available for both Windows (called the License Manager) and Linux (called the License Server, but not to be confused with *license server* in lower case letters reserved for scripts).

Term	Definition
Single-User-Node Locked-License (SUNLL)	A unique license file for one designated computer at one designated site. It cannot be copied or moved outside the site. If the software is installed on a portable computer, it can be temporarily used off-site. The license can be used without network access (to the License Server).
standalone computer	A computer which uses a SUNLL license type.
TC-Toolbox	The short name for the current version of the TC-Toolbox for MATLAB® SDK. This replaces the legacy version.
thin client	An installation where the software is installed on a file server but is run from a client computer. The licensing software may be installed on the file server (consolidated network installation) or on a different computer (distributed network installation).
XQuartz	An open-source X Windows System, which is required to run Thermo-Calc on a Mac.

About the Thermo-Calc Components Being Installed

What is Installed with a Full Standalone or Full Network Client Option?

At the start of the installation process, the following components are installed when you choose either the **Full Standalone** or **Full Network Client** options. If you want to exclude a component (perhaps one of the SDKs), then you would use the **Custom** option.



A full installation means that all listed feature components are installed but the availability of the individual components is based on the license you have. This is also applicable to the databases and software development kits (SDKs).

Thermo-Calc

The Thermo-Calc software includes several add-on features and capabilities that are packaged with the software and included with a full standalone or network client installation. For example, there are the specialized add-on products Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), and Process Metallurgy Module as well as the Steel Model Library. For most of these specialized features, demonstration (*demo*) versions and/or examples are available for all users but advanced features are only available with a license.

Databases

All the latest databases are installed. As with the software features, availability of a specific database in the software itself is based on license. However, several demonstration (*demo*) databases are included and available to all users.

Software Development Kits (SDKs)

When the **Full Standalone** or **Full Network Client** option is chosen, it also installs the software development kits (SDKs) (e.g. TC-Python, TQ-Interface, TC-Toolbox for MATLAB®, etc.).

TC-PYTHON

The TC-Python program is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required to complete the installation as described in the *TC-Python Installation Guide*.

TC-TOOLBOX FOR MATLAB®

If a MATLAB® installation on your computer is found during this installation process, the new TC-Toolbox for MATLAB® (available only for Windows) is automatically installed. However, there are different options based on the version (legacy or new) being installed as described in the *TC-Toolbox for MATLAB Installation Guide®*.

What Does the Custom Option Allow Me to Do During an Installation?

During the installation process, there is some flexibility to choose what to include or exclude with the installation by choosing the **Custom** option. This is primarily to the level of being able to choose the SDKs or to exclude all databases or Thermo-Calc itself. That is, you cannot choose specific Thermo-Calc features or databases as these are controlled by the license and not the installation procedure.

System Requirements

About the Thermo-Calc Components Being Installed

General

A full list of system requirements and program availability is found on the Thermo-Calc website. You can also see the roadmap for platform support to use for planning purposes.

Network Client Installations: Sentinel RMS License Software

Network client installations using the Sentinel RMS license management software require the use of the most recent version, 9.7.

For details of the system requirements to install Sentinel RMS, see Windows: About Installing the License Manager and Linux: About Installing the License Server.

For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

Platforms Tested and SDK Availability

A full list of system requirements and program availability is found on the Thermo-Calc website. You can also see the roadmap for platform support to use for planning purposes.

Platforms Tested

Thermo-Calc and its components are tested on these platforms for Thermo-Calc 2021b:

Windows	macOS	Linux[1, 2]
Windows 10 64-bit	• macOS X Big Sur 11 • macOS X Catalina 10.15	• Ubuntu 20.04 (Focal Fossa) • CentOS 7.8 • OpenSUSE Leap 15.1

[1] Thermo-Calc Software cannot guarantee full functionality if the software is installed on other Linux distributions.

[2] If you are installing on CentOS 7, it is recommended you install gtk2 before you run the installation script.

SDK Availability by Platform

The software development kits (SDKs) are available as follows for the indicated platforms:

SDK	Windows	macOS	Linux
TC-Python	x	x	x
TQ-Interface	x	not available	x
TC-Toolbox for MATLAB®	x	not available	not available
TC-API	x	not available	x

License and Installation Types

In this section:

License and Installation Types 12
About License Keys and Files 13
Standalone Installations (SUNLL) 14
Multi-User Network Installations (NWL) 15

License and Installation Types

Installation procedures are based on the license type, the installation type, and the operating system.

- Visit our website for more information about Licensing Options.

For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

License type	Installation Type	Windows	macOS	Linux
SUNLL	Standalone	Yes	Yes	Yes
NWL	Consolidated network	Yes	No	Yes
	Distributed network	Yes	No	Yes
	License installations on a server network	Yes	Yes	Yes

Sentinel RMS License Management Software: Use Current Version

The most recent version (9.7) of the Sentinel RMS License Manager (Windows) and License Server (Linux) is included with the network license Thermo-Calc software download.

However, due to security issues reported by the vendor, it is important that previous network license installations of the Sentinel RMS are upgraded to this version number.

For more information for your operating system, see Windows: About Installing the License Manager and Linux: About Installing the License Server

About License Keys and Files

To run Thermo-Calc and its components you need a valid license key for each product. The license keys are included in the license file emailed to you by Thermo-Calc Software.

You can copy the license file to the applicable computer(s) before or after installing the software—the license file itself is not required during the installation process. However, it is required to make calculations in Thermo-Calc.

- Request a License File from Thermo-Calc Software

Standalone Installations (SUNLL)

The standalone installation is used with the Single-User Node-Locked License (SUNLL). The Thermo-Calc software and a Thermo-Calc license file are installed on a standalone computer. You can do a full (all operating systems) or a custom installation (Windows and Linux only).



- To get started, go to First Steps of Installation and then Standalone Installations.

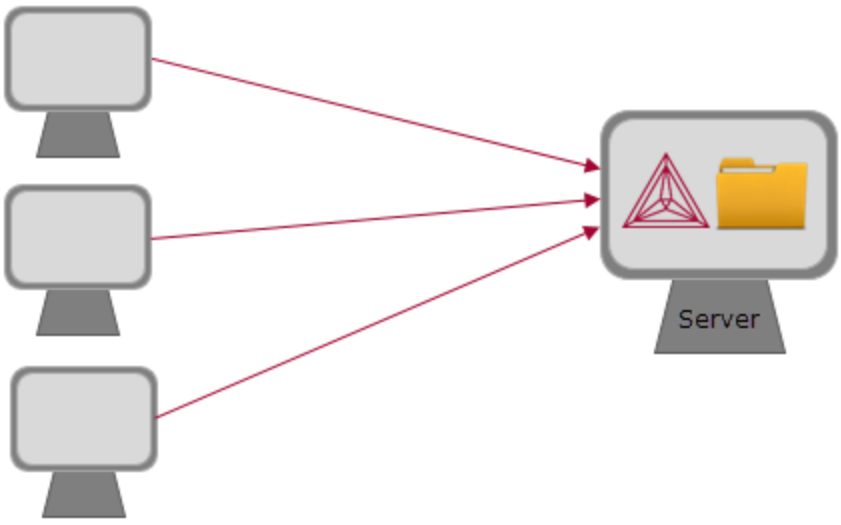
Multi-User Network Installations (NWL)

There are different types of multi-user network installations: consolidated, distributed, and where the licensing software is installed on a computer network. There is also a subtype of installation called thin client, which is a step done with the consolidated and distributed network installations.

Thin client installations: A thin client installation is where the Thermo-Calc software is installed on a computer server but is run from a client computer. The licensing software can be installed on the computer server (a consolidated network) or on a different computer (a distributed network). This type of installation is available for Windows and Linux operating systems. The client computer must have the Thermo-Calc software installed. This type of installation mainly sets environmental variables and paths on the client computer.

Consolidated Network Installations

The consolidated network installation is used with a Network License (NWL) and it is available for Windows and Linux operating systems.

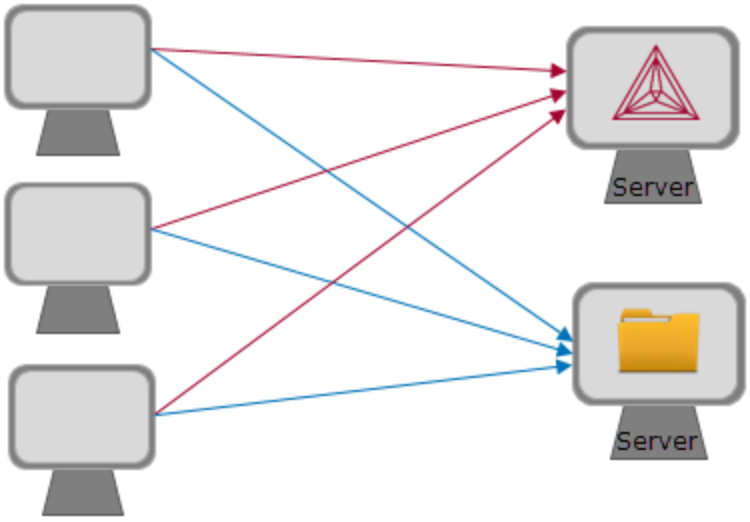


The Thermo-Calc software and the license management program are installed on the same server where the license file is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the same computer server.

- To get started, go to First Steps of Installation and then Network Client Installations.

Distributed Network Installations

The distributed network installation is used with a Network License (NWL) and is available for Windows and Linux operating systems.

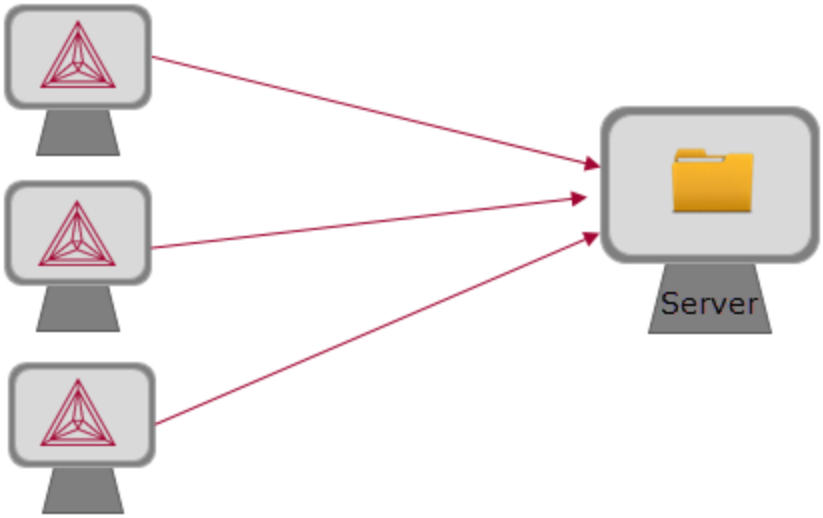


The Thermo-Calc software is installed on one computer server in a network and the licensing software is installed on a different computer server where the license file is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the two computer servers.

- To get started, go to First Steps of Installation and then Network Client Installations.

License Installations on a Server Network

When a license file is installed on a server network, it is used with a Network License (NWL). It is available for all platforms. However, for macOS the server containing the licensing software must be set up on Windows or Linux.



The licensing software is installed on a computer server where the license file is also copied. The Thermo-Calc software is installed on every computer in the network that needs it.

- To get started, go to First Steps of Installation and then Network Client Installations.

Preparing for Installation

In this section:

First Steps of Installation 19

Installation Default Directories and the License File 20

Installation Default Directory: Windows 22

Installation Default Directory: macOS 23

Installation Default Directory: Linux 24

Installation Default Directory: Databases, Database Checker, and TDB Editor 25

Installation Default Directory: Materials 27

Installation Default Directory: Process Metallurgy Materials 28

Installation Default Directory: Custom Property Models 29

Installation Default Directory: TC-Toolbox and the Examples 30

Subnet Information for Network Licenses 31

macOS Installation Notes 32

Linux Installation Notes 33

First Steps of Installation

This section reviews some of the things you need to do before installing the Thermo-Calc software.

- Learn about the different default directories where the software and license files are installed.
- For network installations, collect subnet information.
- Make sure the person installing the software has administrator rights for Windows and macOS.
- For macOS, install XQuartz and make sure the security preferences are set correctly.
- For a Linux Cent OS 7 installation, also install gtk2 before you run the installation script.

```
yum install gtk2
```



Should I get my license file before or after software installation? The Thermo-Calc license file itself is not required during the installation process. However, it is required to make calculations in Thermo-Calc. The license file has details about your computer(s) that in some cases cannot be determined accurately until *after* installation (especially for a network installation). For most users it is recommended you request the file before you start installing.

Installation Default Directories and the License File

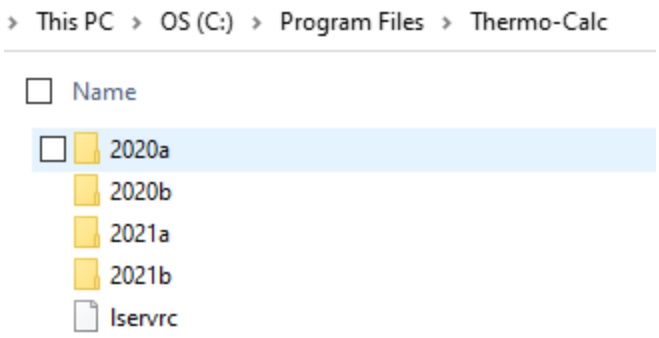
The default directories where the software and its components are installed, including where the license file is stored, vary by platform and user type.

If you want to select specific components to install or if you want to install the software in a non-default installation directory, then do a **custom** installation (Windows and Linux only). In the table, *<user>* stands for the user name and *<version>* for the version of Thermo-Calc, for example 2021b.

License File Installation Location for All Operating Systems

The Thermo-Calc license file is installed outside of the installation program folder. If you have more than one version of Thermo-Calc installed then there are additional folders by version number with only one license file.

For macOS the license file is put in `/Users/Shared/Thermo-Calc`. The example below is for a Standalone Windows installation.



See the following for more information:

- Installation Default Directory: Windows
- Installation Default Directory: macOS
- Installation Default Directory: Linux
- Installation Default Directory: Databases, Database Checker, and TDB Editor
- Installation Default Directory: Materials
- Installation Default Directory: Process Metallurgy Materials

- Installation Default Directory: Custom Property Models
- Installation Default Directory: TC-Python
- Installation Default Directory: TC-Toolbox and the Examples

Installation Default Directory: Windows

Administrative rights are required to install and uninstall Thermo-Calc.

Windows User Type	Default Directory

Administrator	The Thermo-Calc program is installed here:
	`Program Files\Thermo-Calc\<version>`
	The default folders where documents, materials files, examples, and other folders that sometimes require additional licenses are installed under **Public Documents** for ALL USERS.
	For a local user these files are copied to the user's **Documents** folder where this local copy is associated to the user login. The **Public Documents** folder always contains the original set of contents as per the installation.
	`C:\Users\Public\Public Documents\Thermo-Calc\<version>`
	After installing Thermo-Calc, and when you first open the program, the set of folders is copied from the source Public Documents location into a user Documents folder:
	`C:\Users\<user>\Documents\Thermo-Calc\<version>`
	It is recommended that you work with the files that are copied to the *user* folder.

Server network	License software installations on a server network (the License Manager software) `C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS License Manager\WinNT\`

Installation Default Directory: macOS

macOS User Type	Default Directory

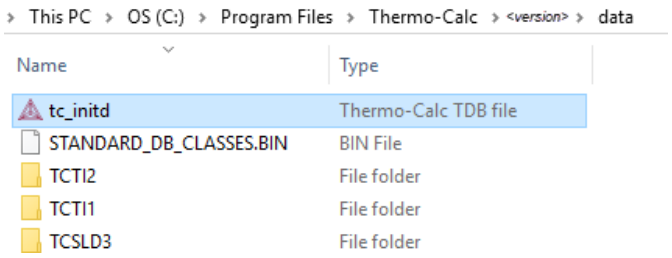
Administrator (user name and password required)	The Thermo-Calc program is installed in the **Applications** folder:
	`Thermo-Calc-<version>.app and uninstall-Thermo-Calc-<version>.app`
	The documents, materials, examples, and other folders that sometimes require additional licenses are installed here:
	`/Users/Shared/Thermo-Calc/<version>`
	To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.

Installation Default Directory: Linux

Linux User Type	Default Directory
Non root user	The Thermo-Calc program including the documents, materials, examples, and other folders that sometimes require additional licenses are installed here: `/home/<user>/Thermo-Calc/<version>`
Root user	The Thermo-Calc program including the documents, materials, examples, and other folders that sometimes require additional licenses are installed here: `/opt/Thermo-Calc/<version>`
License software installations on a server network (the License Server software)	If you are doing a network installation then these files are available as a tar-file from the Thermo-Calc website. In the downloaded tar-file, there is a **restart_lserv** script file, which can be used as a template for creating a script that starts up the License Server.

Installation Default Directory: Databases, Database Checker, and TDB Editor

The standard Thermo-Calc databases and the database initialization file `tc_initd.tdb` are located in a subfolder to the Thermo-Calc installation. For example, in a Windows Standalone installation, you can find these in a folder called **data** where the file path is *C:\Program Files\Thermo-Calc\<version>\data*.



Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

Thermo-Calc accepts some deviations from these syntax rules. Although warnings can be ignored, errors must be corrected.

For example, a warning is reported if an abbreviated phase name is found and phase name abbreviations are accepted by Thermo-Calc and its Add-on Modules. However, reported errors must be corrected in the TDB file before the database can be loaded by the application.

With respect to using this tool, the executable `DatabaseChecker` file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu in Thermo-Calc.

TDB Editor

The TDB Editor is an editing tool for those who develop their own custom databases for use with Thermo-Calc or other applications. The tool speeds up the database editing process by providing immediate feedback through syntax coloring, syntax checking, and by allowing formatting and easy navigation to items of interest in the TDB file.

During installation, the `tdb-language-support.vsix` file is installed in the Thermo-Calc home directory.



In order to access the most-up-to-date version of the VSCode plugin, it must be updated every time a *new* version of Thermo-Calc is installed.

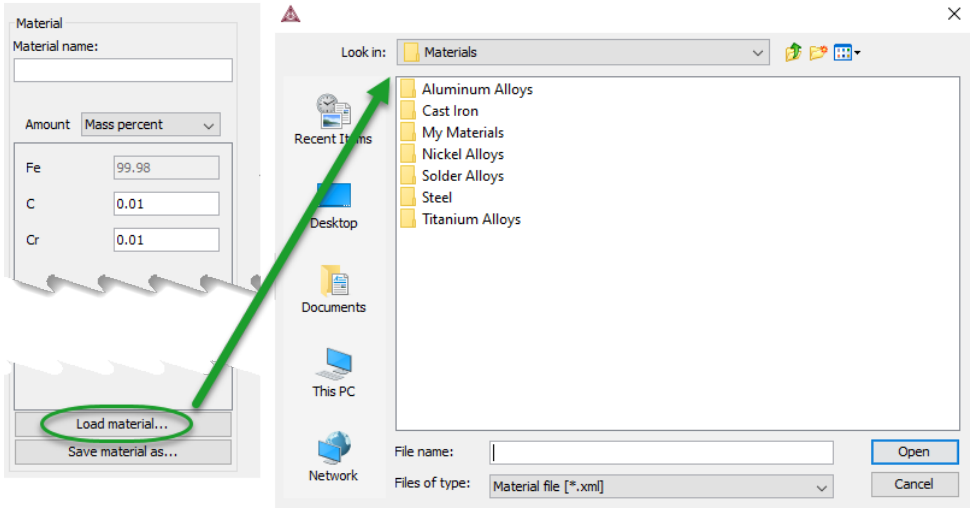
- For information about installing the TDB Editor, which is separate from the main installation and can be done later, see the *Database Manager's User Guide* contained in the *Thermo-Calc Documentation Set* or press F1 in Thermo-Calc and search the help.

Installation Default Directory: Materials

When you are working with the System Definer you can open the default **Materials** folder included with your installation.

At the bottom of the window under **Material**, click **Load material** to navigate to a material file.

There is a separate folder for materials saved using the Process Metallurgy Calculator. See Installation Default Directory: Process Metallurgy Materials.



The default directory where these files are stored is based on operating system:

Operating System	Materials Installation Directory
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2021b\Materials`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2021b/Materials`
macOS	`/Users/Shared/Thermo-Calc/2021b/Materials`

Installation Default Directory: Process Metallurgy Materials

With the Process Metallurgy Calculator you can save materials to work with again. This is the default folder where these are stored based on your operating system:

Operating System	Process Metallurgy Materials Installation Directory
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2021b\ProcessMetallurgyMaterials`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2021b/ProcessMetallurgyMaterials`
macOS	`/Users/Shared/Thermo-Calc/2021b/ProcessMetallurgyMaterials`

Installation Default Directory: Custom Property Models



All Property Models (whether these are predefined or custom models) must be located in a subdirectory of the Property Model directory. You can go to **Tools → Options** and the **Model directory** field displays the default directory.

Predefined models included with the Property Model Calculator are installed in the locations below based on your operating system. If you create your own models using TC-Python, this is the default directory where these are saved.

Operating System	Property Model Installation Directory
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2021b\PropertyModels`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2021b/PropertyModels`
macOS	`/Users/Shared/Thermo-Calc/2021b/PropertyModels`

Property Model Framework

The Property Model Development Framework is now integrated into TC-Python. The Property Models that previously used the Jython API are discontinued. Existing Jython-based Property Models will continue to be supported until the Thermo-Calc 2022a release (January 2022).



It is recommended that you migrate to the new Python Property Model framework that is based on regular Python 3 and has full support for any Python package including numpy, scipy, and so forth. See the TC-Python documentation on the website for more information.



If you install TC-Python with a Python interpreter of your choice, you can also edit the location of this in **Tools → Options → Property model Python interpreter** section.

Installation Default Directory: TC-Toolbox and the Examples

The software component and the examples are installed as described below. There is a difference between legacy and new versions.

The legacy version of TC-Toolbox for MATLAB® will no longer be supported as of Thermo-Calc version 2023a (January 2023) and users are encouraged to migrate their scripts to the new TC-Toolbox.

This is the default path to the installation folder for the TC-Toolbox component on Windows operating systems. Be aware that the initial *installation files and examples* are placed in **Public\Documents**, then after opening Thermo-Calc for the first time, these are copied to the **Documents** folder for each user. The *documentation* is installed elsewhere and as described in TC-Toolbox Documentation.

Version of TC-Toolbox	Path to the TC-Toolbox folder

New TC-Toolbox: Installation files and examples	Both the installation files AND the examples are installed in the following folders.
	The default Windows folders where the new TC-Toolbox examples are installed starts with the original installation placing these under **Public Documents** for ALL USERS.
	For a local user, and after Thermo-Calc is opened for the first time, these files are copied to the user's **Documents** folder where this local copy is associated to the user login. The **Public Documents** folder always contains the original set of contents as per the installation.
	`C:\Users\Public\Public Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB`
	After installing Thermo-Calc, and when you first open the program, the set of folders containing the examples is copied from the source Public\Documents location into a user Documents folder:
	`C:\Users\<user>\Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB\Examples`
	It is recommended that you work with the files that are copied to the *user* folder.

Legacy: Installation files and Examples	The installation file path for the legacy version of TC-Toolbox is to the same location as where you install Thermo-Calc. However, the examples continue to be accessed from a different folder as described below. Examples for the *legacy* TC-Toolbox are placed under MATLAB® in the same documents folder as the Thermo-Calc files (Documents folder): `..\Documents\MATLAB\Thermo-Calc-Toolbox-X\Examples` Where *X* is the installed version number of the toolbox. For most installations the examples are available in the MATLAB® window when the software is opened.

Subnet Information for Network Licenses

This is related to Full Network Client Installations.

For network licenses, the subnet information is also required. Ask your network administrator for the *network address for the subnet*. Additional requirements are included elsewhere for network installations.

- Subnets should be in the format aaa.bbb.ccc*** (for example: 192.168.29.0/24 or 192.168.29.*
- When installing on Sentinel RMS License Server version 9.7, a maximum of seven (7) subnets are permitted.

An alternative way to get this information is to run the command:

- *Windows:* `ipconfig /all`
- *macOS/Linux*: `ip a`

macOS Installation Notes

How to Restart After an Installation

In some types of installations (e.g. a network installation), you may have to restart your Mac to use Thermo-Calc for the first time.

How to Install XQuartz

The XQuartz open-source X Windows system is required to run Thermo-Calc on macOS but it is not required to install Thermo-Calc. Before installing Thermo-Calc, you may also need to ensure that the computer security permissions are set.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, http://xquartz.macosforge.org/landing/.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.7.11.dmg.
4. Click **Download**.
5. Double-click the **XQuartz.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

How to Enable the Security Settings

1. From the Apple main menu, select **System Preferences**.
2. Click **Security and Privacy**.
3. Click **General**. At the bottom of the **Security & Privacy** window, click the lock icon to make changes. Enter the administrator password as required.
4. If you have already tried to launch the Thermo-Calc installer, you can click **Open Anyway** to proceed. Otherwise, under **Allow apps downloaded from:** click **Anywhere** and then **Allow from Anywhere**.
5. Continue with the applicable installation type (standalone or network).



Remember to reset your security after installing Thermo-Calc.

Linux Installation Notes

The following are details you need to know regarding your Linux installation as well as how to open Thermo-Calc.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

Opening Thermo-Calc in Linux

To open Thermo-Calc double-click the **Thermo-Calc-2021b** application or from the Thermo-Calc installation directory enter `$ ./Thermo-Calc-2021b.sh` in the terminal.

Standalone Installations

You can either do a full or a custom standalone installation. The license type is called a Single-User Node-Locked License (SUNLL).

In this section:

Full Standalone Installations 35

Custom Standalone Installations 39

Add New Components to an Existing Installation 42

Full Standalone Installations

The following describes a full standalone installation. These steps assume you have completed the section First Steps of Installation.

Request your License File from Thermo-Calc Software



Updates to Thermo-Calc: Customers who subscribe to the annual maintenance plan can skip this step if you have received your license file in an email from Thermo-Calc Software AB. Save the license file to your computer to use during software installation. The license file name must be the same as the existing file name to ensure there are no errors during the update.

Follow the instructions for your operating system in the section Request a License File from Thermo-Calc Software.

Download your Thermo-Calc Installation Software

- *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
- *DVD installations*: Insert the DVD and follow the instructions.

Run the Applicable Installation File for your Operating System

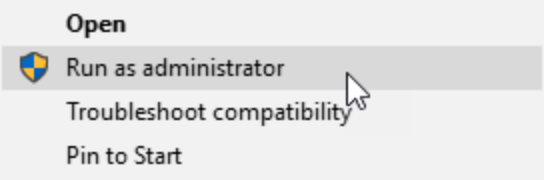
1. Navigate to the folder for your operating system and click the link to download the software package, then go to the folder where you downloaded it.



Administrative rights are required for Windows and macOS installations.

Windows

Right-click the **.exe** file and choose **Run as administrator** to launch the **Setup** program.



macOS

Double-click the downloaded file then follow the instructions.

> For macOS and when you first run the installer, you may see a message that *Thermo-Calc-osx-<version> can't be opened because Apple cannot check it for malicious software*. If this happens, select **Show in Finder**. Then, in the opened **Finder** window right-click the downloaded file `Thermo-Calc-osx-<version>` and select **Open**.

Linux

To start the Setup Wizard in a Terminal window, enter these commands in the directory where the installation file is saved:

```
> chmod +x linux-installation-x64-2021b.run
> ./linux-installation-x64-2021b.run
```

If you are an openSUSE root user, see Linux Installation Notes for some information about your installation.

2. On the **Setup** window click **Next**.
3. On the **License Agreement** window click the button to accept the license agreement then click **Next**.

Select the Installation Type and Upload the License File

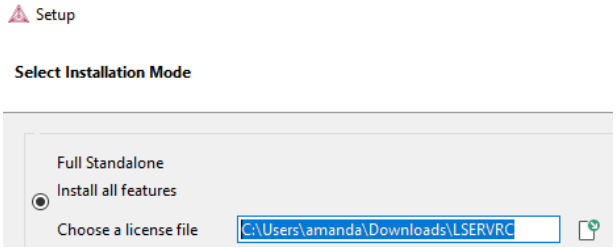
About the Thermo-Calc Components Being Installed

1. In the **Select Installation Mode** window click **Full Standalone: Install all features**.

> If you want to exclude a component (e.g. an SDK), then use the **Custom** option. See Custom Standalone Installations. For TC-Toolbox for MATLAB®, also see Installing TC-Toolbox with the Custom Option.

TC-Python is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

2. For a **Full Standalone** installation, in the **Choose a license file** field either enter the file path or click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software. The license file is called **lservrc**.



To prevent errors, leave this field blank if you did not get a license file yet.

TC-Python is installed for all users even without a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed.

Install the Software and Start Using Thermo-Calc

1. In the **Ready to Install** window click **Next**.

   See the separate instructions for TC-Toolbox for MATLAB® starting with Which TC-Toolbox Installation Should I Choose?

2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation.



macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

- If you did not get your license file see Request a License File from Thermo-Calc Software.

Custom Standalone Installations

About the Thermo-Calc Components Being Installed

Use the **Custom** option to have more control over what component features to include or exclude, for example, to exclude an SDK.

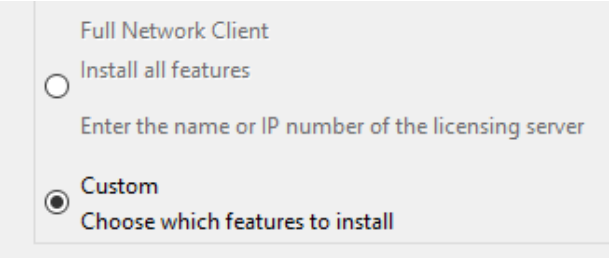
This topic describes how to do a custom installation on a standalone computer for either a Windows or Linux operating system. These steps assume you have completed these sections:

- First Steps of Installation
- Steps 1 to 3 of a Full Standalone Installations where you request your license file, download the software and then have started to set up the program up to the **Select Installation Mode** window.

Select the Installation Mode and the Components to Include or Exclude

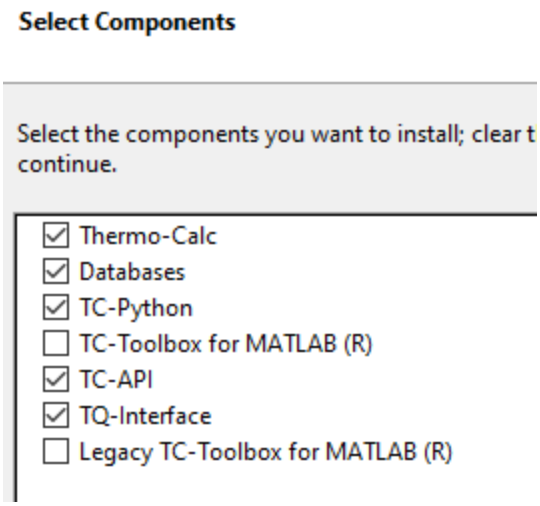
About the Thermo-Calc Components Being Installed

1. In the **Select installation mode** window click **Custom** (the option appears greyed out, but it is available to select). Click **Next**.



2. On the **Specify Configuration** window the **Create Shortcut on Desktop** check box is selected by default. Click **Next**.

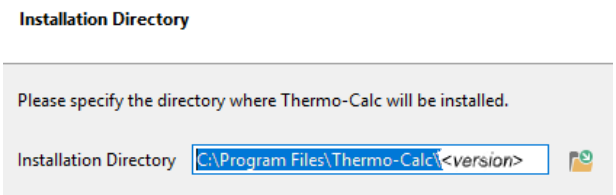
3. In the **Select Components** window, click to select or deselect the check boxes as needed. Click **Next**.



See Which TC-Toolbox Installation Should I Choose? for details about these component options and generally use the separate instructions for this product.

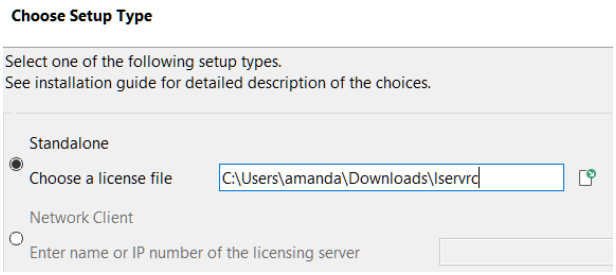
Set the Installation Directory and Choose the License File

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see Installation Default Directories and the License File). Click the file button to **Browse for Folder** and navigate to another directory.



To prevent errors, leave this field blank if you do not have a license file yet.

2. In the **Choose Setup Type** window, click **Standalone**.



3. In the **Choose a license file** field enter the path to your license file (called **lservrc**) or click the file button to navigate to a location on the computer and open the file.
4. TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide* for details.

Install the Software and Start Using Thermo-Calc

1. In the **Ready to Install** window click **Next**.

   See the separate instructions for TC-Toolbox for MATLAB® starting with Which TC-Toolbox Installation Should I Choose?

2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation.

macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

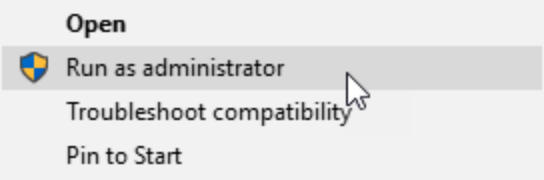
If you did not get your license file see Request a License File from Thermo-Calc Software.

Add New Components to an Existing Installation

If you want to add new components to an existing Thermo-Calc installation (for example, you purchased a license for TC-Toolbox for MATLAB®), run the installation file again as in Step 3 of Full Standalone Installations.

- See Which TC-Toolbox Installation Should I Choose? for details about these component options and generally use the separate instructions for this product.

1. For all OS you need to have administrative level rights. For example in Windows, right-click the executable Thermo-Calc installation **.exe** file and choose **Run as administrator** to launch the **Setup** program.



2. Click **Next**. Click to accept the license agreement.
3. Select the additional component(s) to install.
4. Click **Next** to start the installation, which adds the new component(s).

Use the **Uninstall** program to *remove* components. See Uninstalling Thermo-Calc or Uninstalling TC-Toolbox for MATLAB®.

Network Client Installations

This installation type is available for all operating systems, however for macOS the License Server must be run on a Windows or Linux computer. It is applicable to the consolidated and distributed network types of installations as well as for the licensing installation on a server network.

- About the Thermo-Calc Components Being Installed

In this section:

Full Network Client Installations 44
Windows: About Installing the License Manager 46
Linux: About Installing the License Server 50
Thin Client Installations 55
Custom Network Client Installations 57
Unattended Network Client Installations 60

Full Network Client Installations

The following outlines how to do a full network client installation.

Install the Sentinel RMS Management License Software

Follow the instructions for your operating system:

Windows

- Windows: About Installing the License Manager
- Windows: Installing the Sentinel RMS License Manager

Linux

- Linux: About Installing the License Server
- Linux: Installing the Sentinel RMS License Server

Complete Steps 1 to 3 of a Full Standalone Installation

These steps assume you have completed the instructions for Full Standalone Installations to download and run the software up to the **Select Installation Mode** window. It is up to you whether you get the computer information for the license files before or after installing the software.

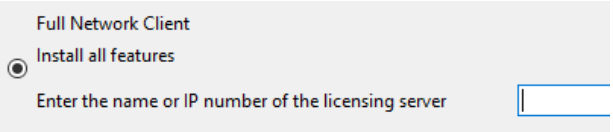
Choose the Installation Type and Enter the Computer Server Details

▶ About the Thermo-Calc Components Being Installed

1. In the **Select Installation Mode** window click **Full Network Client** to **Install all features** (the option appears greyed out, but it is available to select).

> If you want to exclude a component (perhaps one of the SDKs), then use the **Custom** option and see Custom Network Client Installations.

2. In the field, enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



3. TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide* for details.
4. In the **Ready to Install** window click **Next**.
5. When the **Completing the Thermo-Calc Setup Wizard** window opens, click **Finish**. For *Linux* users, log out and log back in to start using Thermo-Calc.

macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

If you did not get your Thermo-Calc license file see Request a License File from Thermo-Calc Software.

Windows: About Installing the License Manager



If you have previously installed an older version of Sentinel RMS License Manager, you must first uninstall the old version then **reboot** the server before starting with a new installation.

The Sentinel RMS License Manager service supplies the client computers in your network with license tokens when it runs Thermo-Calc software. The Sentinel RMS License Manager software is installed on a computer that acts as a license server in your network. This is related to Full Network Client Installations and administrative rights are required for all steps.



Remember to collect subnet information before beginning. See Subnet Information for Network Licenses.



A network license can only be used on one specific computer that hosts the License Manager. The network license determines which client computers receive license tokens using the IP addresses and IP ranges.

Supported Windows Versions

These Windows operating systems are supported for the installation of Sentinel RMS License Manager. When ready, go to Windows: Installing the Sentinel RMS License Manager.



For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

Windows 32-bit Operating Systems

- Windows 7
- Windows 8.1
- Windows 10 v1909
- Windows Server 2008

Windows 64-bit Operating Systems

- Windows 7
- Windows 8.1
- Windows 10 v1909
- Windows Server 2008
- Windows Server 2008 R2
- Windows Server 2012
- Windows Server 2012 R2
- Windows Server 2016
- Windows Server 2019

Windows: Installing the Sentinel RMS License Manager



First review Windows: About Installing the License Manager. Then if this is a new installation of the Sentinel RMS License Manager, start with Step 2.

Uninstall Any Older Versions of Sentinel RMS License Manager

1. With Administrator rights, log onto the server that hosts the Sentinel RMS License Manager.
2. Save a copy of the license file LSERVRC found in the default directory—the license file can be saved as a text file: `C:\Program Files (x86)\Common Files\SafeNetSentinel\Sentinel RMS License Manager\WinNT\`.



After saving the existing license file and uninstalling the old version of Sentinel RMS, ensure you delete the old license file (LSERVRC) in the above folder. This license is not required anymore.

3. Reboot the computer hosting the Sentinel RMS License Manager.
4. Continue with the installation and use the preselected default settings.

Download and Install Thermo-Calc

This step is not required to complete the server installation, however some administrators may want to do it at this point.

1. Download Thermo-Calc.

    - *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
    - *DVD installations*: Insert the DVD and follow the instructions.

2. Install Thermo-Calc. For testing purposes, and in order to confirm the installation is working correctly, install the Thermo-Calc software on the same computer as the Sentinel RMS License Manager. If required after testing, Thermo-Calc can always be uninstalled.

Install the Sentinel RMS License Manager Software

1. From the download, extract the files `license_server_win_9.7.zip` and `LS_tools_win.zip`.
2. Right-click `setup.exe` and select **Run as Administrator** from the menu.

Choose the Installation Directory

1. Click to accept the license agreement.
2. Enter your **User Name** and **Organization** and select to install the License Manager for **All users**.
3. In the **Destination Folder** window click **Next** to accept the suggested destination directory or **Change** to select another directory.

Choose the Setup Type and Install the Software

1. In the **Setup Type** window, select **Complete**. Click **Next**.
2. Select the **Unblock the system firewall for the Sentinel RMS License Manager** check box.



Selecting the check box is required to run Thermo-Calc.

3. Click **Next** and then **Install**.
4. Click **Finish** to exit the InstallShield Wizard.

Install the Thermo-Calc Network License Using WIAdmin



Only the WlAdmin tool can be used to update the network license used by the License Manager.

1. Save the source file containing the license code. The source file can be kept as a .txt file
2. Go to the previously saved file `LS_tools_win.zip`.
3. Right-click the file `WlmAdmin.exe` and select **Run as Administrator** from the menu.
4. If the license server is not found under subnet servers, go to **Edit → Defined Server List**.
5. Enter the host name or IP address of the license server.
6. Click **Add** and then **OK**.
7. Click **View → Refresh All** to update the list.
8. In the left main window right-click the name of a License Manager.
9. From the menu select **Add Feature → From a File → To Server and its File**.
10. To add the license from a file, select **From a File**. This permanently adds the license code to the License Manager license file as well as to the License Manager memory.
11. In the windows that open, browse to the source file that contains the license code and click **Open**.

Install Additional Tool Options

- Sentinel RMS License 9.7 Tools

Linux: About Installing the License Server

The Sentinel RMS License Server service supplies the client computers in your network with license tokens when it runs Thermo-Calc software. The Sentinel RMS License Server software is installed on a computer that acts as a license server in your network. This is related to Full Network Client Installations.

Preparing for Installation

Read and be aware of the following before you begin the section Linux: Installing the Sentinel RMS License Server.



Remember to collect subnet information before beginning. See Subnet Information for Network Licenses.

Uninstall Older Versions of the License Server

- Older versions of the License Server must be stopped by with `lsrvdown` before running the new installation. This is Step 1 in Linux: Installing the Sentinel RMS License Server.
- If you have a license server: Upgrade your license server if the new one is a higher version than the present one. Clients work with newer license servers (managers) but not necessarily with ones older than the client.

Requires Root Access or sudoers List

Root access to your computer is required or you need to be on the `sudoers` list.

Linux 32-bit Installations on a 64-bit OS



To run a license server 32-bit on a Linux 64-bit OS, 32-bit library support is needed.

Thermo-Calc License File



The name of the **license file** must be in lower case letters (**lservrc**) because Linux commands and operations are case-sensitive.

- You need a valid **lservrc** network license file supplied by Thermo-Calc Software (Requesting the License File for Windows or Linux) as well as the actual License Server—a file (program) called **lserv**.
- The Thermo-Calc license file needs to be readable and writable by the license server (license manager).

Differences Between 32- and 64-bit Scripts

Sentinel RMS License Server version 9.7 supports both 32- and 64-bit. However, when writing scripts be aware of script naming and do not mix the scripts.

- All 32-bit scripts are named *<script_name>*, for example `restart_lserv`
- All 64-bit scripts are named *<script_name>64*, for example, `restart_lserv64`



It is not possible to use Linux 32-bit scripts/tools to manage license server 64-bit and vice versa, you cannot use Linux 64-bit scripts/tools to manage license server 32-bit

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

Supported Linux Operating Systems and Versions



For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

Both Linux 32-bit and 64-bit operating systems are supported for the installation of Sentinel RMS License Server.

- Red Hat Enterprise Linux (RHEL) 7.x
- Red Hat Enterprise Linux (RHEL) 8.x
- SUSE Linux Enterprise Server (SLES)12.x
- SUSE Linux Enterprise Server (SLES) 15.x
- Debian Linux 9.x
- Debian Linux 10.x
- Ubuntu Linux 16.x (LTS)
- Ubuntu Linux 18.x (LTS)
- Ubuntu Linux 20.x (LTS)
- OpenSUSE Leap 42.x
- OpenSUSE Leap 15.x

Linux: Installing the Sentinel RMS License Server



First review Linux: About Installing the License Server. Then if this is a new installation of the Sentinel RMS License Server, start with Step 2.

Sentinel RMS License Server version 9.7 supports both 32- and 64-bit. However, when writing scripts be aware of script naming and do not mix the scripts.

- All 32-bit scripts are named *<script_name>*, for example `restart_lserv`
- All 64-bit scripts are named *<script_name>64*, for example, `restart_lserv64`



It is not possible to use Linux 32-bit scripts/tools to manage license server 64-bit and vice versa, you cannot use Linux 64-bit scripts/tools to manage license server 32-bit

Stop Older Versions of the Sentinel RMS License Server

1. To stop an old version of the License Server already running, go to the directory where the old file is found, and enter the commands:

   - 32-bit license server

     ```
     >chmod +x <lsrvdown>
     >./lsrvdown <host_name>
     ```

   - 64-bit license server

     ```
     >chmod +x <lsrvdown64>
     >./lsrvdown64 <host_name>
     ```

2. Edit existing scripts that start the older version of the License Server so that they start the newer version instead.

   For more information about the **lservdown utility**, go to http://sentinelrms.safenet-inc.com/RMSDocumentation/SysAdmin/Content/lsrvdown.htm

Write a Script to Start the License Server

The following is an excerpt from the template script for starting the License Server found in the restart_lserv file.

Replace the paths for LICENSE_SERVER_DIR, LICENSE_FILE_DIR and LOG_DIR to match your system. Save it as a script:

```
# set the directory where the executables are located
LICENSE_SERVER_DIR=/usr/local/Thermo-Calc/2021b/Licensing-files
# set the directory of the license file lservrc
LICENSE_FILE_DIR=/usr/local/Thermo-Calc/2021b/Licensing-files
# set the directory where you wish to save the log-files
LOG_DIR=/tmp
# stop the running server
# (omit this line if calling this script at startup)
$LICENSE_SERVER_DIR/lsrvdown $HOSTNAME
# start the license server
$LICENSE_SERVER_DIR/lserv -s $LICENSE_FILE_DIR/lservrc -l $LOG_DIR/lserv_use.log
-f $LOG_DIR/lserv_err.log
```

Confirm the HOSTNAME variable and open the UDP port

The hostname should always correspond to the DNS record verify this by doing the following.

1. Before starting the License Server make sure that the value of the $HOSTNAME variable is correct. This value can be shown by typing the `> nslookup $HOSTNAME` command in the terminal window:

   The value should be the same IP address that is shown when you use the ifconfig command.

2. Open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting `SELINUX=permissive` in the `/etc/selinux/config` file.

Start the License Server

1. To start the License Server, run the script created as root. Enter these commands in the console:

   ```
   > chmod +x <name_of_script_file>
   > ./<name_of_script_file>
   ```

2. If you want the License Server to start when you boot the system, put a copy of the start script under `/etc/rc.d/init.d` and start the script from the file `/etc/rc.d/rc.local`.

Install Additional Tool Options

- Sentinel RMS License 9.7 Tools

Thin Client Installations

This topic describes how you install a thin Thermo-Calc client to run Thermo-Calc from a file server. It is applicable to consolidated and distributed network installations for either a Windows or Linux operating system.

Installation Requirements

- You need access to the directory where Thermo-Calc is installed on the file server.
- You need the IP number or name of the computer where the license file is installed.
- For *Linux* you may have to disable your firewall. If SELinux is installed, try disabling it by setting `SELINUX=permissive` in `/etc/selinux/config`.

How to Install a Thin Client on Windows

1. Map the file server share as a network drive so that it gets an assigned drive letter (e.g. **E:**).
2. Open the **\Thermo-Calc***<version>*** directory on the file server, where *version* is the current version of the software.
3. Open the directory **Thin-client**. Double-click the `Thermo-Calc-client-windows-<version>.exe` file.
4. Click to accept the terms of the license agreement. Click **Next**.
5. Enter the name or IP number of where the license file and the License Manager software is installed. Click **Next**.
6. By default the **Create Shortcuts on Desktop** check box is selected. Click **Next**.
7. In the **Ready to Install** window, click **Next**.
8. Click **Finish**. To start Thermo-Calc find the program on the server and start it from there.

How to Install a Thin Client on Linux

1. Add the following to the `smb.conf` file, where *<user>* is your user name:

```
[public]
path=/home/<user>/Thermo_Calc/2021b
public=yes
writable=yes
```

```
comment=smb share

guest OK=yes

force user=<user>
```

2. From the client, mount the directory on the server computer that contains the Thermo-Calc server installation (by default, this directory is called **/Thermo-Calc/2021b**). How the directory is mounted depends on the Linux distribution being used as well as how the Thermo-Calc directory on the server computer is shared. Use the Linux command `mount`. For example:

   ```
   > mkdir public

   > sudo mount -t cifs //ip_number_server_computer/public ./public -o
   user=<user>
   ```

3. Open the mounted directory on your computer, and run `client-install-linux-x64.run` or `client-install-linux-x86.run` in the **/Thin-client** directory.
4. If you do this from the terminal window, use the following to start the installation (assuming that the file server is a 64-bit computer):

   > ./client-install-linux-x64.run

5. Click **Forward** and click to select the license agreement. Click **Forward**.
6. Enter the name or IP number of the License Server. Click **Forward**.
7. If you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** check box is selected. Click **Forward**.
8. In the **Ready to Install** window click Forward.
9. Click **Finish**. Log out and log back in to start using Thermo-Calc.

Custom Network Client Installations

This installation type is available for all operating systems, however for macOS the License Server must be run on a Windows or Linux computer.The requirements are the same as for a full client installation.

Install the Licensing Software

Follow the instructions for your operating system:

- Windows: About Installing the License Manager, or
- Linux: About Installing the License Server

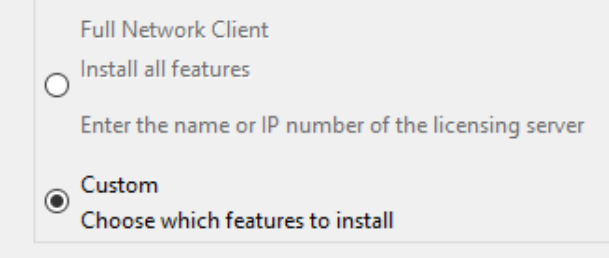
Complete Steps 1 to 4 of a Full Standalone Installation

Follow the instructions for Full Standalone Installations to download and run the software. It is up to you whether you get the computer information for the license files before or after installing the software.

Select the Installation Mode and the Components to Include or Exclude

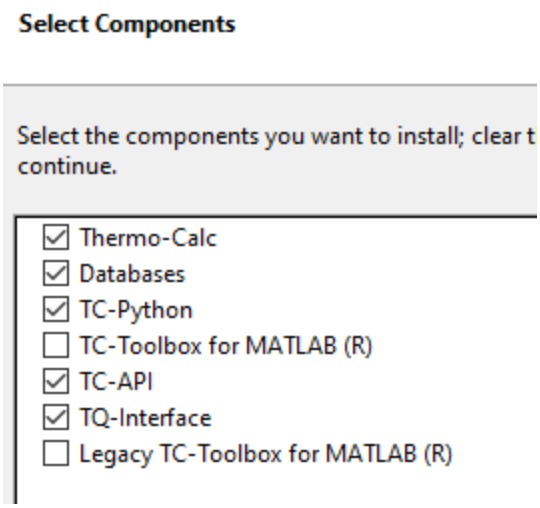
▶ About the Thermo-Calc Components Being Installed

1. In the **Select installation mode** window click **Custom** (the option appears greyed out, but it is available to select). Click **Next**.



2. On the **Specify Configuration** window the **Create Shortcut on Desktop** check box is selected by default. Click **Next**.

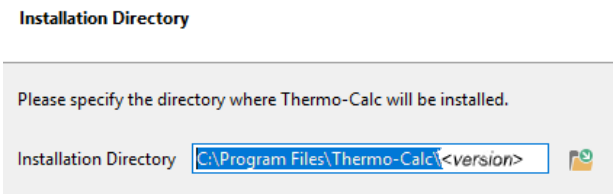
3. In the **Select Components** window, click to select or deselect the check boxes as needed. Click **Next**.



See Which TC-Toolbox Installation Should I Choose? for details about these component options and generally use the separate instructions for this product.

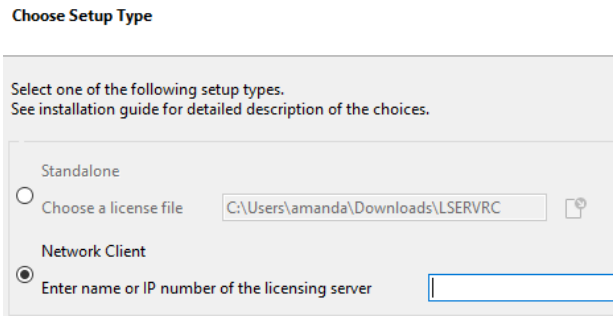
Set the Installation Directory and the File Path to the License

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see Installation Default Directories and the License File). Click the file button to **Browse for Folder** and navigate to another directory. Click **Next**.



To prevent errors, leave this field blank if you do not have a license file yet.

2. In the **Choose Setup Type** window, click **Network Client** and enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



If you have selected to install **TC-Python** there is a reminder window that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

Install the Software and Start Using Thermo-Calc

1. In the **Ready to Install** window click **Next**.

   - See the separate instructions for TC-Toolbox for MATLAB® starting with Which TC-Toolbox Installation Should I Choose?

2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation.

macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

- If you did not get your license file see Request a License File from Thermo-Calc Software.

Unattended Network Client Installations



Terminology note: The use of the term *license server* (lower case letters) is applicable to the option files as described in this section. For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the licensing software.

Sometimes it is convenient to install Thermo-Calc network clients without providing user input after the installation is initiated (an unattended network client installation). This is available for Windows and Linux operating systems.



Make sure you know the name or IP number of the computer where the licensing software and the license file are to be installed.

Create an Option File in a Text Editor to Enter the Options

The following is an example of an option file for a custom network client installation, where *<name/IP number>* is the name or IP number of the computer where the license file is installed:

```
installation_mode=custom
setup_type=client
enable-components=thermo,databases,tq,tcapi,toolbox,tcpython
icons=1
license_server=<name/IP number>
```

Below is a shorter example, specifying that a full Thermo-Calc network client should be installed:

```
installation_mode=full_client
license_server=<name/IP number>
```

Go to the Directory Where the Installation File is Saved



Thermo-Calc can only be installed in unattended mode from the command line prompt.

Start the installation in unattended mode using the option file created with this command:

- For *Windows*: `<installationfile>.exe --mode unattended --optionfile <path\optionfile>`
- For *Linux*: `<installationfile>.run --mode unattended --optionfile <path/optionfile>`

To see other options when you start the Thermo-Calc installation program from the command line prompt, run this command:

- For *Windows*: `<installationfile>.exe --help`
- For *Linux*: `<installationfile>.run --help`

Request License Files

In this section:

Request a License File from Thermo-Calc Software 63
Getting License Information Using Thermo-Calc 64
Requesting the License File for Windows or Linux 65
Requesting the License File for macOS 67

Request a License File from Thermo-Calc Software

The following explains how to retrieve the necessary diagnostic and network adaptor information about your computer and then send an email to Thermo-Calc Software to get your license file(s) containing the license key(s).

To set up the correct licensing:

1. Make a note of your company or organization's *site number*. You can find the site number on an invoice or any correspondence from Thermo-Calc Software.
2. Retrieve your computer diagnostic and network adapter information.
3. Email Thermo-Calc Software with this information.
4. A Thermo-Calc Software representative emails you the license file. Save the license file **lservrc** (there is no file suffix) to a location where you can easily access it later.

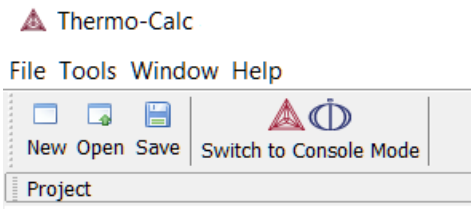
Thermo-Calc Support Center on our website

Getting License Information Using Thermo-Calc

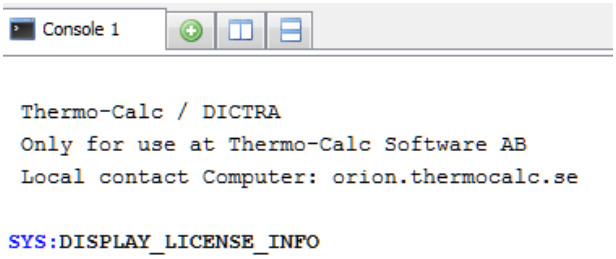
If you have already installed Thermo-Calc, you can view the license information in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command DISPLAY_LICENSE_INFO.

1. Open Thermo-Calc.
2. Click **Switch to Console Mode**.



3. At the `SYS:` prompt, enter `DISPLAY_LICENSE_INFO` (all caps).



4. You can output the information to a `FILE` or to the `SCREEN`.

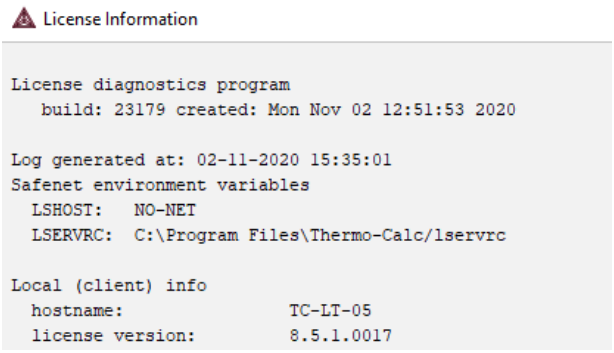
```
SYS:DISPLAY_LICENSE_INFO
OUTPUT TO SCREEN OR FILE /SCREEN/:SCREEN
```

5. For both options, the information is displayed on screen. Copy the section containing the **Ethernet** and **IP address**. You can save it to a text file or paste it directly into an email. If you choose `FILE` as the output, then you can attach the file to an email.

Requesting the License File for Windows or Linux

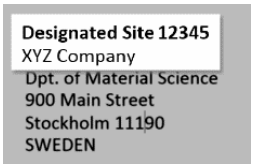
Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

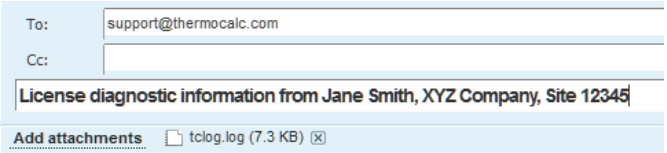
1. To access the computer information you need to provide to get a license, start Thermo-Calc and select **Help → Show License Info**.



2. Copy the information from the **License Information** window. A lot of information may be shown below the initial screen, so make sure you scroll down to the end when you select and copy the window's contents. (Alternatively, you can copy the same information from the console by using the SYS module command DISPLAY_LICENSE_INFO.)
3. Send an email to support@thermocalc.com. Make sure to include the following in the subject line:

   License diagnostic information from <Name> where Name is replaced with your **name**, the **organization name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



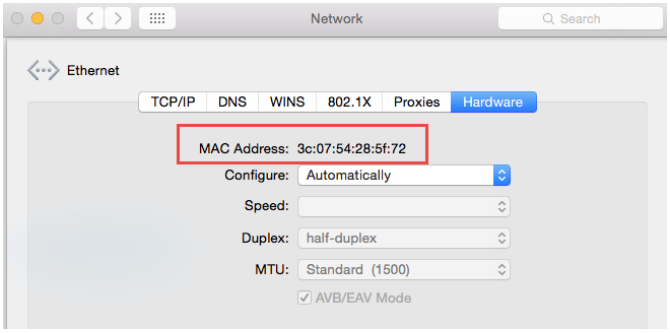


4. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
5. Save the license file(s) to your computer or network.

Requesting the License File for macOS

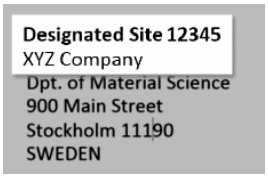
Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

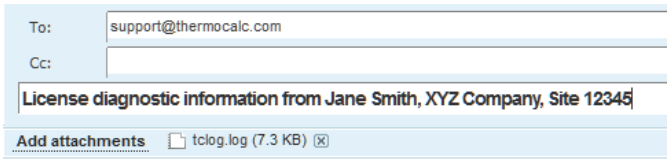
1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.
3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).
4. Click **Advanced → Hardware**. The **Network** window shows you the **MAC Address**. For example, the MAC address (the host ID) might be **3c:07:54:28:5f:72**.



5. Send an email to support@thermocalc.com and copy and paste the MAC address into the body of the email. Make sure to include the following in the subject line:

   License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*





6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Quick Installation Guides

In this section:

Windows® Standalone Quick Install Guide 70

macOS® Standalone Quick Install Guide 74

Windows® Standalone Quick Install Guide

This quick guide helps you do a full standalone installation. A *standalone* installation is used with the Single-User Node-Locked License (SUNLL), where the software and the license file are together on one computer.

This guide is applicable to:

- Windows operating systems
- Full Standalone installation (SUNLL)
- Upgrading to a new standalone version of Thermo-Calc (maintenance plan only)

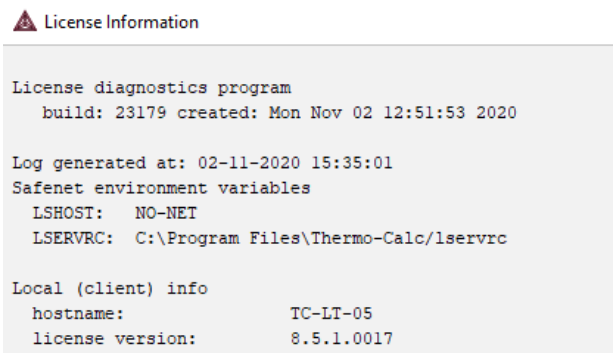
Other Installations

For instructions about other operating systems, network installations, or installing an SDK (e.g. TC-Python or TC-Toolbox for MATLAB®) search the *Thermo-Calc Installation Guide*, which is also available on our website. You can also review the Licensing Options included on our website.

Request a License File

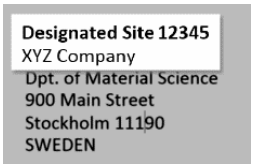
Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

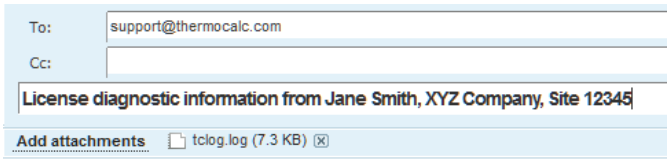
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3. Send an email to support@thermocalc.com. Make sure to include the following in the subject line:

   License diagnostic information from <Name> where Name is replaced with your **name**, the **organization name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*





4. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
5. Save the license file(s) to your computer or network.

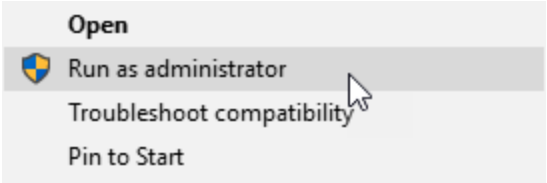
Install the Software

Download and Run your Thermo-Calc Installation Software

Administrative rights are required to complete this installation.

1. For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided. Then navigate to the Windows folder and click the link to download the software.

2. Go to the folder where you downloaded the software. Right-click the **.exe** file and choose **Run as administrator** to launch the **Setup** program.



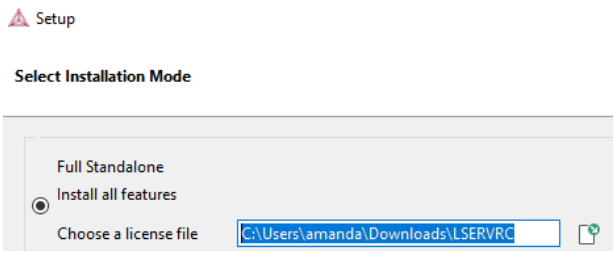
3. On the **Setup-Thermo-Calc** window click **Next**.
4. On the **License Agreement** window click to accept the license agreement. Click **Next**.

Select the Installation Mode

1. In the **Select Installation Mode** window click **Full Standalone: Install all features**.

TC-Python is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

2. For a **Full Standalone** installation, in the **Choose a license file** field either enter the file path or click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software.



The license file is called **lservrc**. Click **Next**. To prevent errors, leave this field blank if you did not get a license file yet.

TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

3. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

macOS® Standalone Quick Install Guide

This quick guide helps you do a full standalone installation. A *standalone* installation is used with the Single-User Node-Locked License (SUNLL), where the software and the license file are together on one computer.

This guide is applicable to:

- macOS
- Full Standalone installation (SUNLL)
- Upgrading to a new standalone version of Thermo-Calc (maintenance plan only)

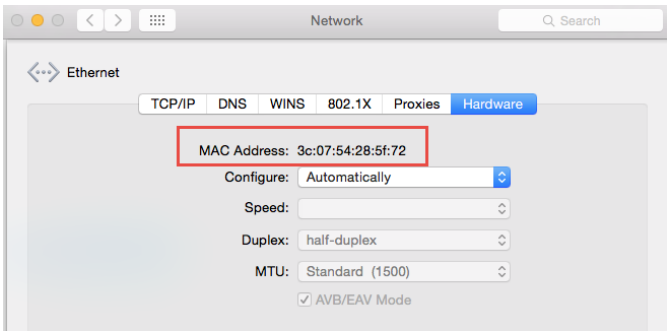
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Request a License File

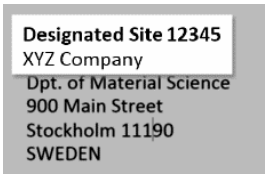
Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

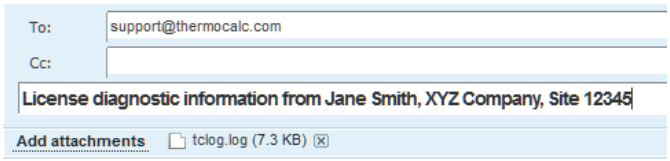
1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.
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6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Install the Software

Download and Install XQuartz

The XQuartz open-source X Windows system is required to run Thermo-Calc on macOS X.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, http://xquartz.macosforge.org/landing/.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.7.11.dmg.

4. Click **Download**.
5. Double-click the **XQuartz.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

Download and Run your Thermo-Calc Installation Software



Administrative rights are required to complete this installation.

1. For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided. Then navigate to the Mac folder and click the link to download the software.

2. Double-click the downloaded file to launch the installation.



For macOS and when you first run the installer, you may see a message that *Thermo-Calc-osx-<version> can't be opened because Apple cannot check it for malicious software*. If this happens, select **Show in Finder**. Then, in the opened **Finder** window right-click the downloaded file `Thermo-Calc-osx-<version>` and select **Open**.

3. On the **Setup-Thermo-Calc** window click **Next**.
4. On the **License Agreement window** click to accept the license agreement. Click **Next**.

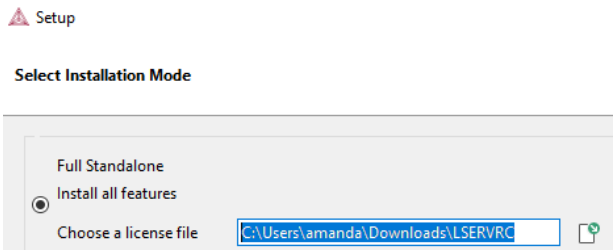
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1. In the **Select Installation Mode** window click **Full Standalone: Install all features**.



TC-Python is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

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The license file is called **lservrc**. Click **Next**. To prevent errors, leave this field blank if you did not get a license file yet.

TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

3. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

TC-Python Installation Guide

In this section:

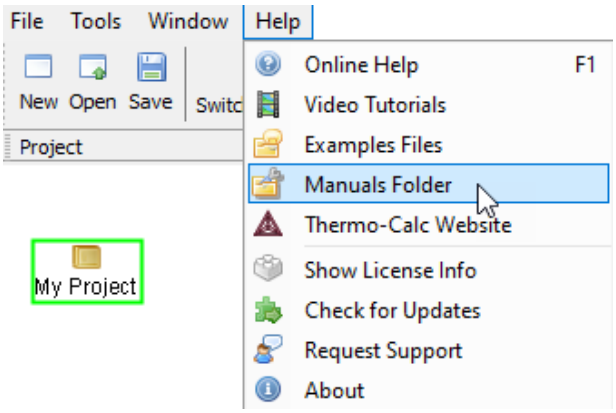
About the TC-Python Documentation 79
Which TC-Python Installation Should I Choose? 81
Installing TC-Python with a Bundled Python-interpreter 82
Installing TC-Python Into a Python-interpreter of Your Choice 85
Installation Default Directory: TC-Python 89
macOS: Setting Environment Variables 90
Fixing Potential Issues with the Environment 91
Updating to a Newer Version 92
TC-Python Diagnostic Script 93

About the TC-Python Documentation

The TC-Python help is available on the Thermo-Calc website where you can also access additional resources. You can alternatively access the locally installed documentation from the **Help** menu in Thermo-Calc.

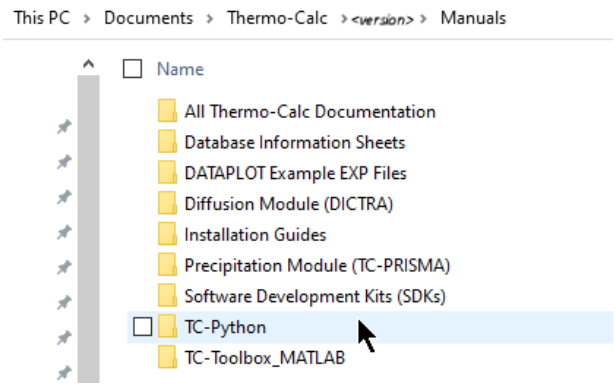
Opening the Locally Installed Documentation

1. In Thermo-Calc from the menu, select **Help → Manuals Folder**.

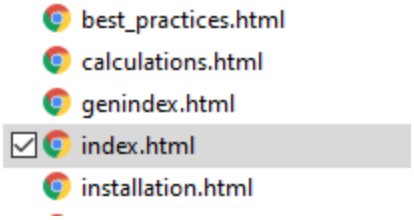


You can also navigate to the **Manuals** folder outside of Thermo-Calc and based on your operating system installation location.

2. In the window that opens, double-click to open the **TC-Python** folder.



3. Double-click the **Index** HTML file (or any of the HTML files).



4. The API reference documentation opens as a searchable HTML file in your local browser.

Which TC-Python Installation Should I Choose?



A license is required to run TC-Python. Also remember to review the System Requirements page on our website.

There are these options to install TC-Python.



See the Videos about TC-Python page for additional learning resources.

Install with the Bundled Python-interpreter

This is a straightforward installation where TC-Python is preinstalled together with some popular Python packages.

This is the recommended option for new users to TC-Python who may only want to run the examples. The available preinstalled packages (e.g. numpy, scipy, scikit-learn, and matplotlib) can also be sufficient for many advanced users.

- Installing TC-Python with a Bundled Python-interpreter.

Install with a Python-interpreter of Your Choice

This installation requires additional steps and is the recommended option for more advanced use and has full flexibility.

- Installing TC-Python Into a Python-interpreter of Your Choice.

Installing TC-Python with a Bundled Python-interpreter

TC-Python can be installed using a Python-interpreter that is bundled to Thermo-Calc. This interpreter has TC-Python preinstalled together with some popular Python packages. This is the recommended option for new users to TC-Python who may only want to run the examples. The available preinstalled packages (e.g. numpy, scipy, scikit-learn, and matplotlib) can also be sufficient for many advanced users.



The bundled interpreter package is also used to run the Property Models in Thermo-Calc. Do not make changes to interpreter packages or this can stop Thermo-Calc from working correctly. To fix issues caused by changes to an interpreter, completely uninstall Thermo-Calc and start over, either with the bundled interpreter package or using interpreters of your choice.



If you are planning to do more advanced calculations that require other external packages then you may want to follow these instructions instead: Installing TC-Python Into a Python-interpreter of Your Choice

Limitations



The following examples cannot be run with the bundled Python-interpreter as additional packages are required: `pyex_M_01_Input_from_file.py` (pandas) and `pyex_M_02_Output_to_file.py` (pandas, lxml, h5py).

The bundled Python 3.7.2 interpreter contains the following major packages.



If you have recommendations for additional packages to include (see below), send an email to Thermo-Calc Support.

Package	Version
matplotlib	3.3.2
numpy	1.19.2

Package	Version
scikit-learn	0.23.2
scipy	1.5.2
TC-Python	2021b

Install an IDE (Integrated Development Environment)

Any editor can be used to write the Python code, but an IDE is recommended, e.g. PyCharm. These instructions are based on the use of PyCharm.

Use of an IDE gives you access to code completion, which helps when you use the API as it gives you the available methods on the objects you are working with.

1. Navigate to the PyCharm website: https://www.jetbrains.com/pycharm/download.
2. Click to choose your OS and then click **Download**. You can use the **Community** version of Pycharm.
3. Follow the instructions. It is recommended you keep all the defaults.



For Mac installations, you also need to set some environment variables as described below in macOS: Setting Environment Variables.

Configure PyCharm to Use the Bundled Python-interpreter

Open PyCharm and configure the interpreter:

1. Go the menu **File→Settings**.
2. Navigate in the tree to **Project: YourProjectName** and choose **Project Interpreter**.
3. Click on the settings symbol close to the **Project Interpreter** dropdown menu and choose **Add**.
4. Select **System Interpreter** and add the bundled Thermo-Calc Python 3 interpreter,

which is located in a folder based on the operating system:

Operating system	Path to the bundled Python-interpreter
Windows	`C:\Program Files\Thermo-Calc\2021b\python\python.exe`
Linux	`/home/UserName/Thermo-Calc/2021b/python/bin/python3`
macOS	`/Applications/Thermo-Calc-2021b.app/Contents/Resources/python/bin/python3`

5. Select the interpreter and confirm.

Run a TC-Python Example

It is recommended that you open one or more of the included examples to both check that the installation has worked and to start familiarizing yourself with the code.

Open the TC-Python Project in PyCharm



When you first open the TC-Python project and examples, it can take a few moments for the Pycharm IDE to index before some of the options are available.

1. Open PyCharm and then choose **File** → **Open**. The first time you open the project you will need to navigate to the path of the TC-Python installation based on your operating system.
2. Click the **Examples** folder and then click **OK**.
3. From any subfolder:
   - Double-click to open an example file to examine the code.
   - Right-click an example and choose **Run**.



If you are not following the recommended approach and create a *new* project (**File→New Project…**), you need to consider that by default the options to choose the interpreter are hidden within the **Create Project** window. For this, click **Project Interpreter: New Virtual Environment** and in most cases choose your *System Interpreter* containing the Python bundled to Thermo-Calc instead of the default *New Virtual Environment*.

Installing TC-Python Into a Python-interpreter of Your Choice

TC-Python can be installed using a Python-interpreter of your choice. This is the recommended option for any more advanced usage and provides full flexibility.

> If you are new to TC-Python and want to mainly run the examples, then it is recommended you install the bundled Python-interpreter. The available preinstalled packages (e.g. numpy, scipy, scikit-learn, and matplotlib) can also be sufficient for many advanced users. See Installing TC-Python with a Bundled Python-interpreter.

Install a Python Distribution

> If you already have a Python distribution installation, version 3.5 or higher, skip this step.

These instructions are based on using the Anaconda platform for the Python distribution. Install version 3.5 or higher to be able to work with TC-Python, although it is recommended that you use the most recent version.

Install Anaconda

1. Navigate to the Anaconda website: https://www.anaconda.com/download/.
2. Click to choose your OS (operating system) and then click **Download**. Follow the instructions. It is recommended you keep all the defaults.

Install Thermo-Calc and the TC-Python SDK

1. Install Thermo-Calc.
2. When the installation is complete, open the TC-Python folder that includes the *.whl file needed for the next step. There is also an **Examples** folder with Python files you can use in the IDE to understand and work with TC-Python.

Operating system	Path to the TC-Python folder
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2021b\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2021b/SDK/TC-Python`
macOS	`/Users/Shared/Thermo-Calc/2021b/SDK/TC-Python`

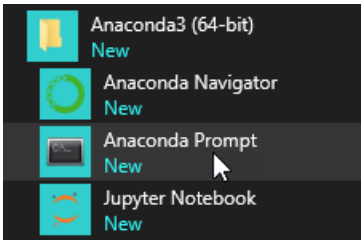
Install TC-Python

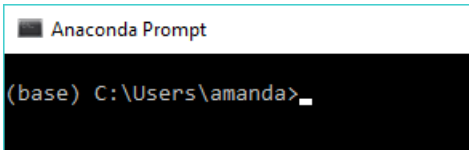
Updating to a Newer Version

On Windows, it is recommended you use the Anaconda distribution prompt (i.e. Anaconda), especially if you have other Python installations.

Do not use Virtual Environments unless you have a good reason to do so. Also see Fixing Potential Issues with the Environment.

1. Open the command line. For example, in Anaconda on a Windows OS, go to **Start** → **Anaconda** → **Anaconda Prompt**.





2. At the command line, enter the following. Make sure there are no spaces at the end of the string or in the folder name or it will not run:

```
pip install <path to the TC-Python folder>/TC_Python-<version>-
py3-none-any.whl
```



On Linux, and depending on the interpreter, *pip3* is typically used.

3. Press <Enter>. When the process is completed, there is a confirmation that TC-Python is installed.



If your computer is located behind a proxy-server, the default pip-command will fail with a network connection error. In that case you need to install the dependency py4j in a special configuration:

```
pip install -proxy user:password@proxy_ip:port py4j
```

Go to the TC-Python Help **Troubleshooting** section for detailed information. This can be found on our website or from the installed documentation where you can search for "pip install fails".

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Use of an IDE gives you access to code completion, which helps when you use the API as it gives you the available methods on the objects you are working with.

1. Navigate to the PyCharm website: https://www.jetbrains.com/pycharm/download.
2. Click to choose your OS and then click **Download**. You can use the **Community** version of Pycharm.
3. Follow the instructions. It is recommended you keep all the defaults.



For Mac installations, you also need to set some environment variables as described below in macOS: Setting Environment Variables.

Open the IDE and Run a TC-Python Example

After you complete all the software installations and set up the pip install path, you are ready to open the IDE to start working with TC-Python.

It is recommended that you open one or more of the included examples to both check that the installation has worked and to start familiarizing yourself with the code.

Open the TC-Python Project in PyCharm



When you first open the TC-Python project and examples, it can take a few moments for the Pycharm IDE to index before some of the options are available.

1. Open PyCharm and then choose **File** → **Open**. The first time you open the project you will need to navigate to the path of the TC-Python installation based on your operating system.
2. Click the **Examples** folder and then click **OK**.
3. From any subfolder:
    - Double-click to open an example file to examine the code.
    - Right-click an example and choose **Run**.

Installation Default Directory: TC-Python

These are the default paths to the TC-Python folder based on your operating system.

Operating system	Path to the TC-Python folder
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2021b\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2021b/SDK/TC-Python`
macOS	`/Users/Shared/Thermo-Calc/2021b/SDK/TC-Python`

For a bundled Python-interpreter installation, these are the paths to this location based on your operating system.

Operating system	Path to the bundled Python-interpreter
Windows	`C:\Program Files\Thermo-Calc\2021b\python\python.exe`
Linux	`/home/UserName/Thermo-Calc/2021b/python/bin/python3`
macOS	`/Applications/Thermo-Calc-2021b.app/Contents/Resources/python/bin/python3`

macOS: Setting Environment Variables

In order to use TC-Python on Mac you need to set some environment variables.

```
TC21B_HOME=/Applications/Thermo-Calc-2021b.app/Contents/Resources
```

If you use a license server:

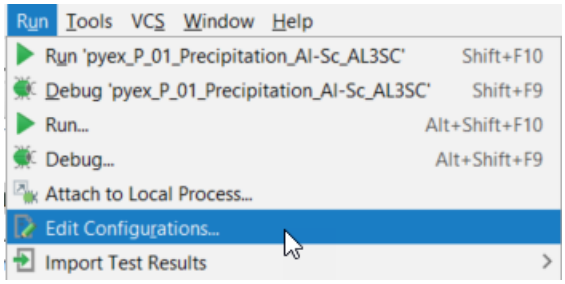
```
LSHOST=<name-of-the-license-server>
```

If you have a node-locked license:

```
LSHOST= NO-NET
LSERVRC=/Users/Shared/Thermo-Calc/lservrc
```

In PyCharm, you can add environment variables in the configurations.

Select **Run** → **Edit Configurations** to open the **Run/Debug Configurations** window. Enter the environment variable(s) by clicking the button to the right of the **Environment Variables** text field. Now the environment variables(s) will be set for each new configuration by default. The same way for configuring the environment variables can be used on other operating systems as if necessary.



Fixing Potential Issues with the Environment

In most cases you should run TC-Python within your **global** Python 3 interpreter and not use Virtual Environments unless you have a good reason to do so.

If there are problems with the interpreter settings, for example, a common problem when you first use TC-Python is the message *No module named tc_python*, which you can resolve in the Settings window as follows:

1. Go the menu **File** → **Settings**.
2. Navigate in the tree to *<Project.YourProjectName>* and choose **Project Interpreter**.
3. Click on the settings symbol close to the **Project Interpreter** drop-down menu and choose **Add**.
4. Now choose **System Interpreter** and add your existing Python 3 interpreter.
5. Select your added interpreter and confirm.



If you are not following the recommended approach and create a *new* project (**File→New Project…**), you need to consider that by default the options to choose the interpreter are hidden within the **Create Project** window. For this, click **Project Interpreter: New Virtual Environment** and in most cases choose your *System Interpreter* containing the Python bundled to Thermo-Calc instead of the default *New Virtual Environment*.



If you really need to use a Virtual Environment, it is recommended you review the hints provided in the **Best Practices** section in the full TC-Python HTML help or PDF.

Updating to a Newer Version

If you are using the bundled Python-interpreter automatically installed with Thermo-Calc, these steps are not required.

These steps are required if you have previously followed the instructions in Installing TC-Python Into a Python-interpreter of Your Choice.

When updating to a newer version of Thermo-Calc, you always need to also install the latest version of TC-Python. It is not sufficient to run the installer of Thermo-Calc (except for bundled versions of the Python interpreter).

```
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl
```

In case of problems you may wish to uninstall the previous version of TC-Python in advance:

```
pip uninstall TC-Python
```

```
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl
```

However, this should not normally be required.

On Linux typically *pip3* is used.

You can check the currently installed version of TC-Python by running:

```
pip show TC-Python
```

TC-Python Diagnostic Script

A diagnostic script is available to help you if you have problems running TC-Python.



It is important to run the diagnostic script EXACTLY the same way as you run your TC-Python script (in the same IDE, same project, same Python environment, same Jupyter notebook, etc).

The script automatically prints useful suggestions that, in many cases, will help you to fix the problem yourself. If you are unable to solve the problem, contact us for support. You can find the script in these locations:

- Miscellaneous example (diagnostics.py)
- In the **Troubleshooting** section of the *TC-Python API Reference Documentation*. Also refer to the **Best Practices** in the same guide to see if there are any other solutions or tips.
- On our website.

TC-Toolbox for MATLAB® Installation Guide

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About TC-Toolbox for MATLAB®

TC-Toolbox for MATLAB® (TC-Toolbox) provides an interface to the commonly used MATLAB® software for scientific and engineering computing. This software development kit (SDK) is ideal for fast realization of ideas and visualization of results during research and development activities. The TC-Toolbox API includes calculation types available in Thermo-Calc such as single point equilibrium, property (step) and phase (map) diagrams, Scheil solidification simulations, as well as all the general Thermo-Calc Property Models (e.g. yield strength, spinodal, driving force, etc.).

With the addition of licenses for the applicable software and databases, you can further maximize your integration with MATLAB® to include the capabilities of the Steel Model Library Property Models (e.g. bainite, pearlite, etc.), as well as access the range of functionality included with the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA). Generally, all the functionality available in Graphical Mode or via the TC-Python SDK is available.

TC-Toolbox for MATLAB® is available on Windows platforms.



A license is required to run TC-Toolbox for MATLAB® and MATLAB® must also be installed on your computer prior to the TC-Toolbox installation. Also remember to review the System Requirements page on our website.

New TC-Toolbox vs Legacy Version

As of 2021b TC-Toolbox for MATLAB® (short name, *TC-Toolbox*) is completely rebuilt. The previous version, now referred to as *legacy TC-Toolbox for MATLAB®* can be installed alongside the new version. You can run both versions at the same time in MATLAB® although there is no communication between the two programs.

Compared to the new TC-Toolbox, the legacy version of TC-Toolbox for MATLAB® can only perform single equilibrium calculations, limiting the scope of simulations available. The rebuild includes significant upgrades compared to the legacy version and allows for easier implementation of new features in the future. If both versions are installed in parallel there is an example available (*Benchmark Toolboxes*) to run a comparison between the two to see that there is no significant change to the speed of calculations, even though there are many other differences making the new version more robust for most users.

The legacy version of TC-Toolbox for MATLAB® will no longer be supported as of Thermo-Calc version 2023a (January 2023) and users are encouraged to migrate their scripts to the new TC-Toolbox.

TC-Toolbox Documentation

There are various locations and formats of the documentation you need related to this SDK. It is important to understand the differences between the new versus the legacy API in order to locate the information you need.

New vs Legacy Content Locations



The new *TC-Toolbox for MATLAB® API Reference Documentation* is available from these general locations (1) within the MATLAB® environment—both as help and as part of the tab completion (2) directly on the Thermo-Calc website, and (3) locally in the Thermo-Calc installation (**Help>Manuals Folder**).

API Reference Documentation

NEW TC-TOOLBOX

The new *TC-Toolbox for MATLAB® API Reference Documentation* is available either as interactive help (in HTML format or when in MATLAB® using tab completion or accessed via different menus or key combinations) or as a standalone PDF. Only information related to the *new* version of the software is included.

There are these ways to access the content:

- Directly in MATLAB® via the Help menu then under **Supplemental Software** click **TC-Toolbox**. Help is also available when writing code and using the tab completion feature and/or pressing different key combinations as described in the *Best Practices* section of the help.
- From the website: HTML Help or PDF
- Locally in a Thermo-Calc installation:
  - HTML: **Help > Manuals Folder > TC-Toolbox_MATLAB**, then click any HTML file.
  - PDF: **Help > Manuals Folder > Software Development Kits (SDKs)**, then double-click to open the *TC-Toolbox for MATLAB® API Programmer Guide*. This is a copy of the HTML API reference documentation.

LEGACY VERSION - PDF ONLY ON THE WEB



Legacy TC-Toolbox for MATLAB® documentation is no longer available in the Thermo-Calc help. *The exception is for installation instructions, which are included as required.* Legacy documentation as a PDF is available from the website documentation archive (for example, see the 2021a PDF on our website). It is also available with any previously installed versions of Thermo-Calc.

Installation Instructions (New and Legacy Versions)

The new and legacy versions of TC-Toolbox for MATLAB® can be installed in parallel with one another. The installation instructions for *both* types of installations are only included in the Thermo-Calc help (press F1), and in the PDF version of the main installation guide found, for example:

- On our website as part of the full Thermo-Calc Installation Guide.
- Once Thermo-Calc is installed:
  - Locally in a Thermo-Calc installation: **Help > Manuals Folder >Installation Guides**.
  - Press F1 in Thermo-Calc to search the help.

Thermo-Calc Help (Limited)

For the new TC-Toolbox, there is limited content included in the Thermo-Calc help (press F1 when in Thermo-Calc) because it is replaced by the *TC-Toolbox for MATLAB® API Reference Documentation*. The exception is installation instructions to describe how to install both versions of the SDK.

Installation Default Directory: TC-Toolbox and the Examples

The software component and the examples are installed as described below. There is a difference between legacy and new versions.

The legacy version of TC-Toolbox for MATLAB® will no longer be supported as of Thermo-Calc version 2023a (January 2023) and users are encouraged to migrate their scripts to the new TC-Toolbox.

This is the default path to the installation folder for the TC-Toolbox component on Windows operating systems. Be aware that the initial *installation files and examples* are placed in **Public\Documents**, then after opening Thermo-Calc for the first time, these are copied to the **Documents** folder for each user. The *documentation* is installed elsewhere and as described in TC-Toolbox Documentation.

Version of TC-Toolbox	Path to the TC-Toolbox folder

New TC-Toolbox: Installation files and examples	Both the installation files AND the examples are installed in the following folders.
	The default Windows folders where the new TC-Toolbox examples are installed starts with the original installation placing these under **Public Documents** for ALL USERS.
	For a local user, and after Thermo-Calc is opened for the first time, these files are copied to the user's **Documents** folder where this local copy is associated to the user login. The **Public Documents** folder always contains the original set of contents as per the installation.
	`C:\Users\Public\Public Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB`
	After installing Thermo-Calc, and when you first open the program, the set of folders containing the examples is copied from the source Public\Documents location into a user Documents folder:
	`C:\Users\<user>\Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB\Examples`
	It is recommended that you work with the files that are copied to the *user* folder.

Legacy: Installation files and Examples	The installation file path for the legacy version of TC-Toolbox is to the same location as where you install Thermo-Calc. However, the examples continue to be accessed from a different folder as described below. Examples for the *legacy* TC-Toolbox are placed under MATLAB® in the same documents folder as the Thermo-Calc files (Documents folder): `..\Documents\MATLAB\Thermo-Calc-Toolbox-X\Examples` Where *X* is the installed version number of the toolbox. For most installations the examples are available in the MATLAB® window when the software is opened.

Which TC-Toolbox Installation Should I Choose?



MATLAB® must be installed before you install TC-Toolbox.

Review the topic About TC-Toolbox for MATLAB® where the differences between the new and legacy versions of the SDK are discussed.

In general, the new version has more functionality and is more robust. However, if you are a long-time user of the legacy TC-Toolbox for MATLAB® you may want to work in parallel as you transfer your scripts, in which case installing these side-by-side can be useful. You can use both versions from within MATLAB® at the same time, although there is no communication between the two.

There are these options to install:

- Install only the *new* version of TC-Toolbox. See Installing the New TC-Toolbox.
- Install only the *legacy* TC-Toolbox for MATLAB®. See Installing TC-Toolbox with the Custom Option.
- Install both versions of the SDK in parallel (these do not interact with each other). Follow the instructions for each installation separately or do it at the same time via the Installing TC-Toolbox with the Custom Option.

Installing the New TC-Toolbox

These instructions are relevant to the new version of TC-Toolbox for MATLAB®.

Automatic Installation of TC-Toolbox

When the following conditions are met, Thermo-Calc automatically installs the TC-Toolbox for MATLAB® component on your computer.

1. MATLAB® is already installed.
2. There is only one Windows user on the computer where TC-Toolbox is being installed.



Administrator privileges are needed when you start the Thermo-Calc installer.

Then follow the regular installation instructions for Thermo-Calc, choosing whether you use a Standalone or Network installation. If required also see Testing a TC-Toolbox Installation.



A reminder regarding the license. Although you do not need to have a license file during the installation process (it can be added after the fact), you do need to have purchased a license for TC-Toolbox for MATLAB® to run the program within MATLAB®.

Manual Installation of TC-Toolbox

The installation is not automatic if:

- There are multiple Windows users on the same machine, or
- The installer cannot find the directory path to the MATLAB installation.

Multiple Windows Users on Same Machine

If there are multiple windows users on the same machine, then the following manual steps are done at the end of the automatic installation.

1. A message at the end of the Thermo-Calc installation process displays with instructions.
2. An Explorer window automatically opens to the `C:\Users\Public\Documents\Thermo-Calc\2021b\SDK\TC-Toolbox-MATLAB` folder.

3. Double-click the `InstallTCToolboxMATLAB.cmd` file to finalize the process. This briefly launches MATLAB® and installs TC-Toolbox. If required see Testing a TC-Toolbox Installation.

Installer Cannot Find the MATLAB® Installation Directory

If the Thermo-Calc installer cannot find the MATLAB® installation directory, follow the instructions for Installing TC-Toolbox with the Custom Option.

Installing TC-Toolbox with the Custom Option



MATLAB® must be installed before you install TC-Toolbox.

As described in Installing the New TC-Toolbox, if MATLAB® is already installed, then Thermo-Calc automatically installs the files you need either using the *Full Standalone* or *Full Network Client* installation where you **install all features**. Otherwise you need to use the **Custom** installation.

The following generally describes the **Custom** option for either a Standalone or Network installation. Use the **Custom** option in these cases:

- To install *Legacy TC-Toolbox for MATLAB®*. The legacy TC-Toolbox needs to be installed on the same computer or on a server with the Thermo-Calc software and database package.
- If MATLAB® is installed but the Thermo-Calc installer is not finding the directory path so you need to enter the path manually.
- If you want to install both the new and legacy versions at the same time.

Some steps are described in more detail in other parts of this guide.

Request your License File from Thermo-Calc Software



A reminder regarding the license. Although you do not need to have a license file during the installation process (it can be added after the fact), you do need to have purchased a license for TC-Toolbox for MATLAB® to run the program within MATLAB®.

Download your Thermo-Calc Installation Software

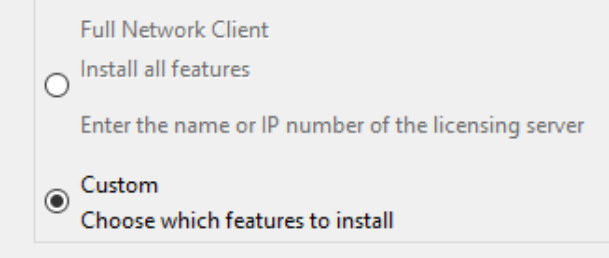
Install MATLAB®

Run the Thermo-Calc Installation File as an Administrator

1. Locate the Thermo-Calc installation file on your computer. Right-click the **.exe** file and choose **Run as administrator** to launch the **Setup** program.
2. Accept the **License Agreement** and click **Next**.

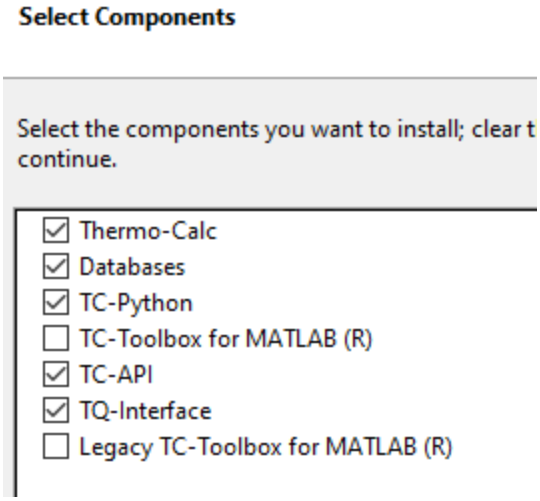
Select the Custom Installation Type

1. In the **Select Installation Mode** window click **Custom** (the option appears greyed out, but it is available to select). Click **Next**.



2. On the **Specify Configuration** window the **Create Shortcut on Desktop** check box is selected by default. Click **Next**.

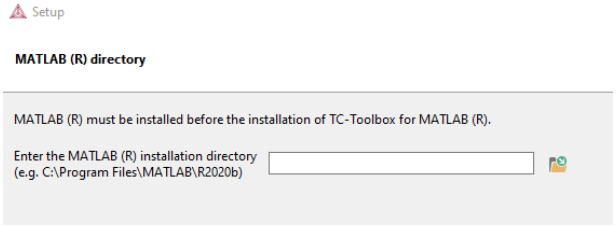
3. In the **Select Components** window, click to select the **TC-Toolbox for MATLAB** check box for the new version and **Legacy TC-Toolbox for MATLAB** for the old one. You can select both at the same time to install these in parallel.



> Remember, you must have MATLAB® already installed and may need to know the file path to the MATLAB® folder. If the **TC-Toolbox for MATLAB** check box is NOT selected, this confirms that the Thermo-Calc installer did NOT locate the MATLAB® installation (or it is not installed yet). The **Legacy TC-Toolbox for MATLAB** check box is never automatically selected.

4. Click **Next**.

5. If you selected one or both of the **TC-Toolbox for MATLAB** check boxes, the **MATLAB directory** window opens.

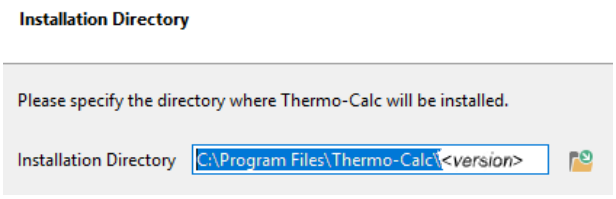


   - If MATLAB® is already installed but the Thermo-Calc installer could not find the path, then enter the file path to the MATLAB® installation directory or click the file button to **Browse for Folder** and navigate to the directory. Click **Next**.

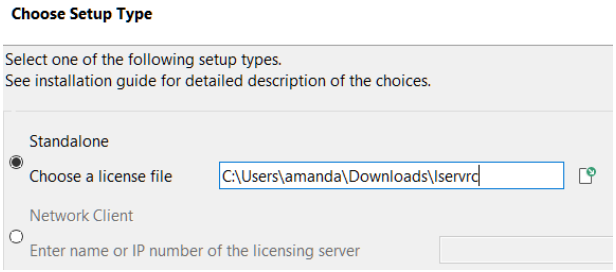
   - If MATLAB® is NOT installed, click **Cancel** to exit the Thermo-Calc installer program. Once MATLAB® is installed you can return to this process.

Set the Thermo-Calc Installation Directory and Choose the Setup Type

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the Thermo-Calc software. Click the file button to **Browse for Folder** and navigate to another directory.



2. In the **Choose Setup Type** window, click **Standalone** or **Network Client**.



   - For a Standalone installation: In the **Choose a license file** field enter the path to your license file (called **lservrc**).
   - For a Network installation: Enter the details as required into the **Enter the name or IP number of the licensing server** field. Click **Next**.

> If the **TC-Python** check box is also selected to be installed (which it is by default), the **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed.

Install and Start Using Thermo-Calc as an Add-on in MATLAB®

1. In the **Ready to Install** window click **Next**.

> If MATLAB® is not installed (and you selected either or both TC-Toolbox check boxes) a message displays to confirm that TC-Toolbox will not be installed until you complete the MATLAB® installation. If MATLAB is installed, click **Back** to confirm that the installation path is correct, otherwise **Cancel** this Thermo-Calc installation, install MATLAB and start again.

2. Click **Finish**.

Test the Installation

- Testing a TC-Toolbox Installation

Testing a TC-Toolbox Installation

There are different ways to test the installation based on whether you are using the new or legacy version of TC-Toolbox.

New TC-Toolbox: Test the Installation

Generally you can check the installation by first looking in the **Home** tab to see if the program is in the menu. Then proceed to running the diagnostic script or another example.

To check the installation, in MATLAB®:

1. From the **Add-Ons** menu, select **Manage Add-Ons**.

   If TC-Toolbox is in the list it is likely it installed correctly but it is recommended you run the diagnostic script or another example to confirm.

2. Run the diagnostics script from the folder `C:\Users\<user>\Documents\Thermo-Calc\2021b\SDK\TC-Toolbox-MATLAB\Examples\Miscellaneous` or open and run any other example to test.

   The TC-Toolbox diagnostic script is also available from our website.

Legacy TC-Toolbox: Test the Installation

Once the legacy installation is complete, you can test the connectivity in MATLAB®.

Start MATLAB and type: **tc_init_root** in the command window and press return. This should result in no return message for a successful installation.

To get a short description of each command type in the command window **help Thermo-Calc-Toolbox** *X* (where *X* is the installed version number of the toolbox).

TC-Toolbox Installation Troubleshooting

Below are some suggestions to help troubleshoot a TC-Toolbox for MATLAB® installation.

Diagnostic Script (New TC-Toolbox)

A diagnostic script is available to help you if you have problems running TC-Toolbox.



It is important to run this script EXACTLY the same way as you run your MATLAB® script.

The script automatically prints useful suggestions that, in many cases, will help you to fix the problem yourself. If you are unable to solve the problem, contact us for support.

The script is based on the version of Thermo-Calc installed and named `tc-toolbox-diagnostic-script-2021b.m`. You can find the script in these locations:

- As an example (`diagnostics.m`) located in this folder `C:\Users\<user>\Documents\Thermo-Calc\2021b\SDK\TC-Toolbox-MATLAB\Examples\Miscellaneous`
- In the **Troubleshooting** section of the *TC-Toolbox for MATLAB® API Reference Documentation*. Also refer to the **Best Practices** in the same guide to see if there are any other solutions or tips.
- On our website.

MATLAB® Installation Directory Not Found

This is applicable to both new and legacy installations.

For Windows installations of the TC-Toolbox for MATLAB® component, you may get an error message or window asking for the MATLAB® installation directory path.



The most common reason for this is that MATLAB® is not installed. If this is the case, exit the Thermo-Calc installation, install MATLAB® and then run the Thermo-Calc installation program again.

If MATLAB® is installed and Thermo-Calc just did not find the file path during the installation setup process, then enter the path in the field when prompted.

Determining the Licensing Software Version (Network Installs)

Sometimes you may need to know the version of License Manager (Windows) or License Server (Linux) software being used. This can be useful while troubleshooting network installations.

- On *Windows* open a command prompt and go to the directory where `lservnt.exe` is found. For example:

  ```
  >C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS
  License Manager\WinNT
  ```

  Type the command `>lservnt.exe –help` and the version is displayed.

- On *Linux* open a Terminal window and go to the directory where the `lserv script` is saved. For example:

  ```
  >cd opt/Thermo-Calc/<version>/Licensing-files
  ```

  Type the command `>./lserv –help` and the version is displayed.

Uninstalling TC-Toolbox for MATLAB®

Uninstalling the New TC-Toolbox

Uninstallation requires that the user is logged in with administrator rights and Thermo-Calc is installed for this same user. Then the uninstallation is automatically completed as part of the uninstallation of Thermo-Calc. Otherwise a manual step is required.

To uninstall TC-Toolbox (when not automatically uninstalled):

1. Start MATLAB®.
2. In the **Home** tab from the **Add-Ons** menu, select **Manage Add-Ons**.
3. Right-click **TC-Toolbox** and choose **Uninstall**.

Uninstalling the Legacy TC-Toolbox

Uninstallation of the legacy SDK requires that the user is logged in with administrator rights and Thermo-Calc is installed for this same user. Then the uninstallation is automatically completed as part of the uninstallation of Thermo-Calc.

Troubleshooting



There are diagnostic scripts available for TC-Python and TC-Toolbox for MATLAB® (these are included as examples in the Miscellaneous folder). These scripts are also available on our website.

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License Errors

Issue	Platform	Installation type	Action or link to more information
How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?	Windows	Standalone	Determining the Current License File Directory Path
How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?	Linux	Standalone	Determining the Current License File Directory Path
How do I add or update a network license on Windows?	Windows	Network	Determining the Current License File Directory Path
How do I add or update a network license on Linux?	Linux	Network	Determining the Current License File Directory Path
No license file found. Copy a valid license file to the installation directory after completing the installation.	All	All	You get this message if the wrong path or no license file is found at a path entered during the installation process. See Installation Default Directories and the License File and Determining the Current License File Directory Path
TC-Toolbox for MATLAB® (new and legacy versions)	Windows	All	TC-Toolbox Installation Troubleshooting
Warning Environment variable “LSHOST” is not set. Software will not function properly.	All	Network	Specifying a New Server Name or IP Number
Problem running post-install step. Installation may not complete correctly. Unable to run post-installation script, run the license initialization script as root after the installation.	Linux and Mac	Standalone	macOS Installations: Running the License Initialization Script or Linux Installations: Running the License Initialization Script
Firewall warnings related to license management software (License Manager and License Server)	Windows and Linux	Network	Firewalls
Client / Server naming mismatches	Windows and Linux	Network	Client/Server Mismatch

Issue	Platform	Installation type	Action or link to more information
InstallScript engine missing	Windows	Network	You are not notified if the InstallScript scripting engine is not installed. Install the ISScript.msi file and then run the downloaded file from Thermo-Calc again as described in Windows: About Installing the License Manager

Determining the Current License File Directory Path

This topic explains how to find out where your license file is installed, either by default or if a different directory was chosen for previously installed versions. For new installations, where you may not have had a license file when you installed Thermo-Calc, you can also use these instructions to determine the correct file path.

From Thermo-Calc

If you have already installed Thermo-Calc, you can view the path to the license file in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command DISPLAY_LICENSE_INFO.

Windows Standalone Installations

How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?

1. Unpack the .zip file that contains your standalone license and save the LSERVRC file on your computer. Find out where to place the new license file by opening a Command Prompt Window (cmd.exe) and type in the command line:

   ```
   >set LSERVRC
   ```

2. Press `Enter`. The output from the command is the path to the license file (including the name of the license file). For example: if the output is

   ```
   LSERVRC=C:\Users\<user>\Documents\Thermo-Calc\lservrc
   ```

   then the new license file should be placed in `C:\Program Files\Thermo-Calc\2021b\`

Linux Standalone Installations

How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?

Find out where to place the new license file by opening a Terminal window and type in the command line:

```
echo $LSERVRC
```

Windows Network Installations

How do I add or update a network license on Windows?

Only the WlAdmin tool can be used to update the network license used by the License Manager. See Install the Thermo-Calc Network License Using WIAdmin.

Linux Network Installations

How do I add or update a network license on Linux?

Replace your current license file with the new license file. The license file is located in the same directory as the license server.

Specifying a New Server Name or IP Number

The Thermo-Calc Setup wizard does not warn you if the name or IP number entered to the server (with the license management software) is incorrect.

If the name or IP number is not set at all, or if it is set to an empty string, then when you start Thermo-Calc the following message displays: *Warning Environment variable "LSHOST" is not set. Software will not function properly*.

Windows

This section explains how to specify or change the name or IP number of the server where the License Manager is installed and for a consolidated network client installation.

To install a license for an existing Thermo-Calc program, follow these steps:

1. Close all running Thermo-Calc programs.
2. Open a command line window.
3. Specify the name or IP number of the licensing software server. Type:

   ```
   set LSHOST=<name/IP number>
   ```

   To display the current name or IP number, type:

   ```
   set LSHOST
   ```

macOS

Permanently set the environmental variable LSHOST to specify a new licensing server name or IP number. Refer to the file `/Applications/Thermo-Calc-2021b.app/Contents/Info.plist`.

In this file, you can manually set the TC21B_HOME variable, which specifies the home directory of the Thermo-Calc program. See the `Info.plist` file for an example.

Linux

You can set or change the name or IP number of the license server at a later time by setting the environmental variable "LSHOST" to this name or number.

Firewalls

Windows

For a Windows License Manager installation you may have to change the system firewall settings to allow the License Manager to communicate with the computers running the client applications. Go to the Windows Firewall settings window to see if there are any problems. If prompted, select Unblock the system firewall for the Sentinel RMS License Manager and click Next.

Linux

For a Linux License Server installation you need to open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting SELINUX=permissive in the /etc/selinux/config file.

Client/Server Mismatch

For some network installations there can be a naming mismatch that causes errors. The server (where the license management software is installed) gets information from its DNS servers that an IP address (aaa.bbb.ccc) belongs to a computer (Computer A). But the client computer identifies itself as having a different IP address (aaa.bbb.ccc.eee) for the same computer (Computer A).

Even if the IP address of the client computer belongs to a subnet range listed in the license file, there is a problem with accessing the license file because the computer name does not match the information.

You may need your organisation's network administrator to assist with this issue.

How to Check

Compare computer names on the client computer and server

1. On the client computer, start a command prompt **cmd.exe** and type `ipconfig /all`. Press `Enter`. A variety of data is displayed on screen. Write down the following information for later comparison:
    - Hostname
    - DNS Suffix
    - Current IPv 4 Address
2. In the command window, type `nslookup` *<client_computer_name>,* where *client_computer_name* is the actual name of the client. Press `Enter`.

    This shows what information is saved on the DNS Servers used by the client computer. This information should match what is shown in the output from the first step.

3. On the server that holds the license management software, open a command prompt and run the command line: `nslookup client_computer_name`. The output lists the information for this server.

    Does it match the information given by the command ipconfig /all on the client computer? If not try the following.

Try these options to correct the issue

1. If the client computer has a dynamic (DHCP) IP address, either change it to a static one or make a reservation on the DHCP Server so that the computer always get the same IP address.
2. Update the records on the DNS Servers used by both the client computer and the server computer.

You can also configure the computer names and IP addresses in the local Hostfile of the client and server:

1. On the client computer, make a backup copy of the file C:\Windows\System32\drivers\etc\hosts.
2. Open the original in a simple text editor.
3. Add a new line which contains the IP and name of the server, for example: 192.168.29.27 license_server.thermocalc.se.
4. Save the changes.
5. On the server, make a backup copy of the file /etc/hosts.
6. Open the original in a simple text editor.
7. Add a new line which contains the IP and name of the client, for example: 192.168.29.47 Computer_A.thermocalc.se.
8. Save the changes.
9. In the host file, there is an example of how the operating system (Windows or Linux) wants the line in the hosts file to look like.

macOS Installations: Running the License Initialization Script

As part of the Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If this part of the installation process did not complete properly for a standalone installation, you must manually run the license initialization script. You need the administrator username and password for these steps.

How to Run the Script

For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the folder:

```
/Users/Shared/Thermo-Calc
```

Installation Default Directory: macOS

1. Open a terminal window. The **Terminal** application is in the */Applications/Utilities* folder.
2. At the prompt, enter this command:

   ```
   $ sudo /Applications/Thermo-Calc-
   2021b.app/Contents/Resources/license-initialization-macOS-x86_
   64.sh
   ```

   If you are not already logged in as an administrator, you probably cannot run the `sudo` command. If this is the case, then you can use the `su` command in the terminal window to login as an administrator. Contact your local system administrator for help.

3. Enter the administrator password and press `Enter`.
4. When you restart your computer and run the license initialization script, you are ready to start using Thermo-Calc.



If you did not install a license file during this procedure, you can still start Thermo-Calc although you will get the **No license file found** message.

Linux Installations: Running the License Initialization Script

As part of a Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If you get a warning message during the standalone installation Unable to run post-installation script, run the license initialization script as root after the installation, then you need to manually run the script as root.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

How to Run the Script



For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the directory where you have installed Thermo-Calc.

Installation Default Directory: Linux

1. In the console, go to the Thermo-Calc installation directory.
   - The license file is put in `/home/<user>/Thermo-Calc` if you are installing as a non-root user, where `<user>` is your user name.
   - If you are installing as root, then this directory is `opt/Thermo-Calc/`.
2. Enter this command:

   ```
   $ sudo sh license-initialization-linux.sh
   ```

   If you are not able to execute the `sudo` command because you are not on the sudoers list, you must log in as a root user with the command `su`, and then use `sh` to run the license initialization script. For example, on a 64-bit computer, enter the following:

   ```
   $ sh license-initialization-linux.sh
   ```

3. Log out of Thermo-Calc and then log back in to save these changes.

Sentinel RMS License 9.7 Tools

These tools relate to Network Client installations of the Sentinel RMS License software.

- Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server

In this section:

GetHostID: Get HostID/Mac Address 122
lsmon: Monitor License Manager Transactions 123
lspool: Maintain Redundant License Manager Pool 124
lsrvdown: Shut Down the License Manager 126
lswhere: Display a List of License Managers 127
WlmAdmin Administrative Tool 128
Sldemo: Show Basic API Functions 132
Wechoid: Get a Computer Locking Code 136

GetHostID: Get HostID/Mac Address

GetHostID is a tool that retrieves the HostID/Mac address from the computer hosting the license server and saves it to a text file.



For Linux the output file is called `gethostid.log`. For Windows it is called `TC_Hostid.txt`.

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.
- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

Windows

1. Extract `getHostID_win.zip`.
2. Right-click `getHostID_win.bat` and select **Run as Administrator** from the menu.

   The output is saved in a file: `TC_Hostid.txt` located in the same folder as `getHostID_win.bat`.

Linux 32-bit

1. Extract `gethostid.tar`.
2. Run the command: `>./gethostid`.

   The output is saved in a file: `gethostid.log` located in the same directory as `gethostid`.

Linux 64-bit

1. Extract `gethostid64.tar`.
2. Run the command: `>./gethostid64`.

   The output is saved in a file: `gethostid.log` located in the same directory as `gethostid64`.

lsmon: Monitor License Manager Transactions

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

Platforms

Windows, Linux 32-bit, Linux 64-bit

The tool retrieves information about all features currently licensed by the Sentinel RMS License Manager, licenses, and clients.

On UNIX computers, you can use "Poll-interval-in-seconds" to specify that lsmon should keep monitoring and reporting usage activity instead of displaying information once and stopping. If specified, lsmon waits for that many seconds between re-polls of the License Manager.

lsmon monitors all licensed applications supported by a License Manager. If the License Manager supports licensed applications from multiple vendors, then all licenses for all vendors are displayed.

- On Windows, use `lsmon` *[Server-host]*
- On Linux 32-bit, use `lsmon` *[Poll-interval_in_seconds] [Server-host]*
- On Linux 64-bit, use `lsmon64` *[Poll-interval_in_seconds] [Server-host]*

OPTIONS

- *Poll-interval_in_seconds*: Enable periodic update at indicated rate. This option is supported on UNIX only).
- *Server-host*: The name of the computer on which the License Manager is running. If Server-host is omitted, lsmon will attempt to talk to the Sentinel RMS License Manager on the computer indicated in the LSHOST environment variable or in the LSHOST (or lshost) file. If the variable or the file does not exist, then it will attempt to contact a License Manager using the broadcast mechanism. If lsmon fails to find a Sentinel RMS License Manager, it will display an error message and exit.

lspool: Maintain Redundant License Manager Pool

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

lspool is a redundant License Manager administration utility (command-line) for Windows and UNIX.

OPTIONS

- `h` Displays a list of lspool usage options.
- `a` *<license manager>* Adds the License Manager to the redundant License Manager pool. Specify the hostname or IP address of the License Manager system. Modifies the redundant license file.. On Windows, dynamic addition of License Manager in an existing redundant pool is not supported.
- `d` *<license manager>* Deletes the License Manager from the redundant License Manager pool. Specify the hostname or IP address of the License Manager system. Modifies the redundant license file. On Windows, dynamic deletion of License Manager in an existing redundant pool is not supported.
- `l` Displays the host name of the leader redundant License Manager.
- `p` Displays the list of License Managers in the redundant License Manager pool.
- `g` *< feature> <version>* Displays the license token distribution criteria for the specified feature/version. If the version is not specified, it must be replaced with empty quotation marks: " ".
- `L` *<event> <OFF|ON>* Disables/enables logging for an event. The events you select will be logged into the License Manager trace log file (only if error logging is enabled).

LSPOOL - L OPTIONS

Events that can be logged using the -L option are given below. The following events are temporarily logged (except 1) and need to be set each time the License Manager is restarted.

- `0` Logs all events.
- `1` Logs when the License Manager is up. On by default. 2 Logs election of the leader License Manager.
- `3` Logs the two-way redundant License Manager heartbeat:> Leader License Manager periodically logs the update status received from all its followers

  > Follower License Manager periodically logs the update about the contact established with the current leader License Manager

- `5` Logs the usage information event, shared by the leader, regarding the number of tokens issued. 7 Logs the license token distribution information synchronization event.
- `9` Logs when the License Manager is down.
- `11` Logs addition of a license into the file or memory. Also logs deletion of a license from the memory.

lsrvdown: Shut Down the License Manager

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

lsrvdown utility is used to shut down the named License Manager.

Platforms

Windows, Linux 32-bit, Linux 64-bit

- On Windows and Linux 32-bit use `lsrvdown host-name`
- On Linux 64-bit use `lsrvdown64 host-name`

lsrvdown can be run from the operating system command prompt by an administrative user on a client or License Manager computer.

- On UNIX, only the user logged in as “root” can use lsrvdown.
- On Windows, any user with administrative privileges may use lsrvdown unless the License Manager was started by a user logged in as Administrator, in which case only Administrator can shut the License Manager down. The computer on which you are running lsrvdown must be in the same network domain as the License Manager computer.



The same user must install the Sentinel RMS License Manager and also run this utility.

lswhere: Display a List of License Managers

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

Platforms

Windows, Linux 32-bit, Linux 64-bit

lswhere command displays the network names of the computers running the License Manager. By default, lswhere displays for each License Manager the address of the computer on which that License Manager is running as well as its host name.

lswhere can be run on Windows and UNIX. lswhere should be run from the operating system command prompt by an administrator or application user on a standalone, client, or License Manager computer.

lswhere should be run in the following format:

- Windows and Linux 32-bit: `lswhere` *[option]*
- Linux 64-bit: `lswhere64` *[option]*

OPTIONS

- `d` Displays details on the License Managers found on the network.
- `r` Displays only the IP addresses of the License Managers found on the network (resolves the host names). lswhere can also be run without specifying any command line options.

WlmAdmin Administrative Tool

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager for Windows, version 9.7.
- The tool is applicable to Windows operating systems. See Windows: Installing the Sentinel RMS License Manager.

WlmAdmin performs a variety of administrative functions for the license management activities. It displays elaborate information that includes the License Manager information, feature information, and license and client information.

Platform

Windows



WlmAdmin can administer a remote Linux license server.

WlmAdmin Functions

- Provides information on the License Managers.
- Details on licenses and clients using them in the network. For example, the administrator can see which users have acquired that license and who are in a queue waiting for the license.

If you are using redundant License Managers, you can use WlmAdmin as an informational tool to:

- Add or delete a redundant License Manager from the redundant License Manager file.
- Display a list of all License Managers in the redundant License Manager pool and display the name of the License Manager leader.
- Display the distribution criteria for specific licenses (only high assurance model is allowed, where the reigning leader server keeps all the license tokens).

View License Manager Information

- Click the name of a License Manager in the left-hand pane of the main window. In the right-hand pane of the display, you see the IP address of the computer containing the License Manager and its host name.

Add or Remove a License Manager from the Defined Server List

- To add a License Manager: Right-click the name of a License Manager in the list of Subnet Servers. From the menu select **Add to Defined List**.
- To remove a License Manager: Right-click the name of a License Manager in the list of Defined Servers. From the menu select **Remove from Defined List**.

Add a License Code to the License Manager from a File

1. Right-click the name of a License Manager in the left-hand pane of the main window.
2. From the menu select **Add Feature > From a File > To Server and its File**.
3. To add the license from a file, select **From a File**. This permanently adds the license code to the License Manager license file as well as to the License Manager memory.
4. In the new windows, browse to the source file that contains the license code and click **Open**.
5. Select the license code file.

Delete Old License Features from the License Manager

1. Right-click the file `WlmAdmin.exe` and select **Run as Administrator**.

   If the license server is not found under subnet servers, go to **Edit > Defined Server List**.

2. Enter the host name or IP address of the license server.
3. Click **Add** and **OK**.
4. Click **View > Refresh All** to update the list.
5. Right-click the name of a License Manager in the left-hand pane of the main window.
6. From the menu select **Remove all Features**

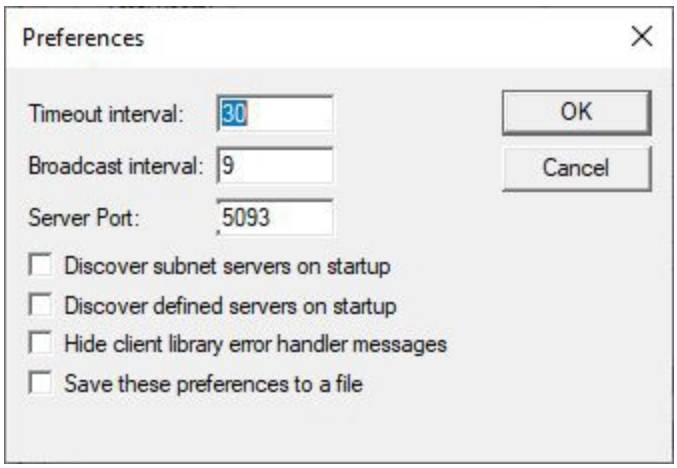
Shut Down a License Manager

- Right-click the name of a License Manager in the left-hand pane of the main window. From the menu select **Shutdown Server**.

Setting WlmAdmin Preferences

WlmAdmin allows you to choose what to display when it starts.

From the **Edit** menu, select the **Preferences** command to view WlmAdmin Preferences:



- **Timeout Interval**: The number of seconds after which WlmAdmin will stop trying to contact a License Manager. If you have a large network or a slow one, you might want to increase this number if you find WlmAdmin has difficulty retrieving information from License Managers.
- **Broadcast Interva**l: Specify the number of seconds between broadcasts to the network to discover License Managers.
- **Server Port**: To set any custom port (other than the default port 5093) on which the RMS License Manager is running.

  Set this port number before you add that License Manager in the list of defined servers.

- **Discover subnet servers on startup**: To automatically discover and display the License Managers on your subnet.
- **Discover defined servers on startup**: To always show the License Managers you have defined.
- **Show client library error handler messages**: To pass license management error

messages from Sentinel RMS to WlmAdmin.

- **Save these preferences to a file**: To save your choices.

Sldemo: Show Basic API Functions

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager for Windows, version 9.7.
- The tool is applicable to Windows operating systems. See Windows: Installing the Sentinel RMS License Manager.

slmdemo is a Windows-based graphical sample program to show basic API functions. Evaluate it using the steps described here to understand the basic API calls and test the connectivity between client and license server

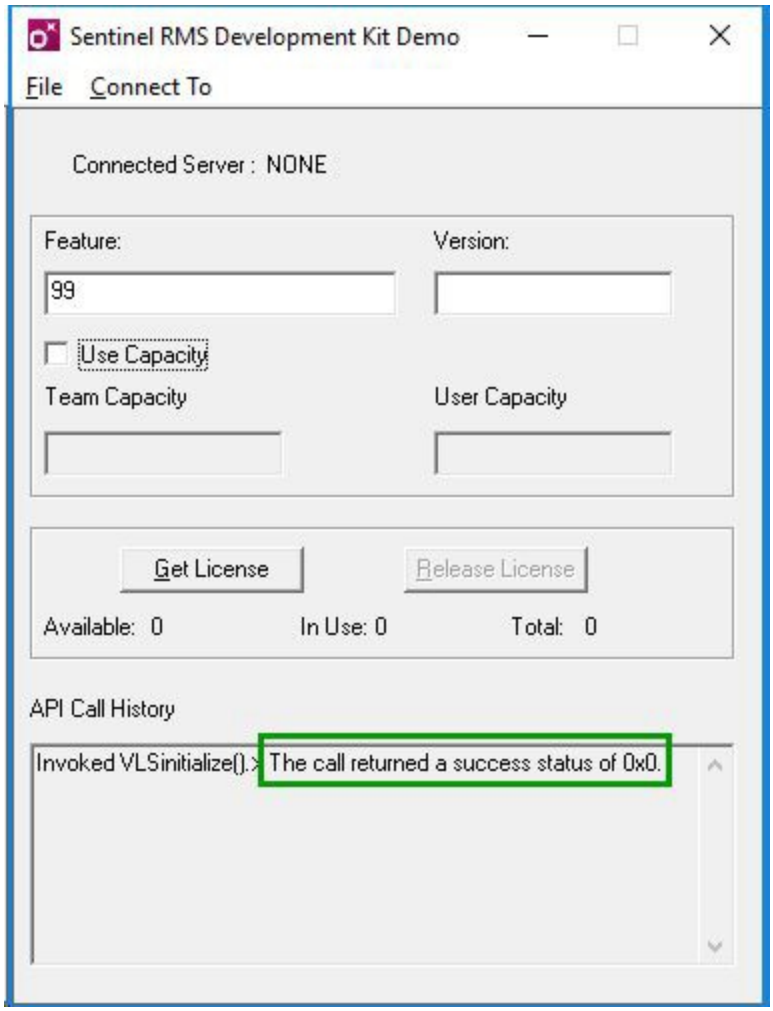


slmdemo can be used to test the connectivity to a remote Linux license server

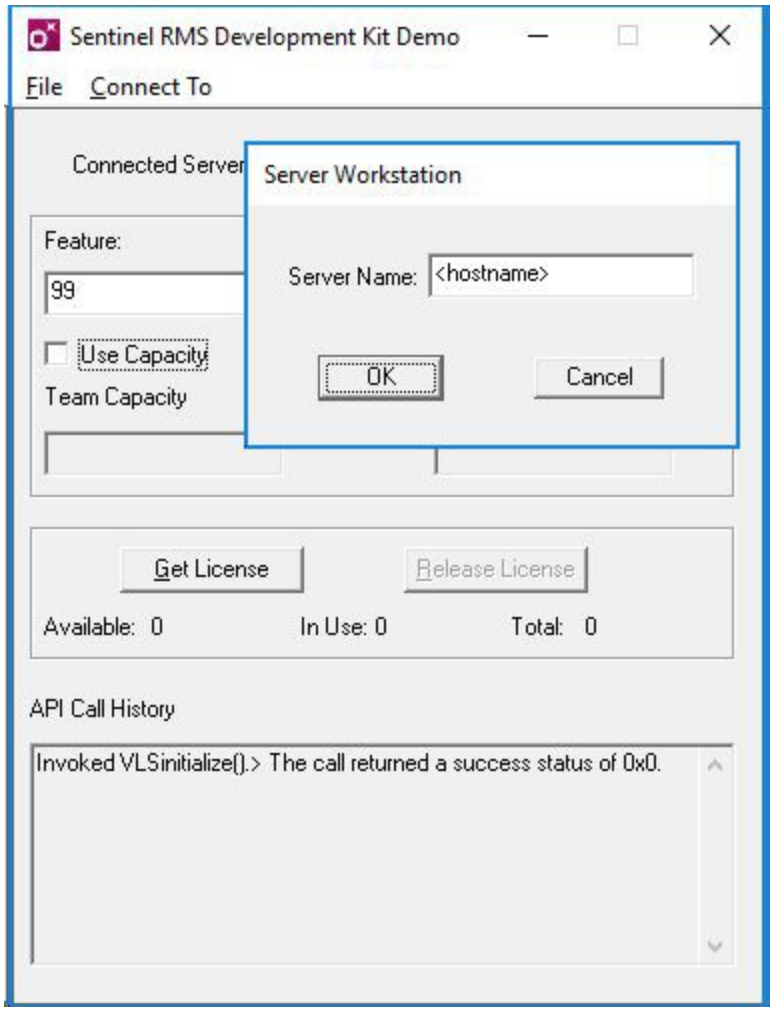
Platform

Windows

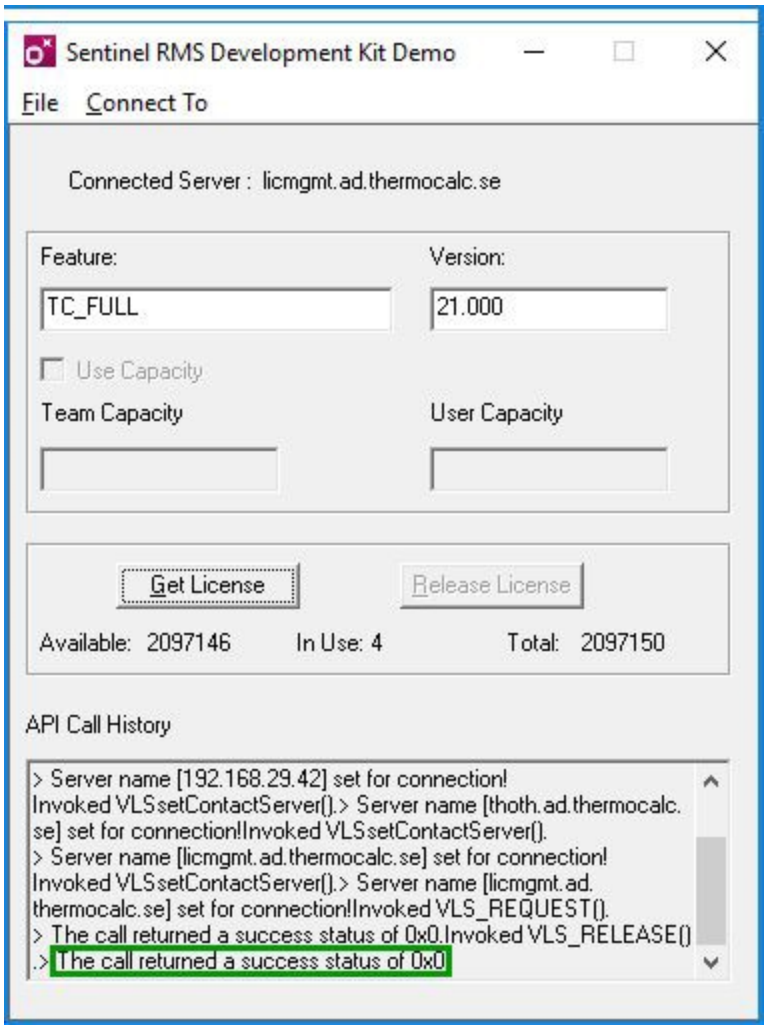
Right-click on the executable and select **Run as administrator**. slmdemo calls the VLSinitialize API when the application is invoked successfully.



Set the contact server (License Manager) under the **Connect To > Server** menu option. Enter a `hostname` , which is the hostname or IP address of the License Server.



Click **OK** and enter in the field one of the license features available in the network license file. Where *Feature* is the name of the feature ex. **TC_FULL** and *Version* is the license version in the NWL (Network) license. Click **Get License**. The message `The call returned a success status of 0x0` means that the connection client <> license server works.



To save the log, click **File > Save log**.

Wechoid: Get a Computer Locking Code

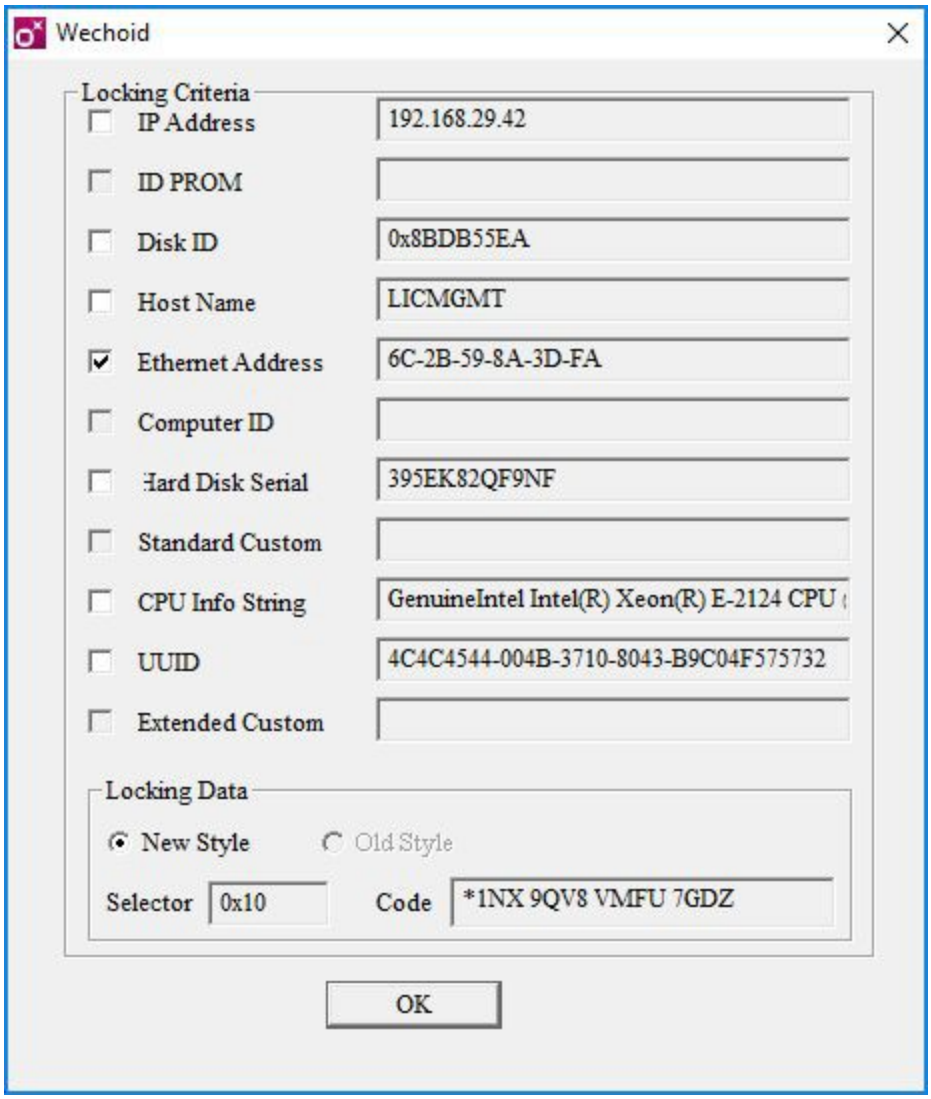
- This is related to the Full Network Client Installations using the Sentinel RMS License Manager for Windows, version 9.7.
- The tool is applicable to Windows operating systems. See Windows: Installing the Sentinel RMS License Manager.

Before your software vendor creates a license code with any computer restrictions, you must get the locking code for your computer with the Wechoid program. Your software vendor will tell you which computers you must run Wechoid on. The Wechoid utility outputs either one or two hexadecimal locking codes depending upon how your software vendor has configured it. You will send all locking information to your software vendor. Your software vendor will use this information, which is specific to your computers, to generate new license codes.

Platform

Windows

When launched, the utility shows the available lock criteria (a checkmark is added next to each) and the values. Click to clear (uncheck) all check boxes except for **Ethernet Address**.


Wechoid
Locking Criteria
IP Address
192.168.29.42
ID PROM
Disk ID
0x8BDB55EA
Host Name
LICMGMT
Ethernet Address
6C-2B-59-8A-3D-FA
Computer ID
Hard Disk Serial
395EK82QF9NF
Standard Custom
CPU Info String
GenuineIntel Intel(R) Xeon(R) E-2124 CPU
UUID
4C4C4544-004B-3710-8043-B9C04F575732
Extended Custom
Locking Data
New Style
Old Style
Selector
0x10
Code
*1NX 9QV8 VMFU 7GDZ
OK

Uninstalling the Software

Also see Uninstalling TC-Toolbox for MATLAB®

In this section:

Uninstalling Thermo-Calc 139

Uninstalling Thermo-Calc

Uninstalling TC-Toolbox for MATLAB®

Windows 10

1. From the **Control Panel** Desktop app, go to **Programs → Programs and Features → Uninstall or change a program**.
2. In the list of programs, locate the version of Thermo-Calc you want to uninstall. Click to highlight that row.
3. Click **Uninstall/Change**.
4. In the **Setup** window, **Uninstallation Mode** dialog box, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

macOS

Deleting the program from the Applications folder does not remove the program from your operating system. Run the **Thermo-Calc-**<*version*>**-uninstaller** program located in the Applications folder.

1. Go to the **Applications** folder and double click the file that starts with **Thermo-Calc-**<*version*>**-uninstaller**. Enter the administrator's user name and password.
2. Click **Yes** to choose **Entire application** or select individual components. Otherwise click **No** to quit.
3. The **Uninstalling Thermo-Calc** window shows the progress. Click **OK** when prompted.

Linux

1. To start the uninstallation procedure, in the Thermo-Calc installation directory use the command
   ```
   ./Thermo-Calc-2021b-uninstaller.run
   ```
   For *Thin Client* installations, use the command
   ```
   ./Thermo-Calc-client-2021b-uninstaller.run
   ```
2. To remove the whole application, including all its components, select **Entire application** and click **Forward**, or to remove specific components, select **Individual components** and click **Forward**.



If you intend to reinstall Thermo-Calc 2021b it is important to (1) Restart the computer before you reinstall the software and (2) remove the environmental variable TC21B_HOME.

Thermo-Calc User Guide: Graphical Mode

Thermo-Calc Version 2021b



Working in Graphical Mode

In this section:

The Graphical Mode Desktop Layout 3

Menu, Toolbar and Keyboard Shortcuts 4

Organizing the Windows on the Desktop 7

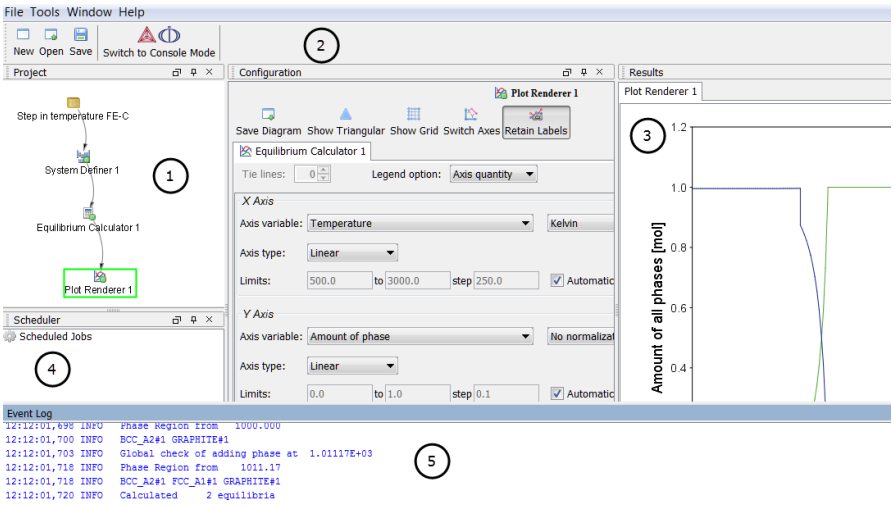
The Graphical Mode Desktop Layout

Open Thermo-Calc to view the default graphical user interface (GUI) layout for Graphical Mode.

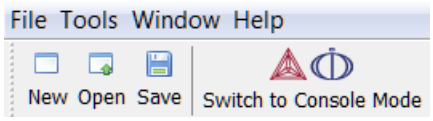
The windows are:

1. **Project**: Create, manipulate and navigate between the activities that make up a project. Click the **My Project** node to access the Quick Start wizard and a variety of templates.
2. **Configuration**: Shows the settings that can be configured for the currently selected activity.
3. **Results**: Shows the results of a calculation, either plotted as a diagram or displayed in table format. In this example, there is a Plot Renderer *tab* in the Results window.
4. **Scheduler**: Displays information about jobs, such as calculations, that are being performed or are scheduled to be performed. You can cancel scheduled jobs and if a job has failed, then you can view information about the error.
5. **Event Log**: By default this window is closed but it displays during calculation processes. You can always open it to view progress of calculations and to troubleshoot.

   In this example, the **Results** window also has a **Plot Renderer** tab. You can also have a **Table Renderer** tab.



Menu, Toolbar and Keyboard Shortcuts



The **File** menu and toolbar are reserved for Graphical Mode but in Console Mode the **Tools**, **Window** and **Help** menus have the same options.

In Console Mode you use commands to access the other options, for example see Main Menu Commands.

Graphical Mode Menu and Toolbar Options

Option	Description	Action (s)
New	Create a new project.	Click **New** on the toolbar Select **File → New Project** Windows: Press <Ctrl+N> Mac: Press < ⌘N>
Open	Open an existing project. See Saving and Opening Project Files.	Click **Open** on the toolbar Select **File → Open Project** Windows: Press <Ctrl+O>. Mac: Press < ⌘O>
Save	Save a project. See Saving and Opening Project Files.	Click **Save** on the toolbar Select **File → Save Project** Windows: Press <Ctrl+S>. Mac: Press < ⌘S>
Save Project As	Save an existing project with a new name.	Select **File → Save Project As** Windows: Press <Ctrl+Shift+S> Mac: Press < ⇧⌘S>
Switch to Console Mode	Launch Console Mode and the command prompt.	Click the button to exit Graphical Mode and open Console Mode.
Switch to Graphical Mode	Launch Graphical Mode to work with the GUI version.	Click the button to exit Console Mode and open Graphical Mode.

Option	Description	Action (s)
Append Project	Combine two projects into one project file. See Saving and Opening Project Files.	Select **File → Append Project** Windows: Press <Ctrl+Shift+O> Mac: < ⇧⌘O>
Exit	Exit the program.	In the upper right-corner of the program, click the X. Select **File → Exit** Windows: Press <Ctrl+Q>. Mac: < ⌘Q>
Options	Change the global defaults for a variety of settings. See Global Settings.	Select **Tools → Options**
Database Checker	Open the Database Checker, a program to check that the syntax of Thermo-Calc database files is correct. This is for advanced users who develop and manage databases.	Select **Tools → Database Checker**
Window menu	Highlight a specific window on the GUI	From the **Window** menu, select an option to refocus on that specific window.
Help	Open the online help system where you can browse or search all the Thermo-Calc documentation.  This does not require an Internet connection. The content is stored locally.	Press <F1> Select **Help → Online Help**
Video Tutorials	Open a link to the Thermo-Calc website where a variety of video tutorials are available.	Select **Help → Video Tutorials**
Examples Files	Open the examples folder based on whether you are in Console Mode or Graphical Mode.	Select **File →** or **Help → Examples Files**
Manuals Folder	Open the folder on your computer that has the PDF documentation and guides.	Select **Help → Manuals Folder**
Show License Info	Open the License Information window.  Also see Displaying Thermo-Calc License Information and the *Thermo-Calc Installation Guide*	Select **Help → Show License Info**
Check for update	Check for updates to the software.	Select **Help → Check for Updates**
Request	Open a link to the Support on the Thermo-Calc website. There are	Select **Help → Request Support**

Option	Description	Action (s)
Support	instructions about how to submit your question.	
About	Includes the version number of the installed software and information about third party software licenses.	Select **Help →About**

Organizing the Windows on the Desktop

The windows on the Thermo-Calc desktop can be fixed or free-floating. By default, most windows are fixed and open.

Auto-Hiding a Window

When a window is fixed it can also be set to auto-hide. Auto-hiding means that the window is minimized when you select another window. The minimized window is then shown either along the bottom or side of Thermo-Calc. A free-floating window is shown on top of the other windows and can be moved outside the frame of Thermo-Calc.



The **Event Log** window is set by default to auto-hide.

Resetting the Desktop Layout

To return to the standard desktop layout, from the main menu, select **Windows → Reset Windows**.

Floating, Hiding and Minimizing Windows in the GUI

For each window you can rearrange, resize, minimize and close it. At the top right corner are the buttons listed in the table.

Button(s)	Description
	Click to toggle on/off free-floating
	Click to toggle on/off auto-hide.
	Click to minimize an open window that has auto-hide turned on. The window automatically minimizes if another window is selected.
	Click to close the window. You can open the window again from the Window main menu.

Projects and Activities

In this section:

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Graphical Mode Activity Node Workflow 12
Creating Activities and Successors 13
Cloning Activities and Trees 15
Moving or Grouping Nodes and Using the Grid 17
Node or Window Status Markers 20
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Working with Batch Calculations 34
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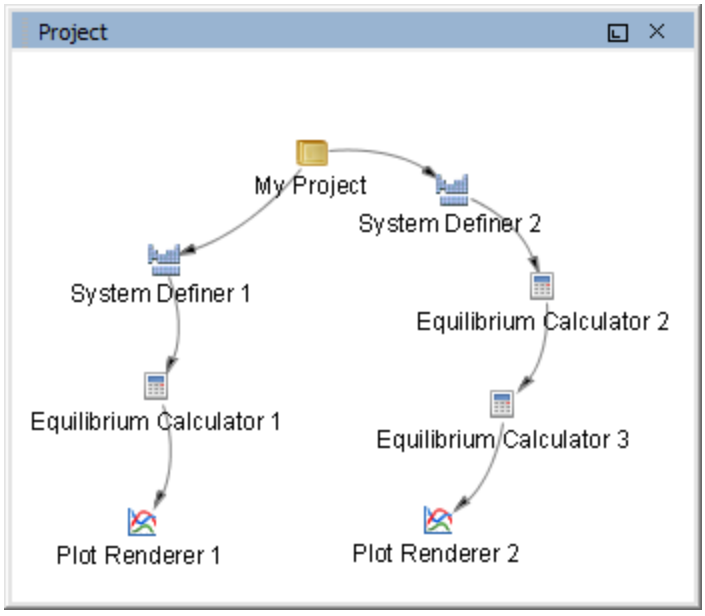
About the Activity Nodes

Graphical Mode Activities vs Console Mode Modules

In a *project*, a set of linked activities is called a *tree*. A result calculated within a tree is fed as input into the next *activity* in the tree. Consequently, if you have an Equilibrium Calculator with another Equilibrium Calculator as its *successor*, the successor takes the calculation results of the *predecessor* as the starting values for its calculation. When working with activities in the Project window these are also referred to as *nodes* (or *activity nodes*) in the tree structure.

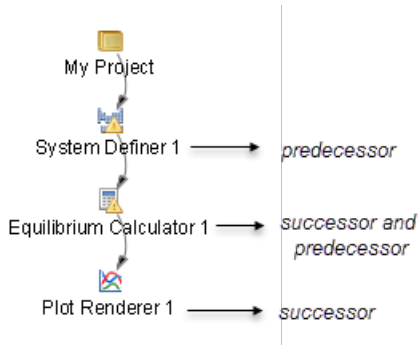
The example below shows a *My Project* node with two trees. In each tree, settings and calculation results are propagated downward until the calculation and the visualization of the results are completed in the *Plot Renderer* nodes.

The system definitions, settings and calculation results of the two trees are independent of each other.



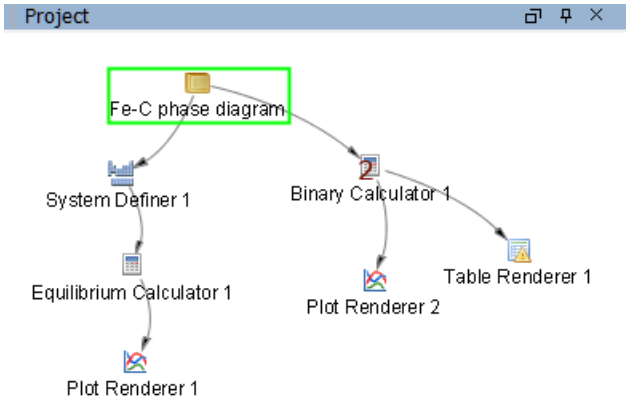
Activity Successor and Predecessor Nodes

An activity node located below another activity node in a tree is referred to as that activity's *successor*. An activity located above another activity is called that activity's *predecessor*. A predecessor is performed before the predecessor's successors and its result is fed forward to any successor activities.



For example, to calculate and display a phase diagram, create a branch with three linked activities: A **System Definer** activity linked to an **Equilibrium Calculator** activity, which in turn is connected to a **Plot Renderer** activity.

You can determine the available successors by right-clicking a node in the **Project** window and choosing **Options** from the menus. The example below shows that **Binary Calculator 1** is a predecessor to the successors, **Plot Renderer 2** and **Table Render 1**.



Creating Activities and Successors and Cloning Activities and Trees

Activity Node Descriptions

The table below is a brief description of the activity types you work with in the **Project** window. When working with activities these are referred to as *nodes* in this documentation.

These are the project activity nodes available in Graphical Mode.

Activity type	Description
System Definer	Define a certain thermodynamic system and read it from file into memory.

Activity type	Description
Property Model Calculator	Choose one or more **General models** and **Steel models** to predict and optimize material properties. You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot.
Equilibrium Calculator	Set thermodynamic conditions and define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions.
Precipitation Calculator	Set the conditions for, and perform, a precipitation calculation using the Precipitation Module (TC-PRISMA). You can also use this in DEMO mode with up to three components.
Diffusion Calculator	Using the Diffusion Module (DICTRA), this activity is where you set the geometry, add one or more regions, enter grids and phases in the regions, and then enter compositions of phases. You can also use this in DEMO mode with up to three components.
Process Metallurgy Calculator	This calculator allows for efficient setup of advanced calculations involving slag, metal and gas. Define the composition of a steel and slag system using material groups: one each for steel, slag and gas.
Plot Renderer	Determine the layout of non-text based output.
Table Renderer	Use it for text-based output.
Binary Calculator	Use it for some calculations involving two components only. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on binary systems.  To perform this activity, you need a database designed for the Binary Calculator, such as the TCBIN database.
Ternary Calculator	Use it for some calculations involving three components. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on ternary systems.  To get a reliable result you need a database that fully assesses binary and ternary systems.
Scheil Calculator	Perform Scheil-Gulliver calculations (also known as Scheil calculations). A default Scheil calculation is used to estimate the solidification range of an alloy assuming that i) the liquid phase is homogeneous at all times and ii) the diffusivity is zero in the solid. However, it is possible to disregard the second assumption for selected components.
Experimental File Reader	Read experimental data files (*.EXP). This type of file contains information specifying a plotted diagram, written in the DATAPLOT graphical language.

Graphical Mode Activity Node Workflow

You can set up a tree in the **Project** window (starting with the **My Project** node) and then perform all the activities at once, or create and perform one activity at a time.



You can also use the templates to add all the necessary activity nodes based on your simulation needs. See Creating a Project from a Template.

The typical workflow is to:

1. *Define a System:* Add a System Definer activity (in the **Project** window) where you select a database and the elements to have as system components (in the **Configuration** window).
   - To the **My Project** node, you can alternatively add and define a Binary Calculator, Ternary Calculator, or Experimental File Reader or Process Metallurgy Calculator activity node.
2. *Set up and run a calculation:* Add an Equilibrium Calculator activity (a successor to the **System Definer**), where calculation conditions are set (temperature, pressure, etc.). This is where axis variables are set to create a property or phase diagram. These settings are also made in the **Configuration** window. You can also add a Property Model Calculator, Precipitation Calculator, Diffusion Calculator or Scheil Calculator to the System Definer.

   ▶ Property Model Calculator Workflow
3. *Visualize the results:* Add either a Plot Renderer or a Table Renderer activity in the **Project** window. When calculated, this creates a plot or table in the **Results** window. The results are shown in a **Plot Renderer** or a **Table Renderer** tab.

   You need to **Perform** a Plot Renderer or a Table Renderer activity to visualize the calculation results from an Equilibrium Calculator.

   ▶ The Quick Start Wizard and Templates

   ▶ About the Activity Nodes

Creating Activities and Successors

You can create a new activity in these ways:

- In the **Project** window, right-click an activity and choose **Create New Activity** (**My Project** node only) or **Create New Successor** (all other nodes).
- Select the activity you want to create from the submenu.
- At the bottom of the **Configuration** window, click **Create New Activity** or **Create New Successor** and select the activity to create.
- Use the **Templates** or the **Quick Start Wizard** (click the **My Project** node and select templates from the **Configuration** window) to quickly add a set of activity nodes to the tree.

Activity	Possible Predecessors	Possible Successors
My Project	None; this is the first node of the tree structure. You can add activities using the Quick Start wizard or templates.  The Quick Start Wizard and Templates	System Definer, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, Experimental File Reader. Also choose templates from this level.
System Definer	My Project, System Definer	Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Scheil Calculator
Experimental File Reader	My Project	Plot Renderer
Binary Calculator	My Project	Plot Renderer, Table Renderer
Ternary Calculator	My Project	Plot Renderer
Process Metallurgy Calculator	My Project	Plot Renderer, Table Renderer
Property Model Calculator	System Definer	Plot Renderer, Table Renderer
Equilibrium Calculator	System Definer, Equilibrium Calculator	Equilibrium Calculator, Plot Renderer, Table Renderer
Precipitation Calculator	System Definer	Plot Renderer, Table Renderer
Diffusion Calculator	System Definer	Plot Renderer, Table Renderer
Scheil Calculator	System Definer	Plot Renderer, Table Renderer

Activity	Possible Predecessors	Possible Successors
Plot Renderer	Equilibrium Calculator, Property Model Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, Process Metallurgy Calculator, Diffusion Calculator, Precipitation Calculator, Experimental File Reader	None
Table Renderer	Equilibrium Calculator, Property Model Calculator, Binary Calculator, Scheil Calculator, Process Metallurgy Calculator, Diffusion Calculator, Precipitation Calculator	None

Cloning Activities and Trees

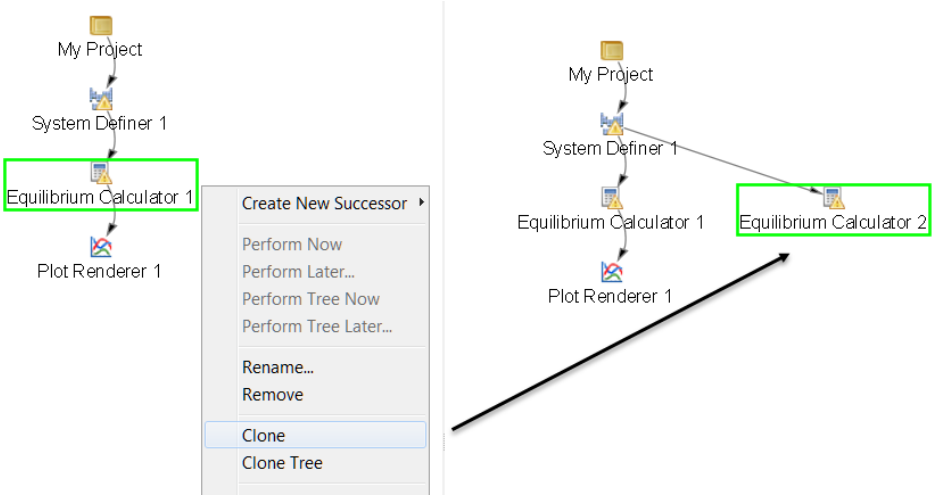
As described in Creating Activities and Successors, you can clone a single activity or the selected activity and all the activities that come after it (successors). The predecessor of the selected activity also is the predecessor of the clone.

Cloned activities are configured exactly like the activities that they were cloned from, and any results of calculations or plots are also cloned. To clone a selected activity, right-click the activity and select **Clone**.

For example, if you clone the Equilibrium Calculator in this project the result is an **Equilibrium Calculator 2** created as a successor to **System Definer 1**.

The following applies to clones.

- The new Equilibrium Calculator has the same settings for conditions, functions and options as its Equilibrium Calculator 1 clone.
- If the Equilibrium Calculator is already performed, then the calculation results are cloned.
- If the activity is a Plot Renderer or a Table Renderer, then the plot or table is cloned.
- If you want to clone all the successor activities that follow a selected activity, then right-click and select **Clone Tree** instead.



Cloning an Equilibrium Calculator activity node

About Equilibrium Calculator Clones and Successors

If you create an Equilibrium Calculator as a successor to another Equilibrium Calculator, then the successor inherits all the settings for conditions, functions and options from its predecessor. In this respect, it is similar to a clone.



The Equilibrium Calculator successor is different from a clone in that it does not inherit any calculated results and it is a successor to the Equilibrium Calculator instead of a successor to its predecessor.

The calculated result from an Equilibrium Calculator that is the predecessor to another Equilibrium Calculator is the starting value for the latter's calculation. The clone of an Equilibrium Calculator on the other hand, does not receive any data as input from the Equilibrium Calculator that it is cloned from.

Moving or Grouping Nodes and Using the Grid

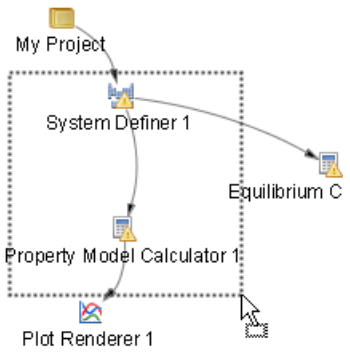
In the **Project** window, you can work with the activity nodes in these ways.

Select and Move Individual Nodes

- Click an activity node to *select* it.
- To move activities, click and hold the activity node and move the cursor.

Select Several Nodes at a Time

- To select several activity nodes, hold down <Ctrl> while clicking on each node you want to select.
- Click and hold the mouse button and draw a square around the activity nodes to select. Both the name and the icon that represents an activity must be within the square.

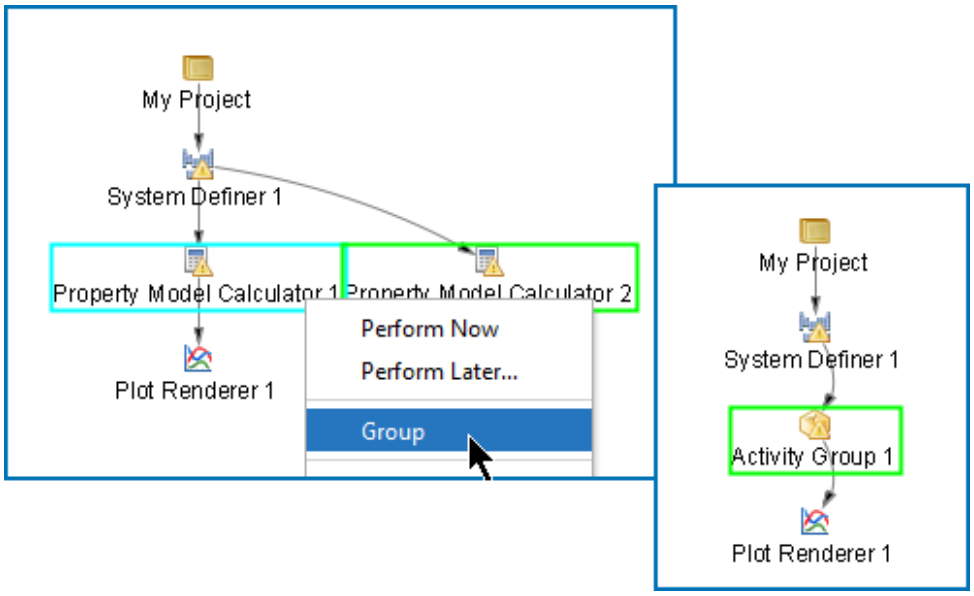


Group Activity Nodes

You can group activity nodes together on the **Project** window. This also creates separate tabs on the **Configuration** window so you can more easily edit the settings for each one. It is important to have logical groupings of nodes because the calculation relies on this connectivity.

In the **Project** window, control+click to select each node, then right-click and select **Group**. An **Activity Group** node is created (you can rename it) and on the **Configuration** window

there are two tabs created, named for each of the group nodes. For example, Property Model Calculator 1 and Property Model Calculator 2. The order of the tabs is based on the order of when you select each node.



Apply Auto Layout

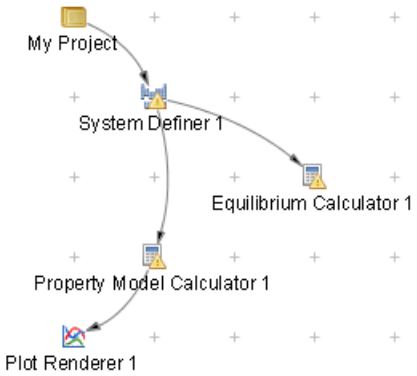
In the **Project** window, right-click anywhere and choose **Apply Auto Layout** from the menu. The nodes and the tree default to the center of the Project window.

Show Grid and Snap to Grid

To show a grid of light-grey cross-hairs overlaid on a project, click **Show Grid** in the toolbar. Click the button again to turn the grid off. Or right-click in the **Project** window and select **Show Grid**.

Click **Snap to Grid** in the toolbar or right-click in the **Project** window and select **Snap to Grid** to automatically position each activity in the Project window at a cross-hairs point in the grid.

The Project window with the grid turned on and activity nodes moved from the default location. These nodes are snapped to the grid.


My Project
System Definer 1
Equilibrium Calculator 1
Property Model Calculator 1
Plot Renderer 1

Node or Window Status Markers

Status markers indicate whether an activity is ready to be performed, is being performed, or has been performed. The markers are overlaid on the activity nodes in the **Project** window. The status markers are displayed on a **System Definer** node.

- About the Activity Nodes

Status Marker Descriptions

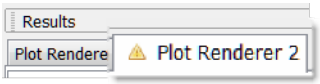
Node Status Markers for the Project and Scheduler Windows

Window	Status marker	Description
Project window		No status marker means the activity is ready to be performed (it has not been performed).
		A yellow triangle means the activity cannot be run. The necessary configurations for the activity may not be set or other prerequisites are not met.
		A green disc means the activity is performed.
		A red circle with a dial (a clock face) means the activity is currently being performed.
Scheduler window		No status marker means the activity (the job) is scheduled to be performed (the job has not started).
		A yellow triangle means there an error happened during the activity job.
		A green disc means the activity (the job) performed successfully.
		A green right-facing arrow means the activity (the job) is being performed.

Results Window Status Marker

If you have plotted a diagram and then modify something in the tree that the Plot Renderer is associated with, then a notification —an exclamation mark enclosed in a yellow triangle— is shown in the Plot tab.

▶ Node or Window Status Markers



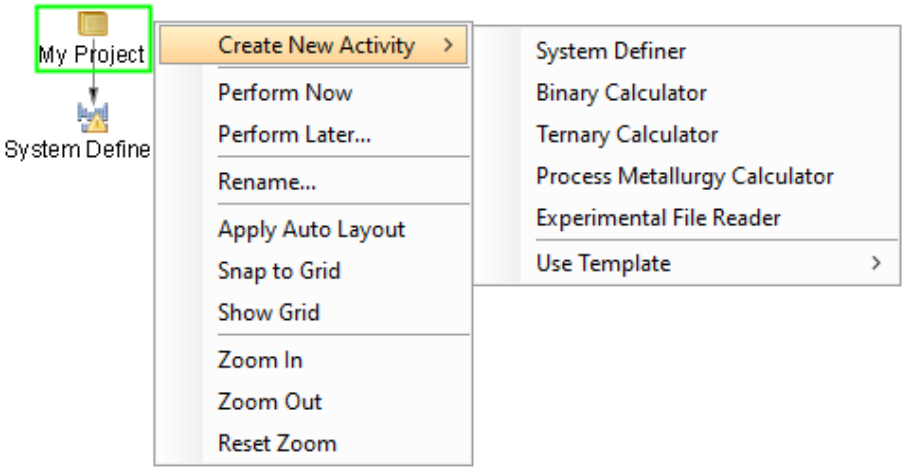
My Project and Activity Menus

When working in the Project window you can right-click nodes to open menus with the available actions. For example, click the **My Project** node to open the menus. Most nodes in the tree have a common menu with differences due to placement in the tree and the activity type.

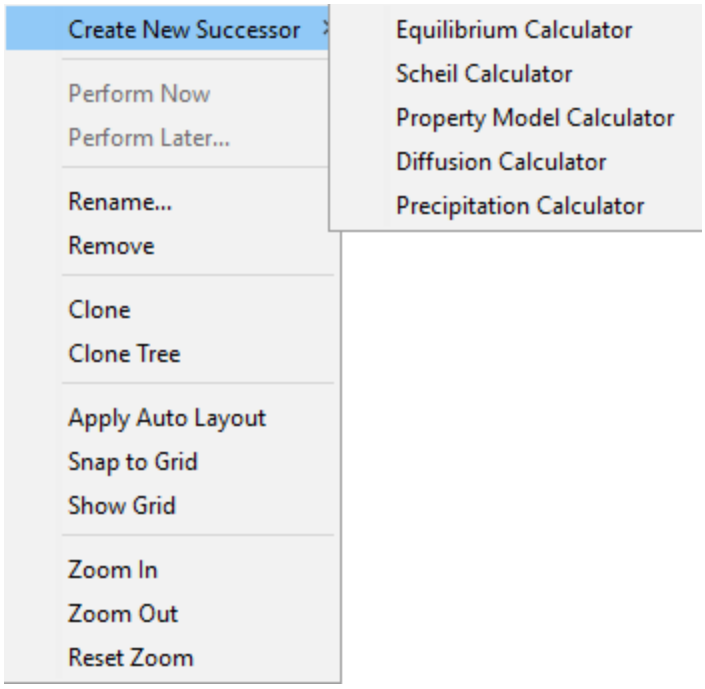
- About the Activity Nodes

Menus

MY PROJECT NODE



ACTIVITY NODE GENERAL



Menu Options for Activity Nodes

Option	Description	Action (s)
Create New Activity	Add System Definer, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, and Experimental File Reader nodes.	Right-click **My Project** and from the **Create New Activity** menu choose an option. Creating Activities and Successors
Create New Activity → Use Template	Choose from the available templates to use the Wizard or add predefined nodes.	Right-click **My Project** and from the **Create New Activity→ Use Templates** menu choose an option. The templates are also available on the **Configuration** window, which you can access by clicking the **My Project** node, or from the **Window** menu.

Option	Description	Action (s)
		Creating a Project with the Quick Start Wizard or Creating a Project from a Template
Create New Successor	Add a successor to the selected node.	Right-click the **System Definer**, any **Calculator** node or the **Experimental File Reader**. Then from the **Create New Successor** menu choose an option. Creating Activities and Successors
Add a Predecessor	Add a predecessor to the selected node.	Right-click a node to add a predecessor to it (when available).
Perform Now or Perform Later	Perform a calculation or create a plot or table immediately, or schedule it for a time in the future.	Right-click any node. Using the Scheduler
Rename	Change the name of the node.	Right-click any node.
Remove	Delete the selected node from the tree.	Right-click any node except My Project.
Clone	Duplicate the selected node and add it to the same tree.	Right-click any node except My Project. Cloning Activities and Trees
Clone tree	Duplicate a tree and add it to My Project.	Right-click any node except My Project.
Apply Auto Layout	Apply an automatic layout to the nodes in the tree.	Right-click any node.
Snap to Grid	Snap a node to align it with the grid.	Right-click any node. Moving or Grouping Nodes and Using the Grid

Option	Description	Action (s)
Show Grid	Turn the grid on or off in the Project window.	Right-click any node.
Zoom In, Zoom Out, Reset Zoom	Zoom in and out of the Project window or reset the zoom to the default.	Right-click any node.

Saving and Opening Project Files

Thermo-Calc Graphical Mode uses project files with the file name suffix `.tcu`. The Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Process Metallurgy Modules also use the same file format in Graphical Mode.

There are different types of file saving based on the stage of a project set up. For example, as you begin to build and design a project simulation, adding and defining a System Definer with applicable calculator, plot or table nodes, and then once you have run a simulation where you now have the option to save with and without the results.

A project file always includes project activities and the configurations. Optionally, the project file may also include calculation results. This increases the size of the file but eliminates the need for re-calculating results when the file is opened later.

Certain simulation results are also more likely to have large file sizes, particularly when working with the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Process Metallurgy Modules.

Saving a Project File

To save your project, on the toolbar click the **Save** button (or CTRL + S, or **File → Save Project**). This saves the file as it is, so if you have previously generated results, it continues to save these to the file. It is recommended that as you build and design your project that you save as you go.

Saving a Project File with Results

If you have generated results you want to keep every time you open the project file, and not previously saved these, from the menu, chose **File → Save Project As** (or CTRL + Shift + S) and then make sure to select the **Include calculated results in the project file** check box. The check box is not available (it is greyed out) if no results have yet been calculated. In this case, go back to your project and click Perform Tree then repeat the steps above.

Click **More information** to learn about the particular results that are saved for each simulation.

Appending a Project

You can only have one project file open at a time in any one instance of Thermo-Calc. However, you can attach (*append*) the trees from additional project files to the topmost **My Project** node. To append an additional project file in this way, from the main menu select **File → Append Project** and open a project file.

- Saving and Printing the Output (Graphical Mode) and *Saving Tabulated Data* for the Table Renderer

Opening a Project File

There are different ways to open project files.

In Thermo-Calc

- From the main menu select **File → Open Project**.
- On the toolbar, click the **Open** button or press <Ctrl+O> (Windows) or < ⌘O> (Mac) on the keyboard. Then navigate to the file on your computer and click **Open**.

On Your Computer

- Navigate to the project file and double-click to open it. This launches a new instance of Thermo-Calc.

How to Open an Example Project File from Thermo-Calc

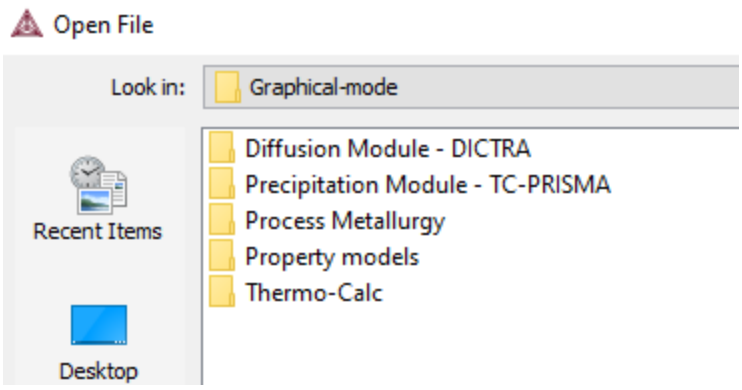


Some Add-on Module examples require additional licenses to run for more than three elements.

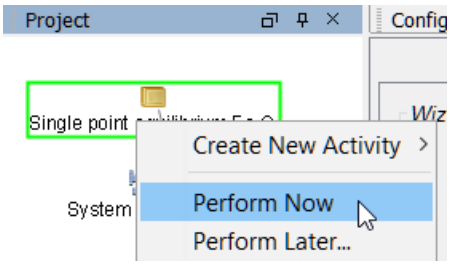
To open an example project file for Thermo-Calc and the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Process Metallurgy Modules:

1. Open Thermo-Calc.
2. Confirm you are in Graphical Mode. If not, click the **Switch to Graphical Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**.

4. The examples are divided into folders. Navigate to the folder and project file you want and double-click to open.



5. The Graphical Mode examples are stored without calculated results so you will want to run the example calculation and generate a plot or table. To do this, click the first node in the tree at the top of the **Project** window. Then right-click and select **Perform now**.



The Calculation Types in Graphical Mode

- Graphical Mode vs Console Mode: Calculation Types

Binary Calculator

The following calculation types are available for a Binary Calculator activity node:

- Phase diagram: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.
- Gibbs energy curves: To calculate at a constant temperature over the whole composition range.
- Activity curves: To calculate at a constant temperature over the whole composition range.
- Phase fractions: To calculate as a function of temperature at a constant composition.

Diffusion Calculator

The following calculation types are available for a Diffusion Calculator activity node:

Detailed simulation of diffusion controlled reactions in multi-component systems. Diffusion calculations are done with the Diffusion Calculator. There are no calculation types you need to choose when setting up your simulation.

Equilibrium Calculator

The following calculation types are available for an Equilibrium Calculator activity node:

- Single equilibrium (no axes): To calculate a single point. The results from this calculation are displayed in the **Event Log**.
- One axis: To vary a quantity on the X-axis.
- Grid: Computes the equilibrium of each grid point in a two-dimensional grid.
- Phase diagram: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Precipitation Calculator

The following calculation types are available for a Precipitation Calculator activity node:

- Isothermal: Precipitation simulation at constant temperature.
- Non-isothermal: Precipitation simulation with user-defined temperature profile.
- TTT Diagram: Time-Temperature-Transformation diagram calculation.
- CCT Diagram: Continuous Cooling Transformation diagram calculation.

Process Metallurgy Calculator

The following calculation types are available for a Process Metallurgy Calculator activity node when doing an **Equilibrium** simulation.

- Single: To calculate a single point. The results from this calculation can be displayed in the **Results** window using a **Table Renderer**.
- One axis: To vary a quantity on the X-axis.
- Grid: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- Uncertainty: Evaluates calculations where the values of the quantities are sampled from Gaussian distributions.

Property Model Calculator

The following calculation types are available for a Property Model Calculator activity node:

- Single: To calculate a single point. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Results** window.
- One axis: To vary a quantity on the X-axis.
- Grid: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- Min/Max: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits.
- Uncertainty: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions.
- Batch: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet. You can include experimental results in the data file, which then can be used to compare to the batch calculation results.

Scheil Calculator

When using a Scheil Calculator activity node, there are no calculation types you need to choose when setting up your simulation.

Ternary Calculator

The following calculation types are available for a Ternary Calculator activity node:

- Isothermal section: To calculate the ternary system for the whole composition range.
- Monovariant lines: To calculate the variation of the liquid compositions with temperature.
- Liquidus projection: The projection liquid surface and the monovariant lines are calculated over the given temperature range.

Working with Batch Calculations

When defining a **Batch** calculation for a Property Model Calculator, you choose to load (import) a configuration data file that contains predefined data. The columns that can be included in the data file are:

- Element compositions and the associated unit
- Temperature and the temperature unit
- Experimental data and a key word
- Parameters (as long as these are both available and selected for a Property Model)
- An identifier (ID) for each row of data



Only these types of data are read / used in calculations. It is important that the data file contents are correctly entered in order for the calculation to perform smoothly. The software runs a validation of the data file prior to allowing you to perform a calculation. Warnings related to this validation display on the Property Model Calculator. You can also skip this data file validation for composition or parameter inconsistencies. See below for details.

The *Batch Control* settings, which are further described in this section, are found on the Property Model Calculator **Configuration** window. See Configuration Window Settings.

Batch Controls



For the settings in this section, it is recommended you read the Data File Rules, Data File Requirements, and Skip Validation of Data File sections prior to importing the data file.

In the **Data file** field, either enter a file path or click the load data file button () to navigate to a data file such as an Excel spreadsheet (with `*.xls` or `*.xlsx` extensions) or a `*.csv` file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software.

Click **Open** to import the data. In the **Data file** field you can see the file path to the selected file. The next time you click the load data file button ( ) the program remembers the last location from where the file is opened.

Choose the delimiter—**Comma** (,), **Colon** (:), **Equals sign** (=), **Semicolon** (;), or **Tab**—that matches the delimiter in the data file and click the **Reload** ( ) button.

The data is imported and displays on the Property Model Calculator:

- The data are used for the applicable fields that must match what already exists as a Property Model parameter (e.g. critical radius, grain size, etc.) as well as the composition, temperature, and units that you want to run the calculation for. Also, if the dependent element composition is not included in the data file, the batch calculation then sets the dependent element to be the same as defined in the user interface.
- The calculation runs once for every row of data included in the file.



When the data file is imported into Thermo-Calc, there is also a **Row** column autogenerated by Thermo-Calc.

Select the **Set zero amount to value (in mole-/mass-fraction)** to enter a small value for the mole/mass-fraction in cases where a Property Model has problems calculating zero amounts of elements.

Select the **Skip validation of data file** check box to allow a calculation to perform using the data file even when certain criteria are not met.

When selected, the validation of the data file is skipped:

- If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator.
- If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation.

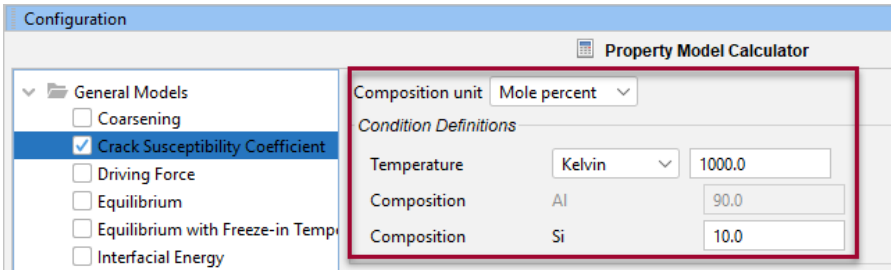


If there are any data file validation error(s), a tooltip on the **Perform** button lists and describes these.

Data File Rules

General Rules

- No abbreviations are allowed.
- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file.
- For the settings on the Property Model Calculator (**Composition unit**, **Composition**, **Temperature**, and **Temperature unit**) when there is nothing specified in the data file, the default is taken from the GUI and used in the calculation. Also, if the dependent element composition is not included in the data file, the batch calculation then sets the dependent element to be the same as defined in the user interface.



Parameter, Parameter Name, and Parameter Value Rules



Only numeric parameters available on the **Configuration** tab for the selected Property Model can be included in the calculation.

The column entries for the Parameter + *<parameter name>* plus the row entries for the *<parameter value>* must adhere to these rules. The validation checks for inconsistencies, which could be the result of any of the following criteria not being met.

- When including **Parameters** in the data file, these must be existing Property Model parameters and the applicable Property Model must be selected on the GUI.
- The *<parameter name>* is case sensitive and must be entered exactly as you see on the GUI, no abbreviations are allowed.
- The *<parameter value>* must be numeric or it is not included in the calculation.

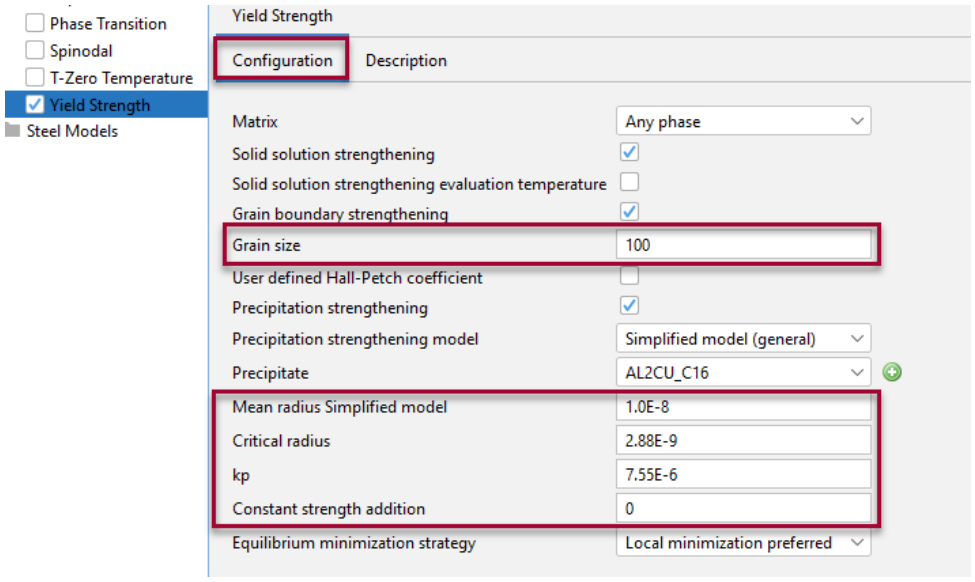


Figure 1: An example of the Yield Strength Property Model numeric parameters available for the Batch calculations. These are available on the Property Model Calculator Configuration tab after selecting Yield Strength under General Models. The parameter name must be entered in the data file exactly as you see on the GUI. No parameters from other calculators are accepted.

Data File Requirements

Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. It is recommended that the data file is cleaned up before importing / loading it and performing calculations. All header text must also be written in English, i.e. no translations into other languages will be read correctly by the data file.

In the table below, `code font` indicates something entered into the data file (or it is an example) and any *<text in italic with angle brackets>* is a generic name for an entry.

Column Heading Description	Column Heading Requirements and Options	Row Cell Requirements and Options
Composition	Enter an *<element short name>*. It is not	Valid format and entries of the *<composition*

Column Heading Description	Column Heading Requirements and Options	Row Cell Requirements and Options
Each element of the composition is in a separate heading column using the *<element short name>* e.g. Fe, C, Mn, Si, etc.	case sensitive. For example: `Fe`. It is not case sensitive, so alternatives in this example are `fe` or `FE`.	*value>*: • A number for the composition e.g. `0.1`, `8.7`, `1.00E-05`, etc. • Text entry `Bal` to define the balanced element. • Empty cells are read as zero (`0`) amounts.
Composition unit	Enter the text `Composition unit`. No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `composition unit` or `Composition Unit`, or `COMPOSITION UNIT`, etc.	Valid format and entries of the *<composition unit>*: • `mass_pct` • `mass_frac` • `mole_pct` • `mole_frac`
Temperature	Enter the text `Temperature`. No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `temperature` or `Temperature`, or `TEMPERATURE`.	Valid format and entries – • Any number e.g. `273.15`
Temperature unit	Enter the text `Temperature unit`. No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `temperature unit` or `Temperature Unit`, or `TEMPERATURE UNIT`, etc.	Valid format and entries – • `C` • `F` • `K`
Parameters with numerical values only. The heading column is defined with `Param` in front of a Property Model *<parameter name>*	`Param` + *<parameter name>* For example: `Param Critical radius` The *<parameter name>* has requirements– • It is case sensitive based on the available and selected Property Model parameter • It must be an existing Property Model parameter and be included with any selected Property Model • No abbreviations	Valid format and entries – The *<parameter value>* must be numeric or it is not included in the calculation. An example of an accepted Property Model parameter is for the **Yield Strength** model where *Grain size* and *Critical radius* are accepted (these have fields for numerical entries) but you cannot use *Matrix* or *Precipitate* as these are text choices from a drop down list.
Experimental value. The heading column is defined	`Exp` + *<keyword>* where the *<keyword>* is defined by the user.	Valid format and entries –

Column Heading Description	Column Heading Requirements and Options	Row Cell Requirements and Options
with `Exp` followed by any *<keyword>*.	For example: `Exp Ms`.The keyword is not case sensitive so alternatives are `MS` or `ms`.	• Each *<experimental value>* must be numeric
Identifier (i.e. an alloy name). The heading column is defined as `Id`	Enter the text `Id`. It is not case sensitive so alternatives are `id` or `ID`.	Valid format and entries – • An *<identifier>* can be any text or number defined by the user.

Data File Example and Column Definitions

	A	B	C	D	E	F	G	H	I
1	Id	Fe	C	Cr	Exp Ms C	Exp Ms	Composition unit	Temperature unit	Param Critical radius
2	2	Bal	0.000928	0.0149	529.85	803	mole_frac	K	2.88E-09
3	3	Bal	0.000928	0.0449	489.85	763	mole_frac	K	3.88E-09
4	4	Bal	0.000324	0.0422	499.85	773	mole_frac	K	4.88E-09

This is an example of data entered into an Excel spreadsheet. When this is imported into Thermo-Calc, an additional "Row" column is automatically added and is a way for you to locate any errors in the data file that are identified as needing correction or adjustment to allow the program to read the file.

- A1 to A4 is the **Identifier** column and rows. The heading text is `Id` and then in the entries in rows A2 to A4 can be text or numbers, for example it might be an alloy name or another user-defined *<identifier>*.

  When the data file is imported into Thermo-Calc, there is also a **Row** column autogenerated by Thermo-Calc.

- B1 to B4 is the **Composition** column and rows for the element `Fe`. In this example, `Bal` indicates that the balance of the composition will be calculated for this column after the *<composition values>* for `C` and `Cr` are entered.

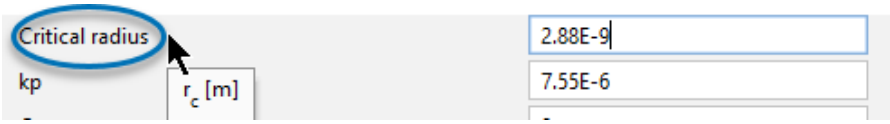
- C1 to C4 and D1 to D4 are the **Composition** columns each for `C` and `Cr` with the specific *<composition values>*, e.g. `0.000928` for `C` and `0.0149` for `Cr` in row 2.

- E1 to E4 and F1 to F4 are the **Experimental Value** columns and rows. The header starts with `Exp` and then user-defined *<keywords>* are added, e.g. `Ms C` and `Ms`. Then specific *<experimental values>* are entered, e.g. `529.85` for `Ms C` and `803` for `Ms` in

row 2.

- G1 and H1 are the headings for the **Composition unit** and **Temperature unit** columns. No abbreviations allowed but it is NOT case sensitive. Then the rows G2 to G4 and H2 to H4 include an accepted text value e.g. `mole_frac` for the composition unit and `K` for the temperature unit.

- I1 is the **Parameter** heading where you need to enter `Param` followed by the parameter name `Critical radius`, which has numeric values entered in rows I2 to I4. The *<parameter name>* matches that on the GUI and is an available and selected Property Model parameter.



Skip Validation of Data File

Select the **Skip validation of data file** check box to allow a calculation to perform using the data file even when certain criteria are not met.

When selected, the validation of the data file is skipped:

- If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator.
- If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation.

If there are any data file validation error(s), a tooltip on the **Perform** button lists and describes these.

Skipping Composition Validation

If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator then the default system composition is used for any missing elements after you select the **Skip validation of data file** check box.

This can occur when there are more elements included in the data file but not entered on the GUI, and then these are excluded from the calculation. For example, you might have too many or too few elements included in the data file compared to the composition entered on the System Definer, which is then further viewed under *Condition Definitions* on the Property Model Calculator **Configuration** window.

When configuring the System Definer, it is recommended you select the composition to match the composition in the data file. However, if this is not possible you can use this check box to override any differences of the composition included in the data file and use the GUI default.

Skipping Parameter Validation

If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation after you select the **Skip validation of data file** check box.

For example, if a data file is uploaded and you are unable to perform the calculation, it means that one of the following criteria are not met for the `Param` columns and related to the *<parameter name>*.

- The parameter name is misspelled (does not match) the one on the GUI
- The parameter is not available with the selected Property Model.
- The parameter is not available with any Property Model.

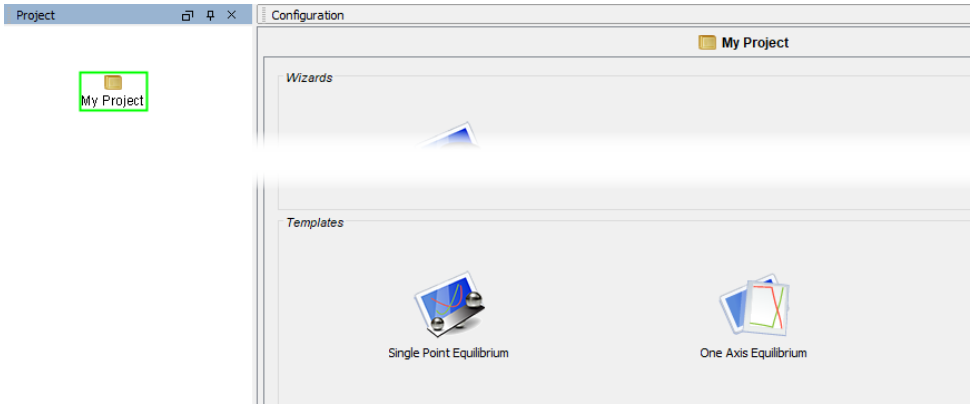
It is best practice to use a data file that only includes available Property Model parameters. However, if this is not possible then use this check box to override the validation. Alternatives to skipping this validation, include removing the prefix `Param` from the data file (or delete this column), and confirming that the parameter you want to calculate is available and selected for the Property Model.

Plotting Experimental Data Against Simulation Results

You can plot experimental values loaded to the Property Model Calculator using the Cross Plot Mode available on the Plot Renderer. For more information, see Plotting Modes.

The Quick Start Wizard and Templates

Use the *Quick Start* wizard or a *Template* to create all the activities for a certain type of calculation. In the **Project** window click the **My Project** node to display the Quick Start and other templates in the **Configuration** window.



Quick Start Wizard

Even before you understand how to work with Thermo-Calc projects, the Quick Start wizard helps you set up a project and run calculations in Graphical Mode. You can set up, calculate and visualize any of the following:

- Single point equilibrium
- One axis equilibrium
- Phase diagram
- Scheil solidification simulation

Creating a Project with the Quick Start Wizard

Templates

A variety of templates are available. You can add these from the **Configuration** window or by right-clicking the **My Project** node and selecting one from the **Create New Activity → Use Template** list:

- **Single Point Equilibrium**: Creates a project for calculating a single point equilibrium. The project consists of a System Definer, Equilibrium Calculator, and a Table Renderer.

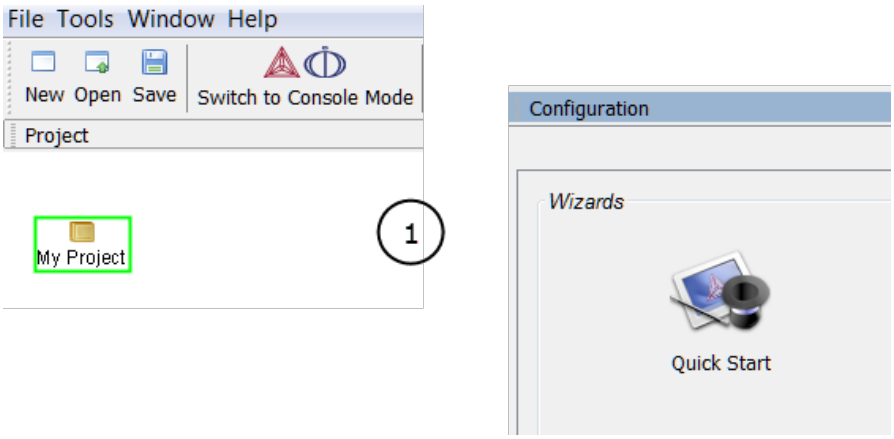
- **One Axis Equilibrium**: Creates a project for calculating a one axis diagram. The project consists of a System Definer, Equilibrium Calculator, and a Plot Renderer.
- **Phase Diagram**: Creates a project for calculating a phase diagram. The project consists of a System Definer, Equilibrium Calculator, and a Plot Renderer.
- **Scheil Solidification Simulation**: Creates a project for performing a Scheil calculation. The project consists of a System Definer, Scheil Calculator, and a Plot Renderer.
- **Binary Calculation**: Creates a project for performing a binary calculation. The project consists of a Binary Calculator and a Plot Renderer.
- **Ternary Calculation**: Creates a project for performing a ternary calculation. The project consists of a System Definer, Ternary Calculator, and a Plot Renderer.
- **Property Model Calculation**: Creates a project for a Property Model Calculator. The project consists of a System Definer, Property Model Calculator, and a Plot Renderer.
- **Diffusion Simulation**: Creates a project for general diffusion simulations. The project consists of a System Definer, Diffusion Calculator, and a Plot Renderer.
- **Precipitation Simulation**: Creates a project for simulating the evolution of particle size distributions. The project consists of a System Definer, Precipitation Calculator and a Plot Renderer.
- **Steel Library - CCT**: Creates a project for a steel package to add all the activities for a Continuous-Cooling-Transformation (CCT) diagram calculation. The project consists of a System Definer, Property Model Calculator, and a Plot Renderer.
- **Steel Library - TTT**: Creates a project for a steel package to add all the activities for a Time-Temperature-Transformation (TTT) diagram calculation. The project consists of a System Definer, Property Model Calculator, and a Plot Renderer.
- **Process Metallurgy**: Creates a project to allow for calculation and efficient setup of advanced calculations involving slag, metal, and gas.

Creating a Project from a Template

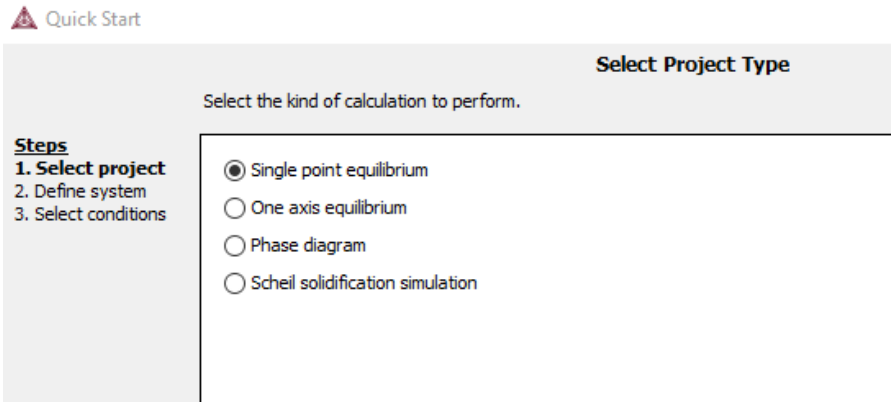
Creating a Project with the Quick Start Wizard

To set up, perform and visualize a calculation using the Quick Start wizard:

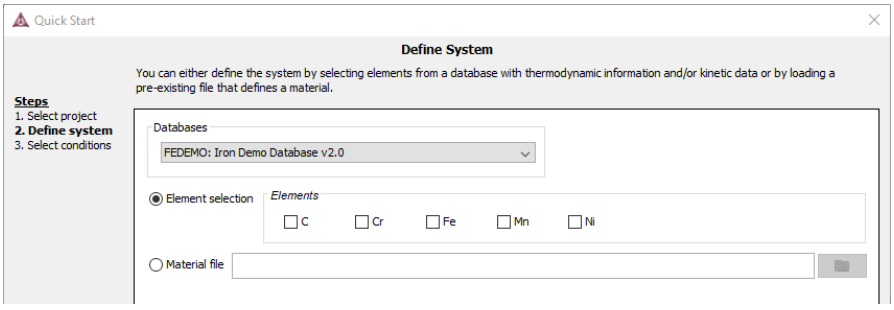
1. In the **Configuration** window click **Quick Start**. If you cannot see the **Quick Start** button, first click **My Project** in the **Project** window.



2. In the **Select Project Type** window click to select the type of calculation to perform. **Single point equilibrium**, **One axis equilibrium**, **Phase diagram** or **Scheil solidification simulation** (a Classic Scheil simulation). Click **Next**.

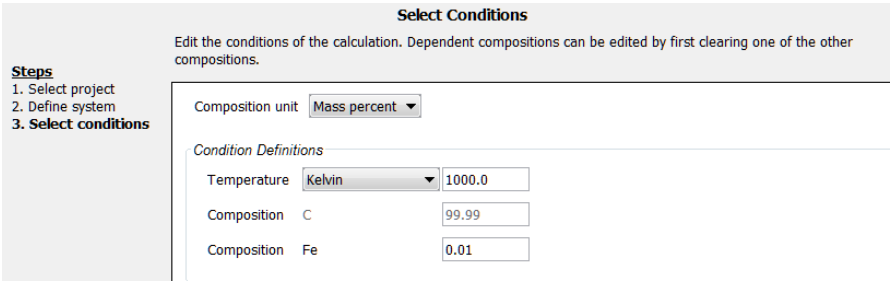


3. In the **Define Systems** window, choose an available **Database**.



4. Click to select **Elements** check boxes to include as system components. To add elements from an existing material file, click the **Material file** button to enter the file path to a material file or click the **Select Material File** button (to the right of the field) to navigate to a file on the computer.
5. Click **Next**. The **Select Conditions** window has different options depending on the Project type and the elements selected.

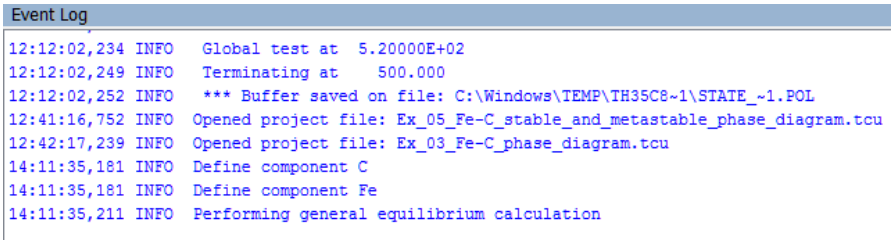
   In this example figure, using a **Single Point Equilibrium**, choose the **Composition unit** from the list and under *Condition Definitions* specify the values of the state variables in the system.



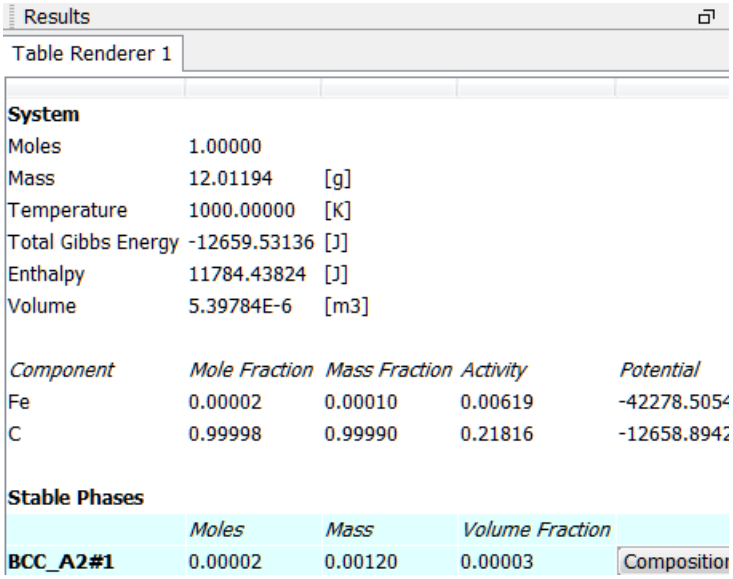
   For a **One axis equilibrium** or **Phase diagram**, specify the **Axis Definitions** of the stepping or mapping operation. Choose minimum and maximum values for the variable(s) (select **Linear – min no. of steps**, **Linear – max step size** or **Logarithmic – scale factors**) and whether it is **Normal** or **Separate phases**. For a **Scheil solidification simulation**, and where applicable, select **Fast diffuser**.

> After using this Quick Start Wizard to do a Classic Scheil calculation (or with fast diffuser components), a Scheil Calculator is added to the Project window. At this point you can review Scheil-Gulliver Solidification Calculations for details about all the options using the Scheil Calculator, i.e. back diffusion and solute trapping.

6. Click **Finish**. Click to expand the **Event Log** window to see information about the progress of the calculation.



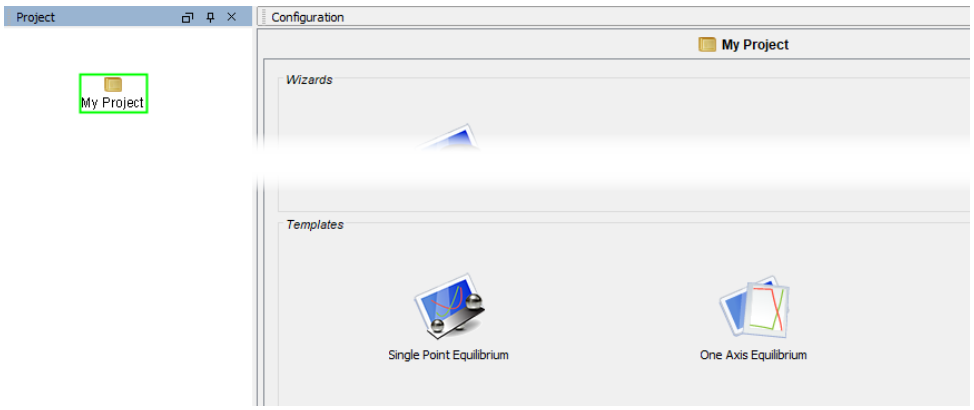
The diagram is plotted in a **Plot Renderer** tab in the **Results** window. If you have calculated a single-point equilibrium, then a **Table Renderer** tab shows information about the equilibrium.



7. To save the project, click **Save** on the main toolbar. To save a diagram or table, right-click the diagram or table and select **Save As**.

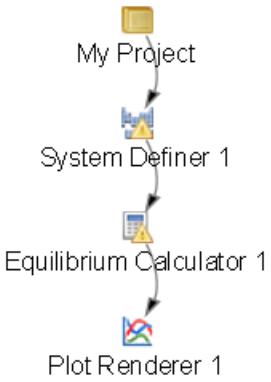
Creating a Project from a Template

Use a *Template* to create all the activities for a certain type of calculation. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.

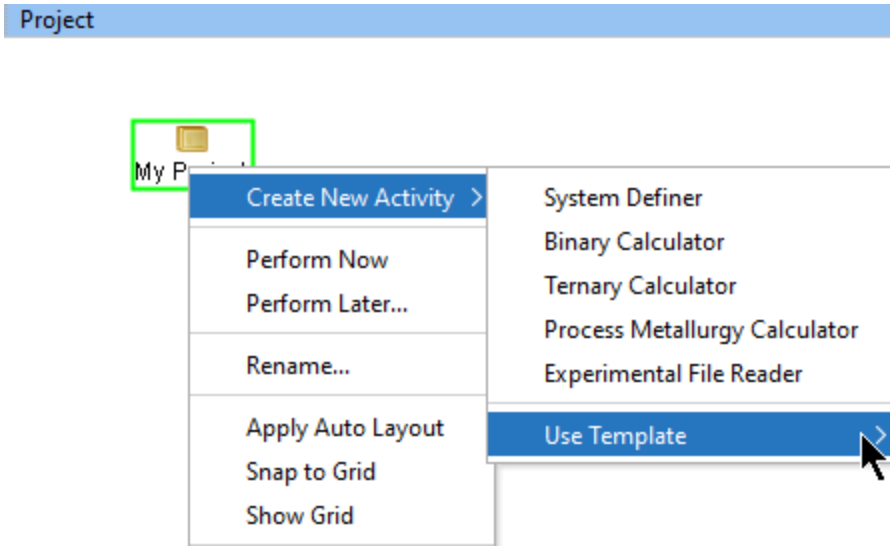


When you click a template, an activity tree is added to the **Project** window. You can then configure and perform the activities or the project.

For example, if you click **One axis equilibrium**, a tree is added to the **My Project** node with **System Definer**, **Equilibrium Calculator** and **Plot Renderer** nodes.



You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



- The Quick Start Wizard and Templates
- Steel Library TTT Diagram Template

Steel Library TTT Diagram Template



The use of this Steel Model Library template requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

Use a *Steel Library TTT* template to add all the activities for a Time-Temperature-Transformation (TTT) diagram calculation. The **TTT Diagram** Property Model is automatically selected with all settings by default on the Property Model Configuration window. This makes it easy to add the project to the tree and examine the progress of transformation as a function of time at a fixed temperature.

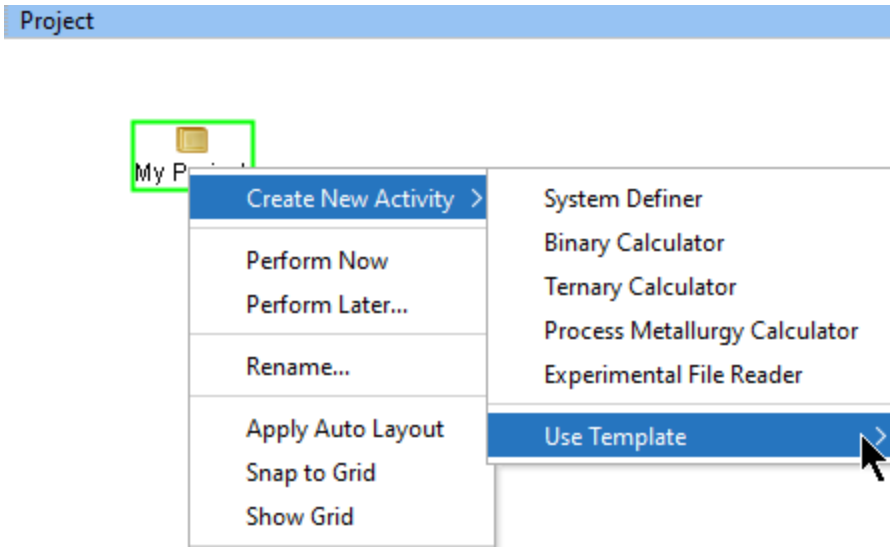
How to Add a Steel Library TTT Template to a Project

1. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.

2. Under *Templates*, click **Steel Library - TTT**.

   A **System Definer**, *Property Model Calculator* (renamed to **Steel Models**) and a *Plot Renderer* (renamed to **TTT**) are added to the **Project** window. Also see Property Model Calculator and Plot Settings: TTT Mode.

You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



Steel Library CCT Diagram Template

The use of this Steel Model Library template requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

Use a *Steel Library CCT* template to add all the activities for a Continuous-Cooling-Transformation (CCT) diagram calculation. The **CCT Diagram** Property Model is automatically selected on the Property Model Calculator with all settings by default. This makes it easy to add the project to the tree and examine the progress of transformation as a function of changing temperature.

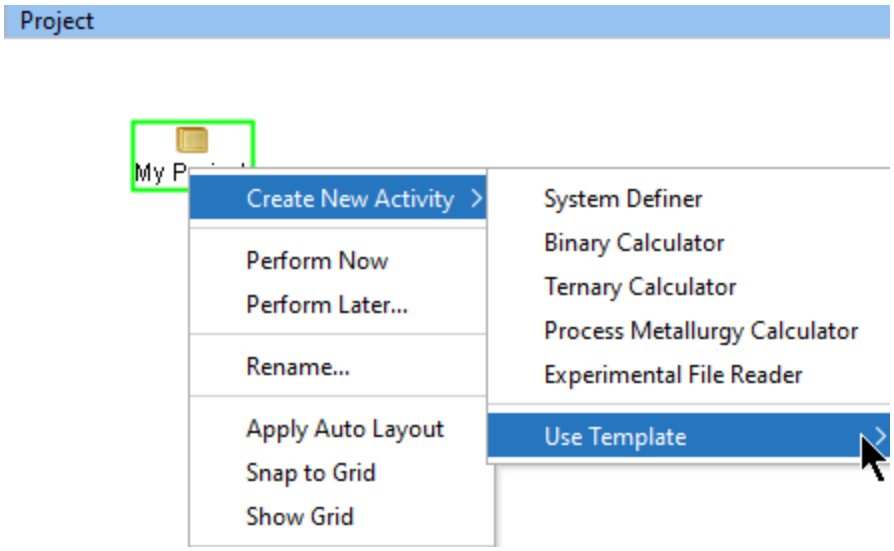
How to Add a Steel Library TTT Template to a Project

1. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.

2. Under *Templates*, click **Steel Library - CCT**.

   A **System Definer**, *Property Model Calculator* (renamed to **Steel Models**) and a *Plot Renderer* (renamed to **CCT**) are added to the **Project** window. Also see Property Model Calculator and Plot Settings: CCT Mode.

You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



Process Metallurgy Template

Use a *Process Metallurgy* template to add the Process Metallurgy Calculator and a Plot Renderer to the **Project** window. The Process Metallurgy Calculator has several preconfigured settings making is easier to setup the different groups and materials needed to define a system for slag, metal and gas used in steelmaking.

- Process Metallurgy Calculator

How to Add a Process Metallurgy Template to a Project

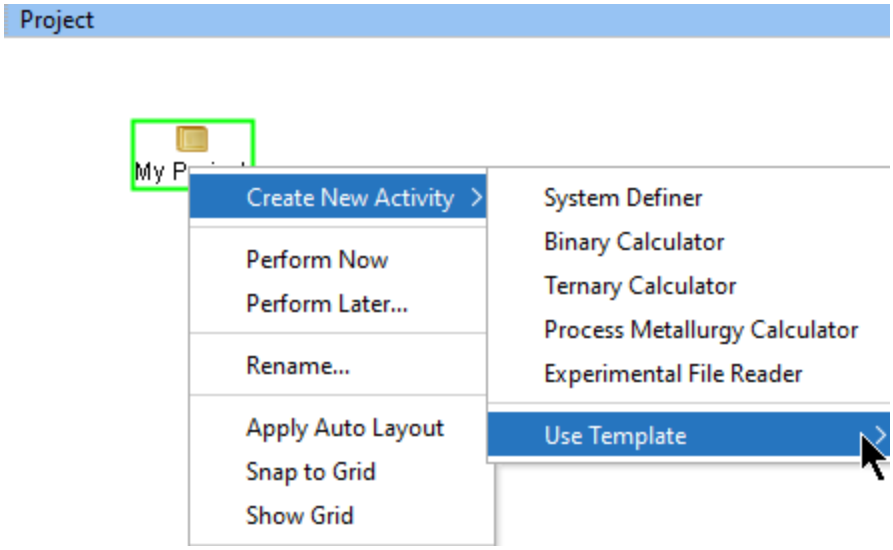
1. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.

2. Under *Templates*, click **Process Metallurgy**.



A **Process Metallurgy Calculator** and a **Plot Renderer** are added to the **Project** window.

You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



Defining and Using the Activity Nodes



For information about the Process Metallurgy Calculator, see The Process Metallurgy Module.

In this section:

System Definer 53

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Binary Calculator 80

Ternary Calculator 84

Scheil-Gulliver Solidification Calculations 87

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System Definer

In a System Definer activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select the species to include as well as change the reference temperature and pressure for your components.

You can add the System Definer directly (right-click **My Project** and select it from the **Create New Activity** menu) or use a variety of the available templates to automatically add the node.



Almost all of the Graphical Mode Examples use the System Definer. For details about the templates, seeThe Quick Start Wizard and Templates and Creating a Project from a Template.

Once you have added a System Definer, the **Configuration** window has these settings tabs:

- Elements
- Species
- Phases and Phase Constitution
- Components
- Data Sources
- Description

Define the System

This topic describes how to define a system, specifically how to select one or more databases and define the elements in the system with the **System Definer** activity node.

1. Right-click **My Project** and from the menu select **Create New Activity→ System Definer** . You can also add any template and a System Definer is added to the Project tree.
2. In the **Project** window, click the **System Definer** activity node.
3. In the **Configuration** window, choose **Databases** from the list or a database **Package**.

   About the Database Files

   OPTIONS:

   - From the **Databases** list, select **<User database>** to define your own.
   - You can choose to add one or more databases by clicking the **Add a database** button.

- From the **Package** list, choose a predefined database package to add multiple databases at a time. Depending on your license, there are predefined database packages available to select.

4. Select the **Elements** tab to choose the elements in the **Periodic Table** or use the **Alphabetic List** to choose elements for the system.

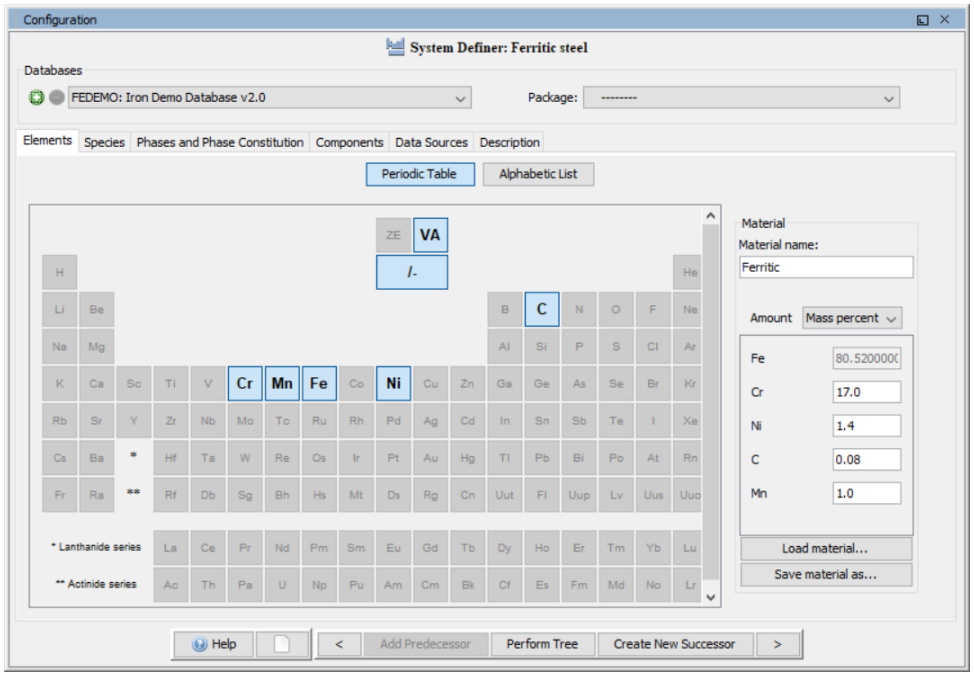
5. As required click the tabs to make edits: **Species**, **Phases and Phase Constitution**, and **Components**. The **Data Sources** and **Description** tabs provide information based on the database.

   Configuration Window Settings

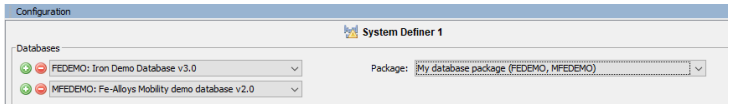
6. Click **Perform** to start the System Definer activity immediately and retrieve data about the system. Click the **Event Log** window to watch the progress of the job.

Configuration Window Settings

The **System Definer Configuration** window has many settings available, which are briefly described below.



Choose Database(s) or a Database Package

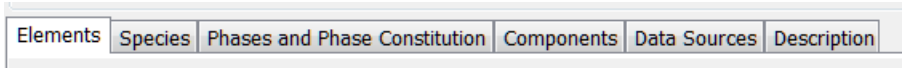


At the top of the **Configuration** window you can choose to add one or more **Databases** by clicking the **Add a database** button. You can also choose a predefined or custom database **Package** from the list. Depending on your license, there are predefined database packages available to select. After adding a database, click **Remove this database** button as required for your simulation.

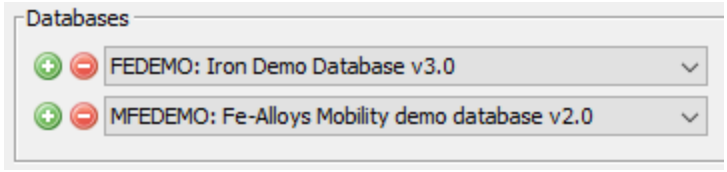
If you have chosen a database package and then remove or change a database, a message displays *Selected databases and selected package may differ*. This means that the original package you selected, which added preset databases, does not match the databases you are using for the project. For information about how to clear the message, see Global Settings: System Definer.

Global Settings: System Definer

There are several settings tabs available for the System Definer activity.



The following example uses the FEDEMO and MFEDEMO databases and Graphical Mode example **PM_G_03**, which you can open from the **Help → Examples Files** menu.

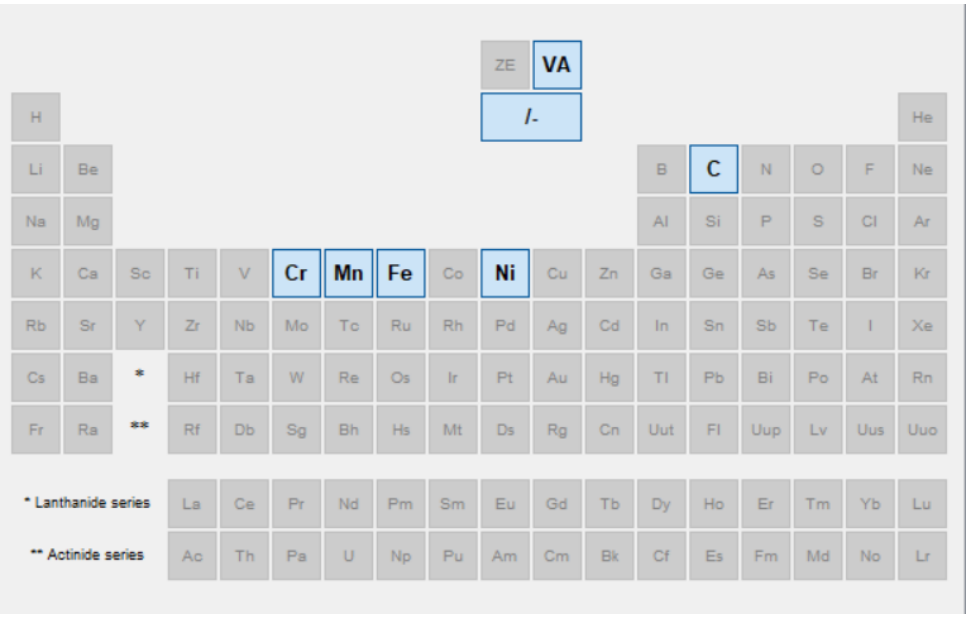


Elements

On the **Elements** tab, and based on the databases or database package selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. Unavailable elements, which are based on the selected database, are greyed out.

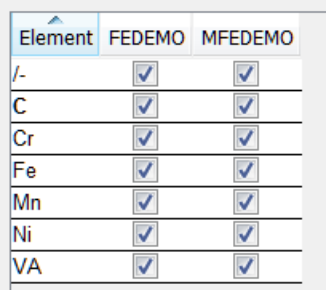
Periodic Table

In this example, using the demonstration databases FEDEMO and MFEDEMO, there are only a select number of elements to choose from.



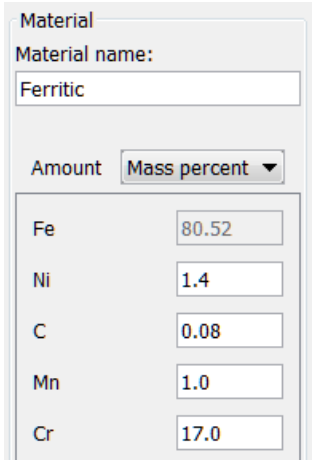
Alphabetic List

Select the elements next to the check boxes for the selected database(s).



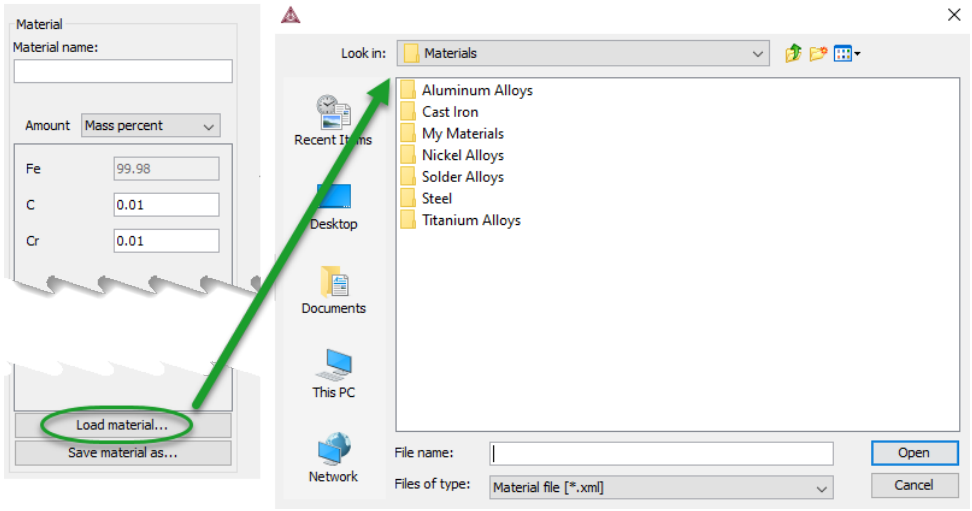
Material Composition

After selecting the elements and in the **Periodic Table** view, under *Material*, you can enter a **Material name** and define the material composition **Amount** in **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.



At the bottom of the window, click **Load material** to open a material file. The default folder opens to the **Materials** folder included with your installation.

- About the Material Files and Examples, Manuals, and Materials Folders



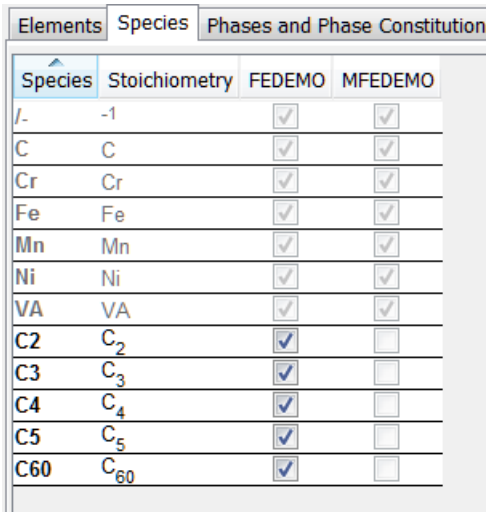
You can also click **Save material as** to save the material you defined, for example **Ferritic**.

- Global Settings: System Definer

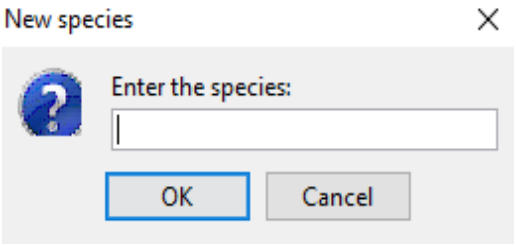
If you load a material file and then change the composition, a message displays *The composition has changed*. This means that the original values/composition do not match the values you are using for the project. The message is cleared by either reloading the material file or editing the composition field to the original value.

Species

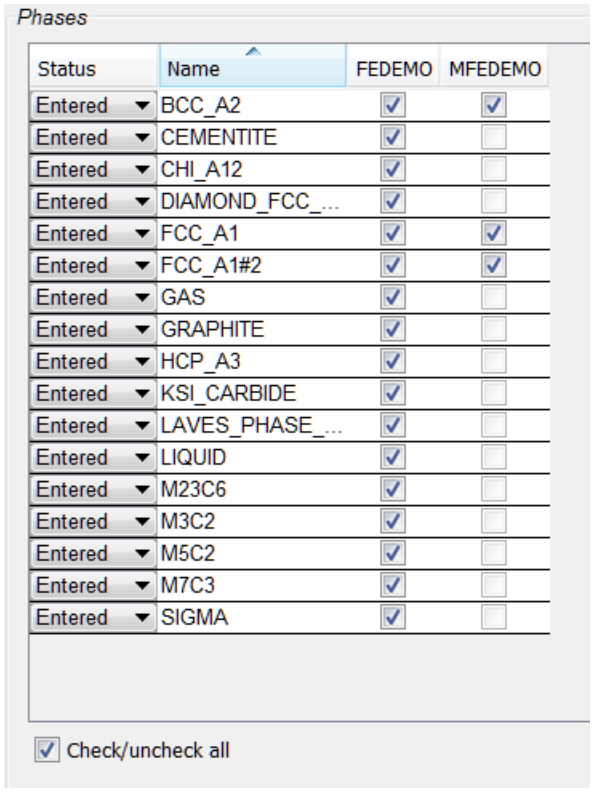
On the **Species** tab for each database you can select and edit the *Species* and view the *Stoichiometry* for the selected database species.



At the bottom of the window, click **Add new species** and enter a **New species** name in the field.

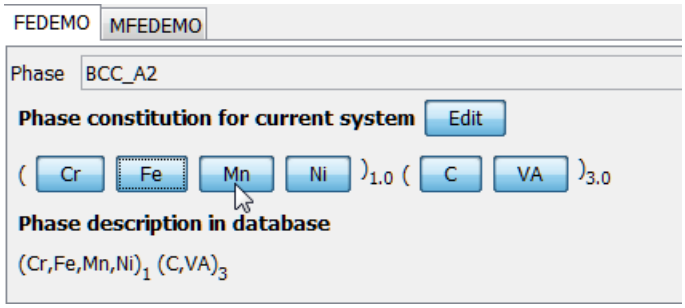


Phases and Phase Constitution



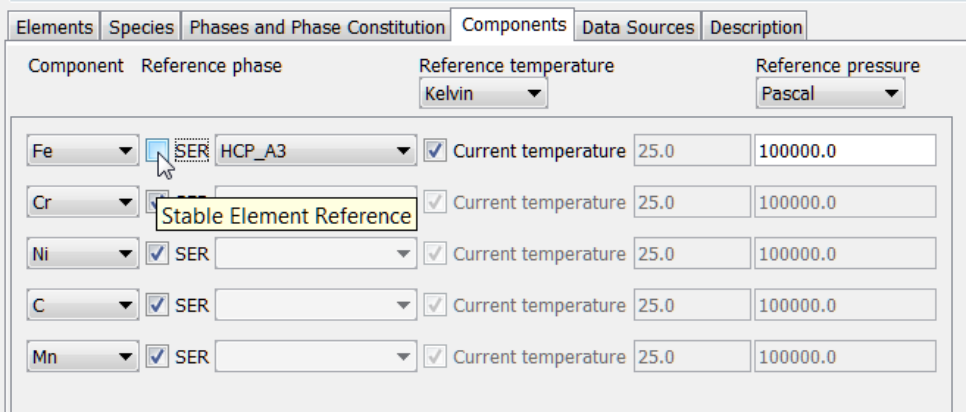
At the top of the **Phases and Phase Constitution** tab for each database you can review and edit the **Status** (**Entered** or **Dormant**) for the selected*Phases*. Select the **Check/uncheck all** check box to toggle between the options.

To review the Phase constitution for a specific phase, click it in the *Phase* list (for example **BCC_A2**) and its details are displayed at the bottom of the window for the database selected. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.



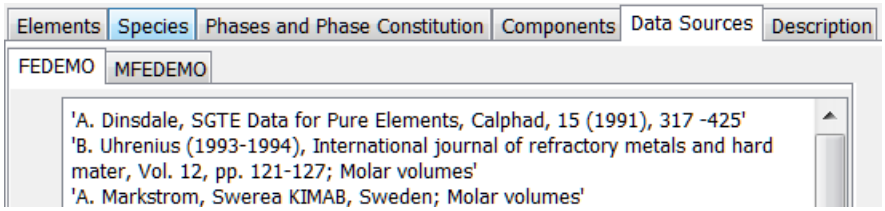
Components

The **Components** tab is where you can review and edit the **Component**, **Reference phase**, **Reference temperature**, and **Reference pressure**. Click to toggle the **SER** (Stable Element Reference) check box on and off. Then choose a **Reference phase** from the list and edit accordingly. Choose a unit for the **Reference temperature** (**Kelvin**, **Celsius** or **Fahrenheit**) and **Reference pressure** (**Pascal**, **Atmospheres** or **Bar**).



Data Sources

Data source references are shown after performing the activity. Click **Perform** or **Perform Tree** at the bottom of the window when your system is set up.



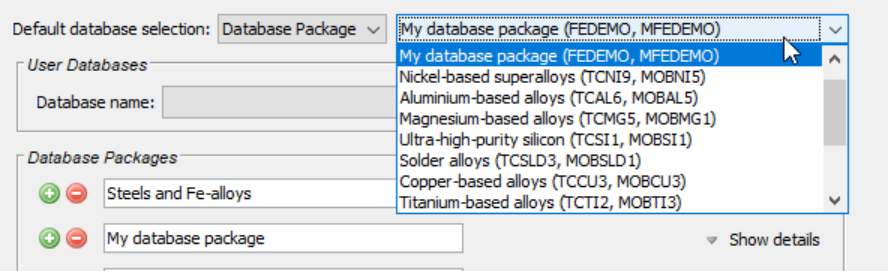
Description

The **Description** tab displays a description of the selected database(s). In this example, **MFEDEMO**.



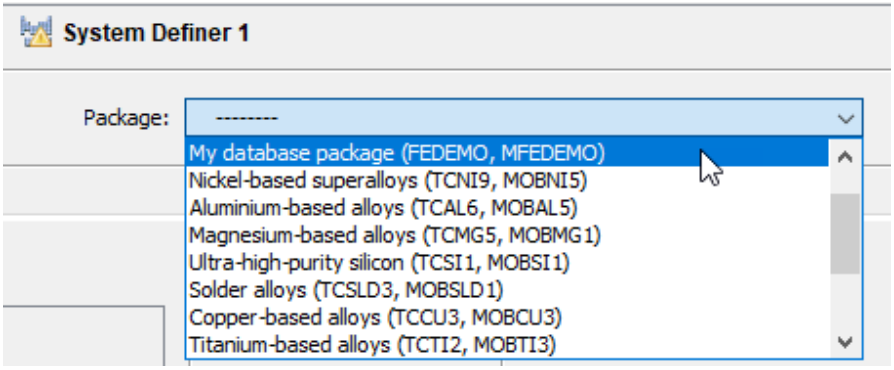
Creating a Database Package

1. From the main menu select **Tools → Options** .
2. Click the **Activities** tab and click **System definition**.
3. Under *Database Packages*, click the **Add a database package** button.
4. Replace the default text with a name for the package, for example **My database package**.
5. Select a database from the **Choose database** list, for example, **FEDEMO Iron Demo Database**.
6. Click the **Add a database** button and from the **Choose database** list, select another database.
7. Click **OK** . The software needs to relaunch for the Database Package to be available to choose as the default for new System Definer activities.



The package is available for new System Definer nodes defined after

adding the package.



Clearing a Database Package Message and Global Settings: System Definer

Clearing a Database Package Message

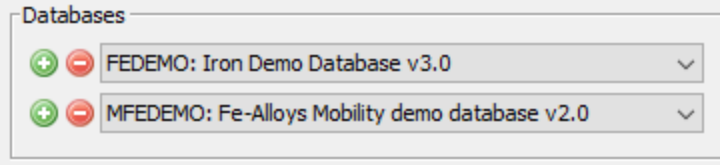
Sometimes when working on the System Definer **Configuration** window, you may add or delete Databases. If you originally added a Database Package, the addition or removal of a database means that the original package you selected does not now match the databases you are using. To clear the message *Selected databases and selected package may differ* and reset the databases you need to either:

- Change the newly added database back to the one that matches the database package, or
- Choose another package from the **Package** list, then select the package you want.

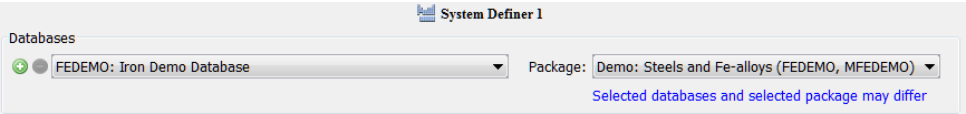
For example, from the **Package** list you select **Demo: Steels and Fe-alloys**.



This adds the **FEDEMO** and **MFEDEMO** databases.



If you add or remove **Databases**, in this example **MFEDEMO** is removed, then this does not match the **Package** and the message displays:



To clear the message, click the **Add a database** button and from the **Choose database** list, select the database that belongs with the package, in this example, **MFEDEMO**. The message is cleared.

You can also choose another package from the list, which changes the databases, and then re-select the original package to reset the message.

- Creating a Database Package and Global Settings: System Definer

About the Material Files

- Examples, Manuals, and Materials Folders

When you are working with the System Definer in Graphical Mode you can open the default **Materials** folder included with your installation. The files are in .xml format and the data contained are from some common alloys. You can also save and create your own materials files from the System Definer, or copy the xml files to the Materials folder.

Aluminum Alloys

- UNS_A95005
- UNS_A96053

Cast Iron Alloys

- UNS_F10007
- UNS_F33101

Nickel Alloys

- UNS_N06600
- UNS_N6600
- UNS_N06625
- UNS_N06690
- UNS_N07001
- UNS_N07718

- UNS_N08800
- UNS_N08825

Solder Alloys

- ASTM_25A
- ASTM_96TS
- UNS_L50134
- UNS_L54321

Steel Alloys

Austenitic Stainless Steel

- ASTM_304_(UNS_S30400)
- ASTM_304L_(UNS_S30403)
- ASTM_304LN_(UNS_S30453)
- ASTM_316_(UNS_S31600)
- ASTM_316L_(UNS_S31603)
- ASTM_316LN_(UNS_S31653)
- ASTM_317L_(UNS_S31703)
- UNS_J92710
- UNS_S30908

Duplex Stainless Steel

- UNS_S31803_A
- UNS_S32750_A
- UNS_S32750_B

High Speed Steel

- ASTM_M10_A5

High Temperature Steel

- UNS_S31008

HSLA Steel

- UNS_K12000

Low Carbon Steel

- UNS_H61180

Maraging Steel

- UNS_K92810

Martensitic Stainless Steel

- ASTM_420
- UNS_J82090
- UNS_J91639
- UNS_S44004

Tool Steel

- UNS_T30106
- UNS_T30109
- UNS_T51620

Training Steel

- Ferritic
- M7_Steel

Titanium Alloys

- UNS_R54520
- UNS_R56260

My Materials

This is where you can add your own material files to be able to load it to the System Definer. When you are in the System Definer **Configuration** window, you define your material then click **Save material as**. You can save the profile to this folder or create a folder with a new name.

Equilibrium Calculator

An Equilibrium Calculator allows you to set the conditions for, and perform, a calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use a variety of the available templates.

Once you have added an Equilibrium Calculator, the **Configuration** window has these settings tabs. An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the settings of the predecessor.

- **Conditions:** Set the conditions for your calculation that define the stepping or mapping axis variables. This tab can be viewed in a simplified mode and in an advanced mode.
- **Functions:** Define your own quantities and functions, which you then can calculate and plot.
- **Options:** Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.



The **Options** tab is where you can locally define specific Equilibrium Calculator settings. These settings can also be applied globally. To open the **Options** window: From the main menu select **Tools → Options** and click the **Activities** tab. Then click **Calculation**.



For an example of how serially coupled Equilibrium Calculators can be used, see example T_06. For details about the templates, seeThe Quick Start Wizard and Templates and Creating a Project from a Template.

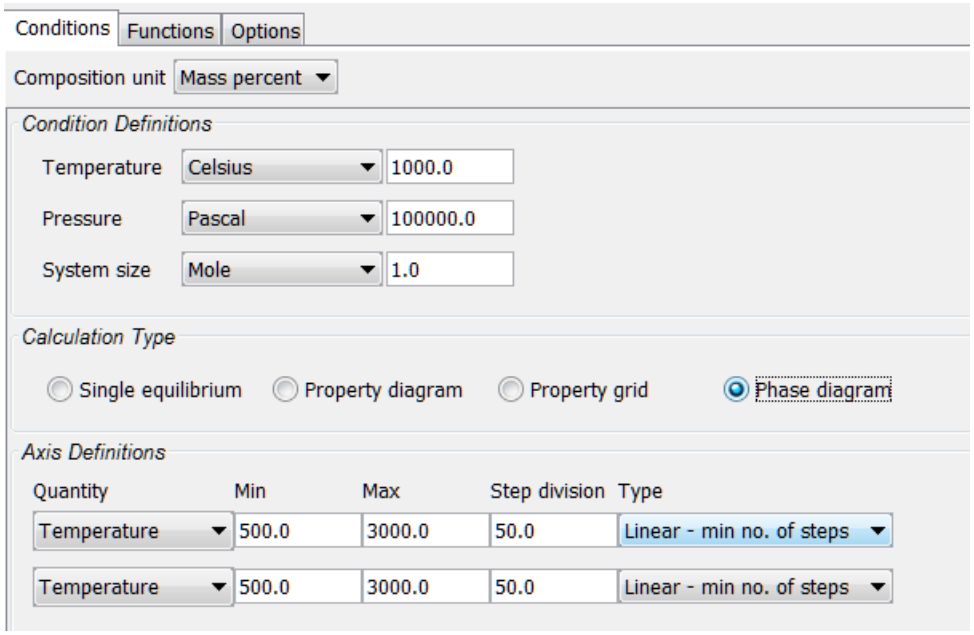
Define the Equilibrium Calculator

1. Add an Equilibrium Calculator node to the System Definer. If you used the **Single Point Equilibrium** , **One-Axis Equilibrium**, or **Phase Diagram** template, click the **Equilibrium Calculator** node to display the **Configuration** settings window.
2. In the **Configuration** window, enter the settings described in Conditions Tab Settings, and as required from the Options Tab Settings. There are also settings you can define on the **Functions** tab. See Calculating and Plotting Functions
3. Once you have finished defining the Equilibrium Calculator, you also choose settings on the Plot Renderer.

▶ Calculating with a Fixed Phase

Conditions Tab Settings

Conditions and axis variables for the Equilibrium Calculator are set in the **Conditions** tab on the **Configuration** window. The tab can be viewed in two modes: **Simplified** (the default) or **Advanced**. The conditions to set depend on the type of calculation.



See examples T_01: Calculating a Single-Point Equilibrium ,T_02: Stepping in Temperature in the Fe-C System and T_05: Stable and the Metastable Fe-C Phase Diagrams.

Options Tab Settings

About Advanced Mode

Click **Switch to advanced mode** to add and remove conditions as well as set additional axis definitions. However, the number and types of conditions set must still conform to the Gibbs' phase rule. The **Number of missing conditions is** field, at the top of the tab shows how many conditions that you have left to set. If the number is negative, then that number of conditions need to be removed.

The following outlines what you can set on the **Conditions** tab in simplified mode.

Click **Switch to advanced mode** for more options.

Composition unit

Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Condition Definitions

Specify the values (and units) of the state variables: **Temperature**, **Pressure**, and **System size** or any other available lists under *Condition Definitions*.

Calculation Type

Select a *Calculation Type*: **Single equilibrium** (no axes), **One axis**, **Grid** or **Phase diagram**.

- Click **Single equilibrium** to only calculate the equilibrium. No additional settings are required. Add a **Table Renderer** to perform the calculation and view the details in the **Results** window.
- Click **One axis** to vary a quantity on the X-axis.
- Click **Grid** to compute the equilibrium of each grid point in a two-dimensional grid.
- Click **Phase diagram** to calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.
- 

  When you use the Equilibrium Property Model Settings with the **Property Model Calculator**, it is the same calculation result as when you are using an **Equilibrium Calculator** with the **Single equilibrium** calculation type.

Axis Definitions

- **One axis**: Define the axis variable using these fields and menus: **Quantity**, **Min**, **Max**, **Step division**, **Type** and **Step Method**.
- **Grid**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**.
- **Phase diagram**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max**, **Step division** and **Type**.



If the Equilibrium Calculator already has a Plot Renderer as a successor and you change the stepping/mapping quantities, then the quantities represented on the X- and Y-axis are automatically updated in the Plot Renderer.



For a **One axis** calculation, on the Plot Renderer, you can choose to plot a **Heat map**, **Contour** or **3D** diagram.

- Heat Map, Contour, and 3D Plots

Step Method (One axis)

From the list, choose **Normal** or **Separate phases**.

- **Normal** allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). Only the step axis value is changed between each step.
- **Separate phases** calculates how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase, etc.).

Number of steps (Grid)

Set a fixed **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point an equilibrium is calculated.

Type and Step division (One axis and Phase diagram)

Type options: **Linear - min no. of steps**, **Linear - max step size** and **Logarithmic - scale factor**.

- For **Linear - min no. of steps**, the **Step division** value specifies a minimum number of steps that is calculated between the minimum and maximum value during the stepping/mapping operation.
- For **Linear - max step size**, the **Step division** sets the maximum size of each step. For **Logarithmic - scale factor**, **Step division** specifies the scale factor of a logarithmic function that distributes the steps from the initial equilibrium to the minimum and maximum values defined.

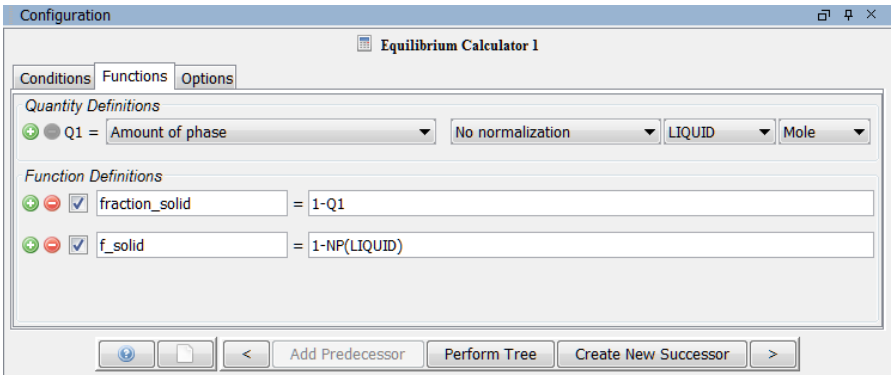
Calculating and Plotting Functions

The **Functions** tab allows you to define your own functions that can be plotted in a Plot Renderer.



For an example of how you can use functions that you define, see T_07: User-Defined Functions.

1. Add an **Equilibrium Calculator** node and click it in the **Project** window.
2. In the **Configuration** window click the **Functions** tab.
3. Under **Quantity Definitions**, define **Q1**. Click the add button to **Add a new quantity**. Then from the lists, choose the variable for each quantity to define. The quantities are called **Q1**, **Q2**, **Q3** and so on. In this example, the quantity **Q1** is defined as the **Amount of phase**, with **No normalization**, **LIQUID** in **Mole** units.

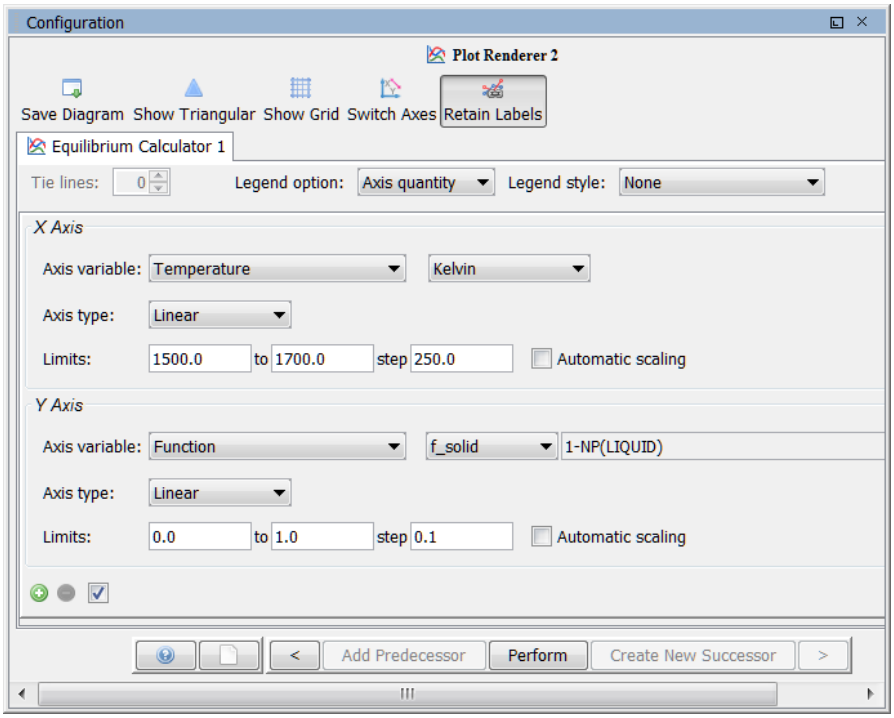


4. Under **Function Definitions**, click the add button to add a new function. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign. In this example, the quantity defined as Q1 is renamed to **fraction_solid**, which gives as its output the fraction of solid phase (**1-Q1**).

   You can also use Console Mode syntax when entering the function. For example, the function above can be entered as `1-NP(LIQUID)`. See Parameters, Functions, and Variables for details.

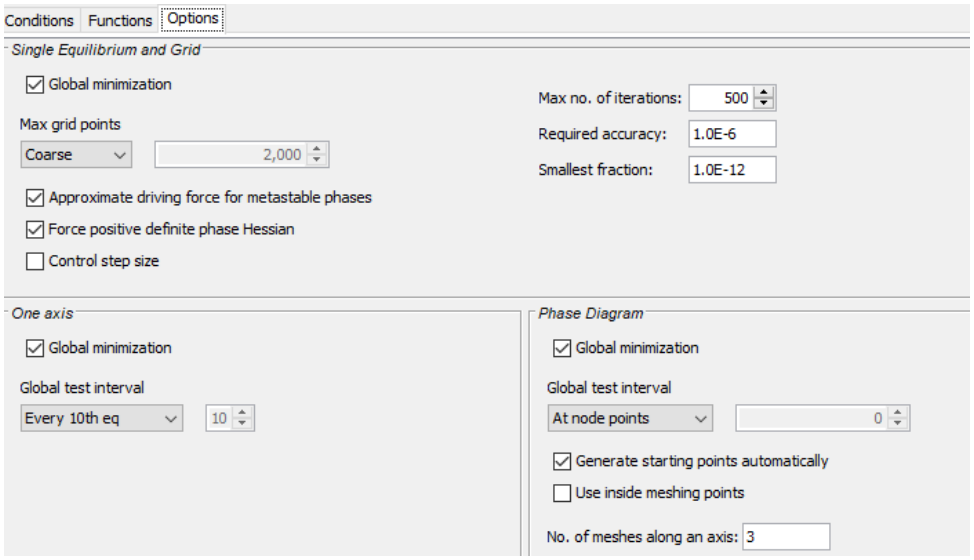
5. To plot the defined function, right-click **Equilibrium Calculator** and choose **Create new successor→Plot Renderer**.
6. Click the **Plot Renderer** node. In the tab for the Equilibrium Calculator that contains the function, set an **Axis variable** to **Function**, then from the menu select the defined function. In this example the Y-axis is set to plot the value of the function **fraction_ solid**.

   When run, the Plot Renderer plots the value of the function.



Options Tab Settings

These settings are for the Equilibrium Calculator and are located on the **Configuration** window → **Options** tab.





You can change these settings locally for a specific Equilibrium Calculator or globally in the **Options** settings. To open the **Options** window: From the main menu select **Tools → Options**. Click the **Graphical Mode** tab then click **Calculation**.

Single Equilibrium and Grid

Under *Single Equilibrium and Grid*, there are these *Calculation Type* setting options.

Global minimization

The **Global minimization** check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.

Max grid points

For the **Max grid points**, the default is **Coarse** (2000 grid points), or choose **Medium** (20,000 grid points), **Fine** (200,000 grid points), or **Custom** to set your own number of grid points.

Approximate driving force for metastable phases

The **Approximate driving force for metastable phases** check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.

Force positive definite phase Hessian

The **Force positive definite phase Hessian** check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

▶ ADVANCED_OPTIONS

Control stepsize

The **Control stepsize** check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

ADVANCED_OPTIONS

Max no of iterations

Enter or choose a value for the **Max no. of iterations**. By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Required accuracy

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Smallest fraction

The default **Smallest fraction** is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.



In Console Mode, the default of 1E-30 for IDEAL phases is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.

One Axis

Under *One axis*, there are these *Calculation Type* setting options.

Global minimization

The **Global minimization** check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.

ADVANCED_OPTIONS

Global test interval

The default **Every 10th eq** is the recommended **Global test interval** i.e. every tenth step and at each phase change during calculations. Or choose **Always** or **Custom**.

If you choose **Custom**, the integer number determines how often the global minimization should be used during step and mapping. Any other positive integer number, n, suggests it performs a global minimization test at every *n*-th step during calculations.

Phase Diagram

Under *Phase diagram*, there are these *Calculation Type* setting options.

Global minimization

The **Global minimization** check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.

Global test interval

The default **At node points** is the recommended **Global test interval** and is used only at node points during the calculations.

- If you choose **Every 10th eq**, this is every tenth step and at each phase change during calculations.
- If you choose **Custom**, the integer number determines how often the global minimization should be used during step and mapping. Any other positive integer number, n, suggests it performs a global minimization test at every *n*-th step during calculations.

Generate starting points automatically

The **Generate starting points automatically** check box is selected by default.

Use inside meshing points

Click the **Use inside meshing points** check box as required. The initial mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If you select the check box, then the initial equilibrium points added are also added to the inside edge.

No of meshes along an axis

The default **No of meshes along an axis** is 3 , which represents how many intervals of initial equilibrium points are added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, center, and end of each axis-variable forming 2 intervals.

Calculating with a Fixed Phase

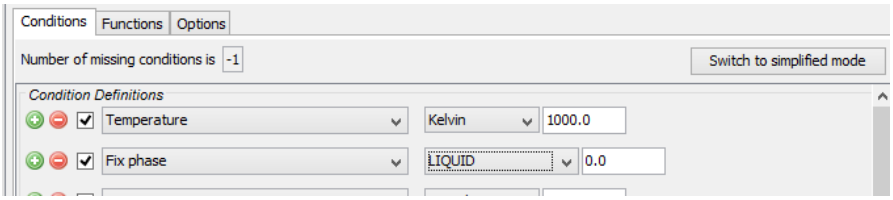
This describes how to use the advanced mode to set a phase to be fixed at a certain amount. This allows you to, for example, find out at what temperature a material starts to melt. If you set the phase to be fixed to liquid phase at zero amount, and do not define the temperature state variable, then you can calculate at what temperature the material enters a state where the liquid phase is no longer zero (that is, when it starts to melt).

For a fixed phase equilibrium calculation, it is recommended to serially couple the Equilibrium Calculators. This is where one Equilibrium Calculator activity is the successor to another Equilibrium Calculator activity that performs an ordinary equilibrium calculation, and then, for the condition you are interested in, you make a rough estimate of the value. This gives the fixed phase calculation better starting values.

1. Right-click a node that can add an **Equilibrium Calculator** to your project.
2. In the **Project** window, click the **Equilibrium Calculator** activity node.
3. In the **Configuration** window, click **Switch to advanced mode**.

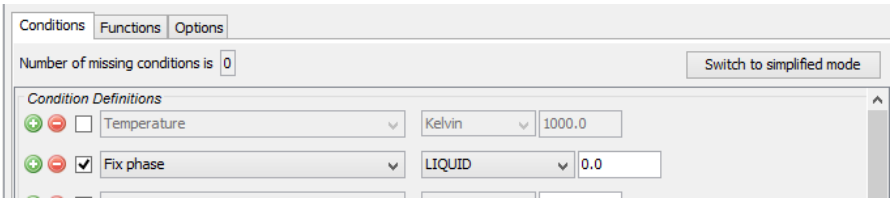
   If the **Default calculation mode** is globally set to **Advanced** then by default the Configuration window is already in advanced mode.

   Global Settings
4. Under *Condition Definitions*, click the **Add quantity** button.
5. Select **Fix phase** from the first menu.
6. Select the phase that you want to fix in the second menu, and set the amount of that phase you want to fix the phase to. For example, if you want to know when your material starts to melt, set the phase to **LIQUID** and the value to **0.0**:



   Above the *Condition Definitions*, the **Number of missing conditions is** field is probably **-1**. This means that you must remove one condition.

7. To remove a condition, either click the **Remove** button, or click to clear the check-box. For example, if you want to know at what temperature your material starts to melt, then you cannot have a fixed temperature, in which case the temperature condition is not selected:



The **Number of missing conditions is** field displays **0**. When you have set all your conditions, you can perform the Equilibrium Calculator (now or later).

Binary Calculator

A Binary Calculator can be used for some calculations involving two components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on binary systems. There is also a **Binary Calculation** template you can use to quickly set up a simulation.

The Binary Calculator relies on some specifications that are not supported by all databases. You need a specially designed database for the Binary Calculator such as the TCBIN database.



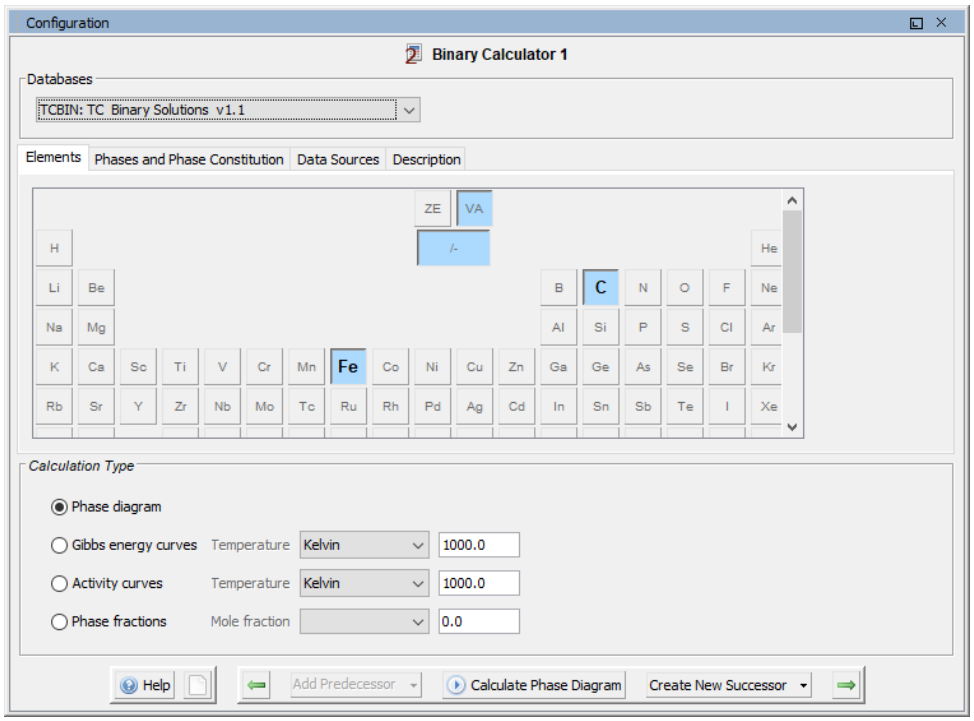
For an example of how a Binary Calculator can be used in a project, see T_03: Fe-C Phase Diagrams. For information about the templates see Creating a Project from a Template.

Configuration Window Settings

The Binary Calculator **Configuration** settings window and the associated tabs are similar to what you see on a System Definer. The database TCBIN is added by default when you use the Binary Calculation template, but you can choose any installed and licensed database from the list.



The various versions of the TCFE (Thermo-Calc Steels and Fe-Alloys) databases are not compatible with the Binary Calculator.


Configuration
Binary Calculator 1
Databases
TCBIN: TC Binary Solutions v1.1
Elements
Phases and Phase Constitution
Data Sources
Description
ZE
VA
/-
H
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Calculation Type
Phase diagram
Gibbs energy curves
Temperature
Kelvin
1000.0
Activity curves
Temperature
Kelvin
1000.0
Phase fractions
Mole fraction
0.0
Help
Add Predecessor
Calculate Phase Diagram
Create New Successor

Elements

On the **Elements** tab, and based on the database selected, select and review elements from the periodic table. Unavailable elements, which are based on the selected database, are greyed out.

Phases and Phase Constitution

At the top of the **Phases and Phase Constitution** tab, and based on the selected database, you can review the *Status* for the selected *Phases*. Select the **Check/uncheck all** check box to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the *Phase* list (for example **BCC_A2**) and its details are displayed below the *Phases* list. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

Data Sources

Data sources are not available until the activity has been performed. Click **Perform Tree** to display available data sources.

Description

The **Description** tab displays a description of the selected database.

Calculation Type

Choose a *Calculation Type*.

Phase diagram

Click **Phase diagram** to calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Gibbs energy curves

Click **Gibbs energy curves** to calculate at a constant temperature over the whole composition range. From the **Temperature** list select a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and enter a value in the field.

Activity curves

Click **Activity curves** to calculate at a constant temperature over the whole composition range. From the **Temperature** list select a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and enter a value in the field.

Phase fractions

Click **Phase fractions** to calculate as a function of temperature at a constant composition. From the **Mole fraction** list select a component and enter a value in the field.

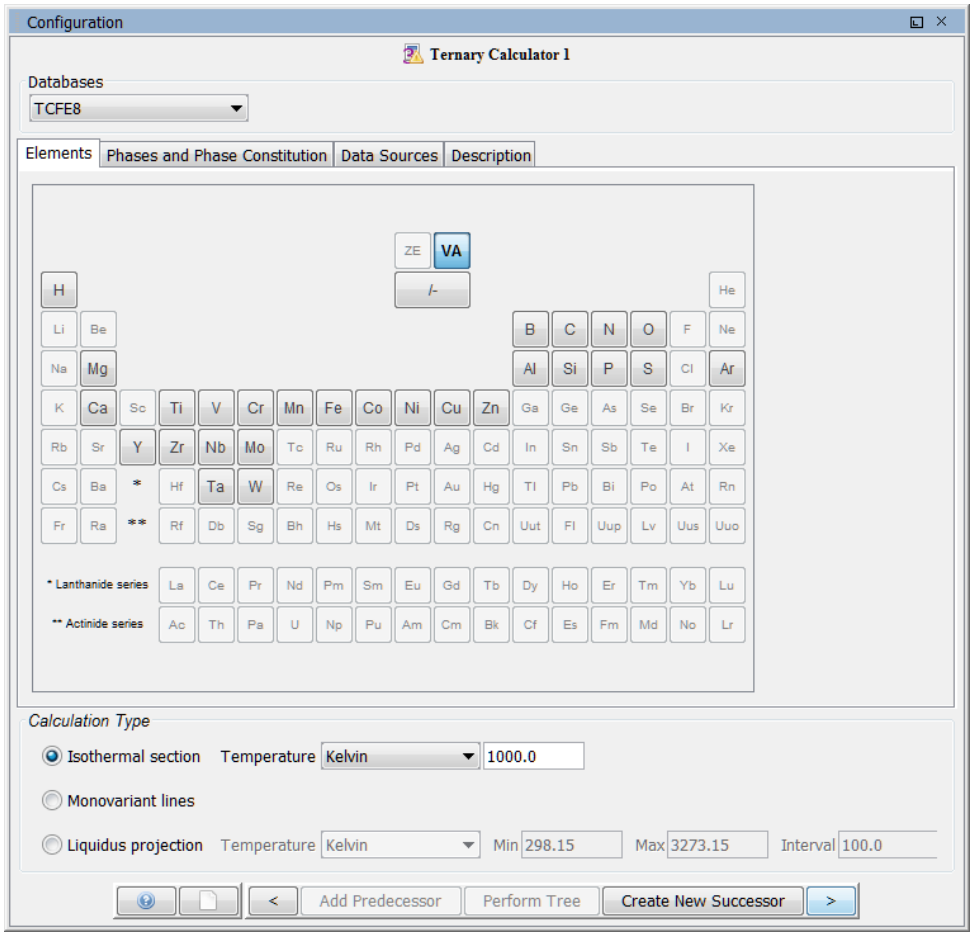
Ternary Calculator

A Ternary Calculator is used for some calculations involving three components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on ternary systems. There is also a **Ternary Calculation** template you can use to quickly set up a simulation.

For an example of how a Ternary Calculator is used in a project, see T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K. For information about the templates see Creating a Project from a Template.

Configuration Window Settings

Below lists the available settings that must be configured before performing the calculation and the image shows the **Configuration** window for a Ternary Calculator activity.



Databases

Select a database that contains specifications dedicated to the Ternary Calculator.

Elements

On the **Elements** tab, and based on the database selected, select and review elements from the periodic table. Unavailable elements, which are based on the selected database, are greyed out.

Phases and Phase Constitution

At the top of the **Phases and Phase Constitution** tab, and based on the selected database, you can review the *Status* for the selected *Phases*. Select the **Check/uncheck all** check box to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the *Phase* list (for example **BCC_A2**) and its details are displayed below the *Phases* list. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

Data Sources

Data sources are not available until the activity has been performed. Click **Perform Tree** at the bottom of the window to display available data sources.

Description

The **Description** tab displays a description of the selected database.

Calculation Type

Choose a *Calculation Type*.

Isothermal section

Click **Isothermal section** to calculate the ternary system for the whole composition range. From the **Temperature** list select a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and enter a value in the field.

Monovariant lines

Click **Monovarient lines** to calculate the variation of the liquid compositions with temperature.

Liquidus projection

Click **Liquidus projection** so that the projection liquid surface and the monovariant lines are calculated over the given temperature range. Then select the **Temperature** unit and in the fields enter a range (**Min** and **Max**) and an **Interval**.

Scheil-Gulliver Solidification Calculations



In Graphical Mode, you use the Scheil Calculator activity node to simulate the various models available in Thermo-Calc or with the Add-on Modules or additional databases.

Thermo-Calc is often used to perform equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can also be simulated.

A well-known example of a non-equilibrium calculation is the *Scheil-Gulliver solidification simulation*. In Thermo-Calc, the available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Classic Scheil Simulation

This is a Scheil simulation based on the well-known *Scheil-Gulliver* model. If this model is used without "fast diffusers" it is *Classic Scheil* simulation with the following assumptions:

- Diffusion in the liquid phase is assumed to be very fast, that is, infinitely fast.
- Diffusion in the solid phases is so slow that it can be ignored, that is, diffusion is assumed to be zero.
- The liquid/solid interface is in thermodynamic equilibrium.

In this Classic Scheil simulation the temperature is decreased step-by-step. When the temperature drops below the liquidus temperature the equilibrium amount and composition of solid and liquid phase is calculated. The solid phase is removed from the system and only the amount and composition of the liquid phase is used for the next calculation step at a lower temperature. Again, the equilibrium amount and composition of solid and liquid phase is calculated and again the solid phase is removed from the system for the next step. This procedure is repeated until the last liquid disappears.

This calculation procedure is equivalent to assuming that there is no diffusion in the solid phase and infinitely fast diffusion of all elements in the liquid phase. It has been shown to be a good approximation of the solidification of most alloys such as Ni-superalloys, Cu alloys, Al alloys, Mg alloys, and others. However, in materials with interstitial elements, such as carbon, ignoring diffusion in the solid causes discrepancies with experimental results.

Interstitial elements have much faster diffusion rates. The assumption of no diffusion in the solid phase during solidification is thus not correct at most industrial or lab-scale solidification rates.

For this reason, a variant of the Scheil simulation was developed and implemented in Thermo-Calc, where one or more elements can be defined as *fast diffusers*. See Other Options: Fast Diffusers and Scheil Simulations.

Scheil Simulation with Back Diffusion in Primary Phase

The *Scheil simulation with back diffusion in primary phase* kinetic model quantitatively takes into account the real back diffusion of all elements in the primary solid phase (typically the FCC or BCC phase). This model requires the use of both a thermodynamic and mobility database. The calculation also requires the cooling rate to be specified; a fast cooling rate allows for less time for back diffusion and the simulation result is similar to the classic Scheil-Gulliver solidification simulation. A very slow cooling rate allows for almost complete back diffusion, the solidification simulation is then close to an equilibrium calculation. It also requires that the size of the solidification domain is specified. In most cases this domain size corresponds to the secondary arm spacing, as this is where typically the liquid is trapped during solidification.



The secondary arm spacing also depends on the cooling rate. For this reason, a simple empirical relation between cooling rate and secondary arm spacing is predefined in Thermo-Calc.

For the *Scheil simulation with back diffusion in primary phase* model the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- The liquid/solid interface is in thermodynamic equilibrium.

Also see Other Options: Fast Diffusers and Scheil Simulations.

Scheil with Solute Trapping

The *Scheil with solute trapping* model simulates deviation from local equilibrium for the primary phase. It is useful for high solidification speeds, such as those seen in additive manufacturing applications and is based on the Aziz [1982] model for solute trapping and extended to multicomponent systems.

The model is based on the main assumption that the primary phase is the only dendrite forming phase affected by solute trapping.

For equilibrium- and Scheil-type solidification simulations thermodynamic equilibrium is established at the solid-liquid interface. This means that solutes are partitioned between the solid and liquid phases according to solidus and liquidus lines of the phase diagram. The assumption of thermodynamic equilibrium at the solid-liquid interface however breaks down for very fast solidification rates, that are encountered for example during additive manufacturing. Aziz [1982, Aziz; 1988, Aziz], proposed a model that links partitioning at the solid-liquid interface to solidification rate / interface velocity. Basically, the faster the solidification rate, the lower is the partitioning at the interface. Put very simply, what is thought to happen, is that the solid-liquid interface moves so quickly, that the solutes in the liquid are trapped in the advancing solid phase, thus the name “solute trapping”.

Aziz [1982] proposed a model to account for solute trapping based on balancing the overall kinetics at the solid-liquid interface. The two terms to be balanced are the velocity of the interface, that is calculated based on the cooling rate and considerations of the solid-liquid geometry (dendrite arm spacing) the interface kinetics, that follows from the trans-interface diffusion (meaning how fast solutes travel from one side of the solid-liquid interface to the other) and the change of phase from liquid to solid without changing the composition.

For a *Scheil with solute trapping* model the following assumptions are made.

- Only one primary solid phase forms dendrite, NOT necessarily the first solid phase
- Solute trapping in primary solid phase only. Other solid phases have equilibrium compositions following Scheil model
- Amounts of solid phases are dependent on solute trapping and solidification speed
- Dynamic liquidus for primary solid phase is dependent on solute trapping and solidification speed

Solute Trapping References

[1982, Aziz] Aziz, M. J. (1982). Model for solute redistribution during rapid solidification. Journal of Applied Physics, 53(2), 1158–1168.

[1988, Aziz] Aziz, M. J., & Kaplan, T. (1988). Continuous growth model for interface motion during alloy solidification. Acta Metallurgica, 36(8), 2335–2347.

Other Options: Fast Diffusers and Scheil Simulations

If a *Classic Scheil* or *Scheil simulation with back diffusion in primary phase* model is selected plus one or more *Fast diffuser* check boxes selected, then Thermo-Calc takes into account the concept of the *fast diffuser*. Typically, C is defined as a fast diffuser, but also other

elements such as N, O, or others can also be defined.



Fast diffuser does not quite define this since diffusion is not actually simulated. It is simply assumed that the “fast diffusers” distribute throughout the solid and liquid phase according to thermodynamic equilibrium. This corresponds to *infinitely fast diffusion* for the selected elements.

For a *Classic Scheil* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the solid phases, except the ones defined as “fast diffusers”, is zero.
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

For a *Scheil simulation with back diffusion in primary phase* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

The Classic Scheil simulation and Classic Scheil simulation with fast diffuser models can be considered *thermodynamic* models. There are clear limitations as a certain amount of back diffusion always takes place in the solid phase at real solidification.

You can also use the more sophisticated *Scheil simulation with back diffusion in primary phase* kinetic model. Adding the fast diffuser option to this can be useful, for example for interstitials like C in steels where these then equilibrate in all phases and not just the primary phase.

Summary

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Scheil in Graphical Mode vs Console Mode



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase

Scheil in Graphical Mode vs Console Mode

Type of Calculation	Console Mode	Graphical Mode
Classic Scheil	Use the START_WIZARD command to answer prompts	Scheil Calculator > select the Classic Scheil button on the Configuration window. Or use the Quick Start template > and select Scheil solidification simulation
Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > select the Scheil with back diffusion in the primary phase button on the Configuration window then enter the settings as needed. A mobility database is required.
Scheil with solute trapping	SOLUTE_TRAPPING command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > select the Scheil with solute trapping button on the Configuration window then enter the settings as needed.
Fast diffusers and Classic Scheil	Use the START_WIZARD command to answer the prompt `Fast diffusing components` where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > select the Classic Scheil button plus one or more of the Fast diffuser check boxes next to the composition(s) on the Configuration window then enter the settings as needed.

Type of Calculation	Console Mode	Graphical Mode
Fast diffusers and Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer the prompt `Fast diffusing components` where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > select the Scheil with back diffusion in the primary phase button plus one or more of the Fast diffuser check boxes next to the composition(s) on the Configuration window then enter the settings as needed. A mobility database is required.

Scheil Calculator

In Graphical Mode, you use the **Scheil Calculator** to set up the various Scheil solidification simulations outlined in more detail in Scheil-Gulliver Solidification Calculations.

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Scheil in Graphical Mode vs Console Mode

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase

There are several options to get started with a Scheil simulation using the Scheil Calculator.

- Use the **Scheil Solidification Simulation** template to add a project tree consisting of **System Definer**, **Scheil Calculator**, and **Plot Renderer** nodes.
- Build your own tree by right-clicking and adding nodes from **My Project**.
- Use the **Quick Start Wizard > Scheil Solidification Simulation** option to set up a Classic Scheil simulation. This adds a tree of nodes where you can then choose to simulate using the other options on the Scheil Calculator.
- Open an example and use this as a template.

By default, a Plot Renderer successor to a Scheil Calculator has the plot axes defined as **Mole fraction of solid** (X-axis) and **Temperature Celsius** (Y-axis). When these default axes are used, the results of normal equilibria calculations are automatically plotted in the same diagram as the Scheil calculations.

For information about the templates see Creating a Project with the Quick Start Wizard and Creating a Project from a Template.

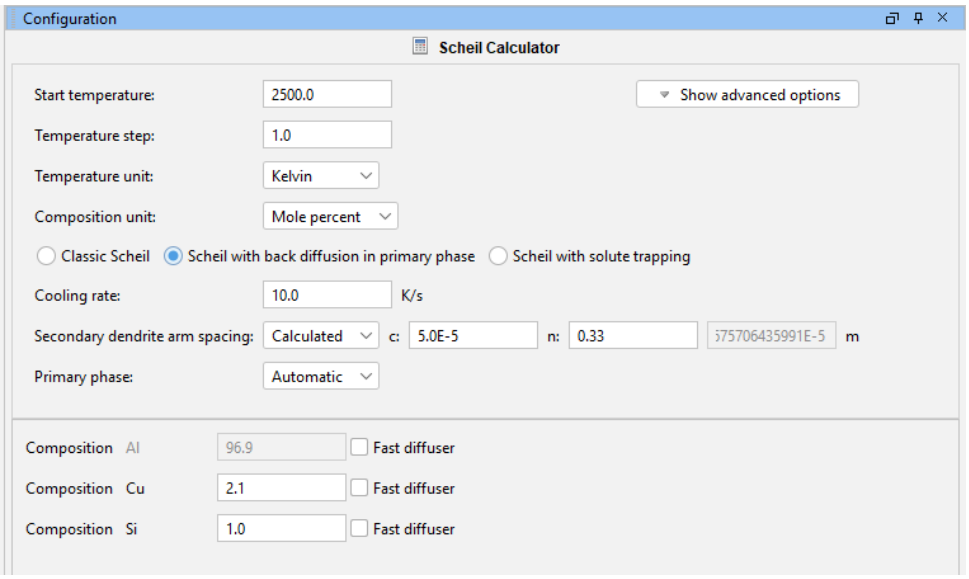
For examples using the Scheil Calculator see T_08: Scheil and Equilibrium Solidification, T_10: Scheil Solidification with Back Diffusion, and T_13: Scheil Solidification with Solute Trapping.

Define the Scheil Calculator

1. Add a **Scheil Calculator** node to the System Definer. If you used the **Scheil Solidification Simulation** template (or opened an example), click the node to display the **Configuration** settings window.
2. Enter the settings described in Configuration Window Settings. This includes details about the *Advanced Options* settings as well as all the permutations related to the types of Scheil simulations available such as back diffusion and solute trapping.
3. Once you have finished defining the Scheil Calculator, you also choose settings on the Plot Renderer.

Configuration Window Settings

An example of the main **Configuration** window of a **Scheil Calculator** activity is shown below. These settings must be configured before performing the calculation.



Start temperature

Enter a **Start temperature** that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.

Temperature step

Enter a **Temperature step**. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.

Temperature unit

Select the **Temperature unit**: **Kelvin**, **Celsius** or **Fahrenheit**.

Composition unit

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Choose a Model - Classic, Back Diffusion, Solute Trapping

- The available settings are based on the chosen model. See Scheil-Gulliver Solidification Calculations for descriptions.

Click to select a model - **Classic Scheil**, **Scheil with back diffusion in primary phase**, or **Scheil with solute trapping**. The settings are described accordingly.



The back diffusion option is available to select after adding a mobility database and once components are defined on the System Definer.

Composition

The **Composition** settings display after you add components to the System Definer.

Fast diffuser

The **Fast diffuser** check boxes are available after you add components to the System Definer. Click the check box to allow redistribution of this component in both the solid and liquid parts of the alloy.

Cooling rate (Back Diffusion)

This field is available when **Scheil with back diffusion in primary phase** is selected.

Specify the **Cooling rate** in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

Secondary dendrite arm spacing (Back Diffusion)

This field is available when **Scheil with back diffusion in primary phase** is selected.

The **Secondary dendrite arm spacing** is the distance in meters between two secondary dendrite arms. It can be either a **Constant** or **Calculated** from the cooling rate as c*(cooling rate)$^{-n}$ where c and n are entered in these fields.

Select **Calculated** or **Constant**.

- For **Calculated**, enter values for **c** and **n**.
- For **Constant**, enter a value (unit = m) in the field.

Primary phase (Back Diffusion and Solute Trapping)

This field is available when **Scheil with back diffusion in primary phase** or **Scheil with solute trapping** is selected.

The primary phase is the phase where the back diffusion or solute trapping takes place.

If **Automatic** is selected (or kept as the default), the program tries to find the phase which gives the most back diffusion or solute trapping.

To override this setting, choose a specific primary phase from the list:

- For back diffusion, only phases with diffusion data can be used as primary phases.
- For solute trapping, only phases that dissolve all elements in the system can be used as primary phases.

Scanning speed, Alpha, and Calculated solidification speed (Solute Trapping)

These fields are available when **Scheil with solute trapping** is selected.

As needed, enter **Scanning speed** and **Alpha** to define the **Calculated solidification speed**.

The **Calculated Solidification Speed** is Vs = $V_{scanning}$ * cos(α) m/s, where $V_{scanning}$ is the user specified **Scanning speed** in m/s and **Alpha** is the alpha angle, α, between the solid/liquid boundary and scanning direction.

Advanced Settings

Click **Show advanced options** to access more settings.

Global minimization

By default the **Global minimization** check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.

Liquid phase

The default in the list is the **Liquid phase** already defined in the database.

Terminate on

From the **Terminate on** list, choose **Fraction of liquid phase** or **Temperature** and enter a value in the field.

Max no. of iterations

Enter or choose a value for the **Max no. of iterations**. By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Required accuracy

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Smallest fraction

The default **Smallest fraction** is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.



In Console Mode, the default of 1E-30 for IDEAL phases is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.

Approximate driving force for metastable phases

The **Approximate driving force for metastable phases** check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.

Property Model Calculator

A **Property Model Calculator** enables you to predict and optimize material properties based on their chemical composition and temperature. The available calculation types are **Single**, **One Axis**, **Grid**, **Min/Max**, **Uncertainty**, and **Batch**.

Using these, you can evaluate models simultaneously over a range of compositions and temperature and cross plot the results, then conduct an uncertainty analysis and plot the results as either a histogram or a probability plot. The **Batch** calculation further enables you to read input from a file, such as a spreadsheet.

- Configuration Window Settings
- There are **General Models** and **Steel Models** available. For more information, see About the Property Models.

> You can also create custom Property Models. Search the TC-Python help on the website for details about creating custom models. In general go to the **Property Model Framework → Best Practices** section.

Property Model Calculator Workflow

At the start when you are designing a project, it is recommended you first test it by performing a **Single** calculation type. This verifies that the configuration of the model is valid, otherwise you will get a *Not a Number* result in the Event Log Window, which indicates the calculation did not work correctly.

Once the Single calculation performs successfully, you can experiment with other calculation types such as **Grid**, **Min/Max**, **Uncertainty**, or **Batch**. Best practice for both Grid and Uncertainty is to start with a small number of steps (Grid) or samples (Uncertainty) to confirm that it works before increasing the number of steps or samples. For Batch calculations, it is good practice to first review the data file requirements described in Working with Batch Calculations.

For a Grid calculation, you can additionally plot a *Heat map*, *Contour* or *3D* diagram. This setting is done on the Plot Renderer, which has several Plotting Options and Plotting Modes available.

In general, the workflow for each model differs. A recommended start point is to do a **One axis** calculation (using the Equilibrium Calculator) to determine what phases you get and where the transitions are before setting up the Property Model Calculator.

- The Quick Start Wizard and Templates and Creating a Project from a Template

About the Property Models

The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information.

General Models

The following General Property Models are available with the Property Model Calculator.

- About the Steel Model Library Property Models

Coarsening

The **Coarsening** Property Model calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase. See About the Coarsening Property Model and Coarsening Property Model Settings for background theory and input parameter details.

Crack Susceptibility Coefficient

The **Crack Susceptibility Coefficient** Property Model calculates the hot tearing tendency during solidification. See About the Crack Susceptibility Coefficient Property Model and Crack Susceptibility Coefficient Property Model Settings for background theory and input parameter details.

Driving Force

The **Driving Force** Property Model calculates the thermodynamic driving force for a phase. See Driving Force Property Model Settings for input parameter details.

Equilibrium

The **Equilibrium** Property Model calculates the equilibrium for the given conditions. Optionally define additional function definitions. See Equilibrium Property Model Settings for input parameter details.

Equilibrium with Freeze-in Temperature

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at all other temperatures. See About the Equilibrium with Freeze-in Temperature Property Model and Equilibrium with Freeze-in Temperature Property Model Settings for background information and input parameter details.

Interfacial Energy

The **Interfacial Energy** Property Model estimates the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. See About the Interfacial Energy Property Model and Interfacial Energy Property Model Settings for background information and input parameter details.

Liquid and Solidus Temperature

The **Liquid and Solidus Temperature** Property Model is for doing a common calculation. For example, you can easily use uncertainty calculations, vary one or more conditions, and see how that affects the liquidus and solidus temperatures. See Liquid and Solidus Temperature

Property Model Settings for input parameter details.

Phase Transition

The **Phase Transition** Property Model calculates the point when a new phase may form by varying set conditions. The Model is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the varied condition. See Phase Transition Property Model Settings for input parameter details.

Spinodal

The **Spinodal** Property Model calculates the spinodal line. See About the Spinodal Property Model and Spinodal Property Model Settings for background information and input parameter details.

T-Zero Temperature

The **T-Zero Temperature** Property Model calculates the so-called T_0 line. See About the T0 Temperature Property Model and T0 Temperature Property Model Settings for background information and input parameter details.

Yield Strength

The **Yield Strength** Property Model calculates yield stress. It returns the calculated yield strength at room temperature for the specified material using the equilibrium values calculated at a particular temperature and by further defining the following contributions to the total yield stress: precipitation strengthening, solid solution, grain boundary strengthening, and constant addition of strength. See About the Yield Strength Property Model and Yield Strength Property Model Settings for background information and input parameter details.

Calculation Types

- About the Uncertainty Calculations and Heat Map, Contour, and 3D Plots

The Property Model Calculator includes these calculation types:

- **Single**: Calculates a single point.
- **One axis**: Varies a quantity on the X-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps. You can then select to create heat map, contour and 3D plots on the Plot Renderer.
- **Min/Max**: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The Mean field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the Model(s) results are shown in the Event log.
- **Uncertainty**: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The Mean field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.
- **Batch**: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet. You can include experimental results in the data file, which then can be used to compare to the batch calculation results.

Examples and Video Tutorials

Website

For videos about the Property Model Calculator, go to our website.

YouTube

You can also go to YouTube channel to review the available training videos. Subscribe to the channel to be updated when new videos are added. Also see the video introduction to the Property Model Calculator.

About the Steel Model Library Property Models



The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information.

These **Steel Models** are available with the Property Model Calculator. The following are available with the Steel Library.

- About the Property Models

Bainite

The **Bainite** Property Model describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. In this Model, bainite is modeled as ferrite or a ferrite-cementite mixture.

See About the Bainite Property Model and Bainite Property Model Settings for background theory and input parameter details. Also see Steel Library TTT Diagram Template and Plot Settings: TTT Mode.

CCT Diagram

The **CCT Diagram** Property Model calculates the concurrent transformations to pearlite, bainite, and martensite under continuous cooling conditions and is used to construct a continuous-cooling-transformation (CCT) diagram.

See About the CCT Diagram Property Model and CCT Diagram Property Model Settings for background theory and input parameter details. Also see Steel Library CCT Diagram Template and Plot Settings: CCT Mode.

Critical Transformation Temperatures

The **Critical Transformation Temperatures** Property Model calculates critical transformation temperatures for steels.

See About the Critical Transformation Temperatures Property Model and Critical Transformation Temperatures Property Model Settings for background theory and input parameter details.

Martensite Fractions

The **Martensite Fractions** Property Model calculates the fraction of athermal martensite based on available driving force.

See About the Martensite Fractions Property Model and Martensite Fractions Property Model Settings for background theory and input parameter details.

Martensite Temperatures

The **Martensite Temperatures** Property Model calculates the martensite start (Ms) temperature based on modeling of the transformation barrier. Martensite half and finish temperatures are also given according to the Martensite Fractions Property Model.

See About the Martensite Temperatures Property Model and Martensite Temperatures Property Model Settings for background theory and input parameter details. Also see Steel Library TTT Diagram Template and Plot Settings: TTT Mode.

Pearlite

The **Pearlite** Property Model calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.

See About the Pearlite Property Model and Pearlite Property Model Settings for background theory and input parameter details. Also see Steel Library TTT Diagram Template and Plot Settings: TTT Mode.

TTT Diagram

The **TTT Diagram** Property Model calculates the concurrent transformations to pearlite, bainite, and martensite under isothermal conditions and is used to construct a time-temperature-transformation (TTT) diagram.

See About the TTT Diagram Property Model and TTT Diagram Property Model Settings for background theory and input parameter details. Also see Steel Library TTT Diagram Template and Plot Settings: TTT Mode.

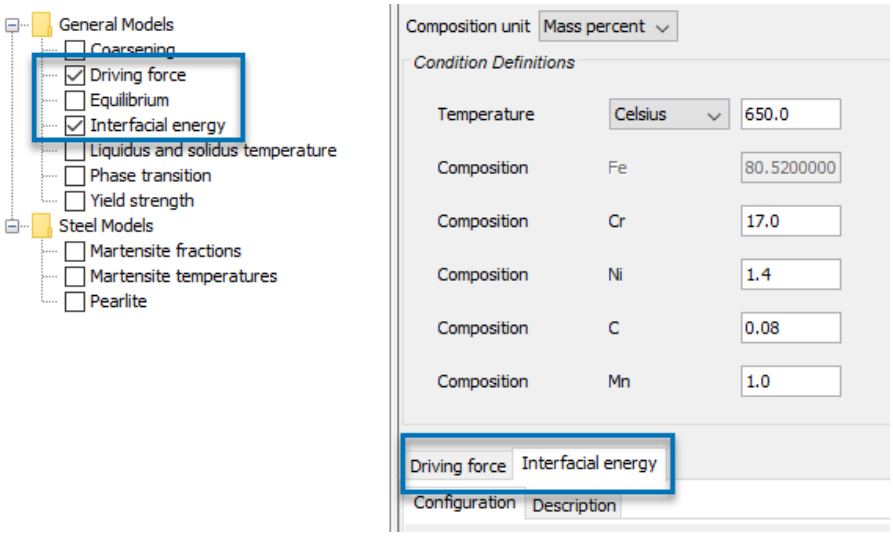
Define the Property Model Calculator

1. Add a **Property Model Calculator** node to the System Definer. If you used the **Property Model Calculation** template, click the node to display the **Configuration** settings window.

2. From the left side of the **Configuration** window, click to select one or more of the check boxes under the **General models** or **Steel models** folders.

   Steel Models are only available if you have a license for the Steel Model Library. If you are interested in learning more about the available models, go to our website.

   A tab with the same name as the Property Model opens in the right side of the window under *Condition Definitions*. When you select more than one Model, a matching tab is added in the same order that the check box is selected.



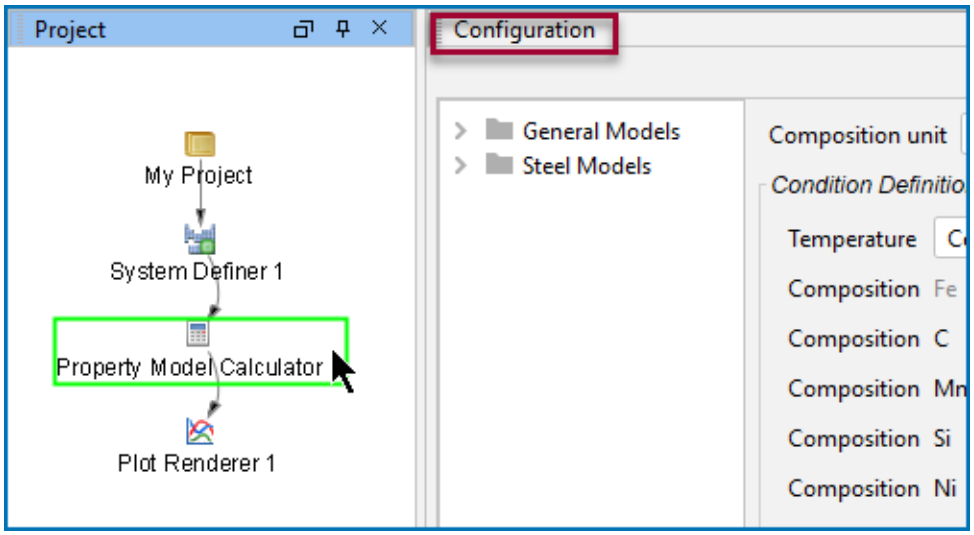
3. Enter the settings described in Configuration Window Settings and for each *Calculation Type*.
4. For each Model on the **Configuration** tab, select or enter settings as required.

> When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

5. Once you have finished defining the Property Model Calculator, you also choose settings on the Plot Renderer.

Configuration Window Settings

Click the **Property Model Calculator** node in the **Project** window to view the **Configuration** window. The settings available vary based on such choices as the Property Model and calculation type selected.



Composition unit

Choose a unit: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Condition Definitions

Choose a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a value for the **Temperature** and **Composition** for each component.

The values entered in *Condition Definitions* are used as the start values for the different calculation types.

Timeout in minutes

Select the **Timeout in minutes** check box to enter a time when a calculation will stop trying to complete the evaluation. This is useful if it is a complex or unknown calculation outcome and you want to prevent it from taking too much computer time or resources. The number entered in the field means that this is the maximum amount of time that each line can take for an individual calculation. This is useful in particular for Batch or Uncertainty calculations.

Define the Property Model

For each Property Model chosen, select or enter **Configuration** settings as required.

For links to each Model with the settings details, see About the Property Models.



When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Calculation Type

Choose a calculation type: **Single** (no axes), **One axis**, **Grid**, **Min/Max**, **Uncertainty**, or **Batch**.

- Select **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Results** window.

  Equilibrium Property Model Settings

- Select **One axis** to vary a quantity on the X-axis.
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.
- The **Min/Max** calculation evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log.
- The **Uncertainty** calculation evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Renderer activity.
- The **Batch** calculation allows for high throughput calculations with Property Models. Data can be read from a file, such as a spreadsheet, rather than, for example, having a fixed grid or random values. Results from these batch calculations can then be compared to experimental values (as long as this data is included), using the Cross plot mode on the Plot Renderer.

Axis Definition

For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.

Grid Definitions

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.



For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour*, or *3D* diagram.

Heat Map, Contour, and 3D Plots

Min/Max Definitions

For the **Min/Max** calculation type, click to select the applicable check boxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under *Condition Definitions* for the respective quantity.

Enter numerical values in the Δ**Min/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the **Event Log**.

Sampling of Data from Gaussian Distributions

For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

- About the Uncertainty Calculations

Sampling Parameters

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

- About the Uncertainty Calculations

Batch Controls

- For more details about the format of a data file used to define the compositions, parameters, experimental data, or skipping validation, see Working with Batch Calculations.

In the **Data file** field, either enter a file path or click the load data file button (📁) to navigate to a data file such as an Excel spreadsheet (with `*.xls` or `*.xlsx` extensions) or a `*.csv` file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software.

Click **Open** to import the data. In the **Data file** field you can see the file path to the selected file. The next time you click the load data file button (📁) the program remembers the last location from where the file is opened.

Choose the delimiter—**Comma** (,), **Colon** (:), **Equals sign** (=), **Semicolon** (;), or **Tab**—that matches the delimiter in the data file and click the **Reload** (🔄) button.

The data is imported and displays on the Property Model Calculator:

- The data are used for the applicable fields that must match what already exists as a Property Model parameter (e.g. critical radius, grain size, etc.) as well as the composition, temperature, and units that you want to run the calculation for. Also, if the dependent element composition is not included in the data file, the batch

calculation then sets the dependent element to be the same as defined in the user interface.

- The calculation runs once for every row of data included in the file.



When the data file is imported into Thermo-Calc, there is also a **Row** column autogenerated by Thermo-Calc.

Select the **Set zero amount to value (in mole-/mass-fraction)** to enter a small value for the mole/mass-fraction in cases where a Property Model has problems calculating zero amounts of elements.

Select the **Skip validation of data file** check box to allow a calculation to perform using the data file even when certain criteria are not met.

When selected, the validation of the data file is skipped:

- If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator.
- If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation.



If there are any data file validation error(s), a tooltip on the **Perform** button lists and describes these.

Diffusion Calculator



The Diffusion Calculator is available with three elements if you do not have the additional Diffusion Module (DICTRA) license. With the Add-on Module you can use all available elements as per the licensed database selected. See Available Graphical Mode Features for details.

A **Diffusion Calculator** allows you to set the conditions for, and perform, a diffusion calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use the **Diffusion Simulation** template.

Once you have added a Diffusion Calculator, the **Configuration** window has these settings tabs:

- **Conditions:** Set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles and the thermal profile.
- **Options:** Modify the simulation conditions such as the choosing the default solver (automatic or homogenization) and the time integration method. Also define the time step controls and if you choose homogenization as the solver, define further settings such as the interpolation scheme and whether to use global minimization or not.

Available Graphical Mode Features

The Diffusion Module is an Add-on Module to the core Thermo-Calc software.



A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*. This is not available in Console Mode. See Demonstration (Demo) Mode to learn more.

Diffusion Simulation Template

A **Diffusion Simulation** template is available to all Thermo-Calc users when in Graphical Mode.

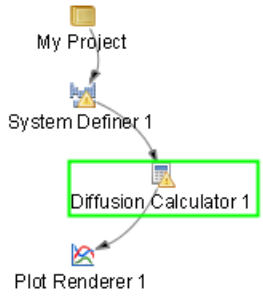


If you are using the Diffusion Module in Demo Mode, see Demonstration (Demo) Mode for what is available to you. Even if you have a license, you may find yourself in Demo Mode if you have a network license and all the licenses are checked out.

USING THE TEMPLATE

When you first open Thermo-Calc in Graphical Mode, on the **My Project** window, click the **Diffusion Simulation** button to add a *System Definer*, *Diffusion Calculator* and *Plot Renderer* to the **Project** tree.

Click the **Diffusion Simulation** icon in the Templates window to add **THESE NODES** to the Project.



Creating a Project from a Template.

Diffusion Calculator

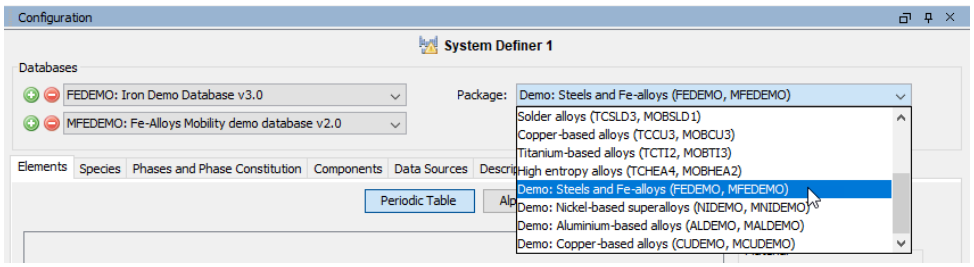
A Diffusion Calculator allows you to set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles and the thermal profile, plus additional options. Many of the settings are automatically set as you define your system. Details about this activity are described in Diffusion Calculator.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Diffusion Module simulation. If you have a Diffusion Module (DICTRA) license you can run all the examples because the demonstration database packages are included with your installation.

Select the database packages from the **System Definer Configuration** window to run a simulation.

If you are in Demo Mode, see Demonstration (Demo) Mode to learn more.



Demonstration (Demo) Mode

The Diffusion Module and some examples are available to all Thermo-Calc users but only for simulations with three elements. If you do not have a license for then you are in *Demo Mode* when using the Diffusion Calculator or Diffusion Simulation template.

DIFFUSION SIMULATION TEMPLATE

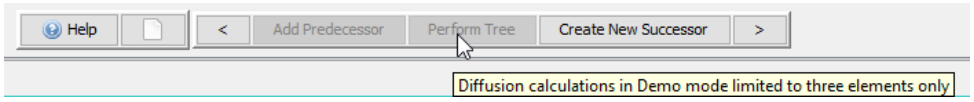
When you are in DEMO mode, in the **Templates** area this is indicated by the text under the logo.



DIFFUSION CALCULATOR

If you are experimenting with the Diffusion Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Diffusion Calculator, the **Perform** button is unavailable and the tooltip explains why.

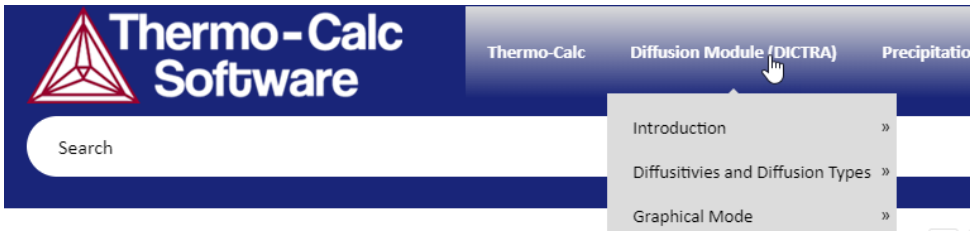


Even if you have more than three elements, the Plot Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Define the Diffusion Calculator

Available Graphical Mode Features

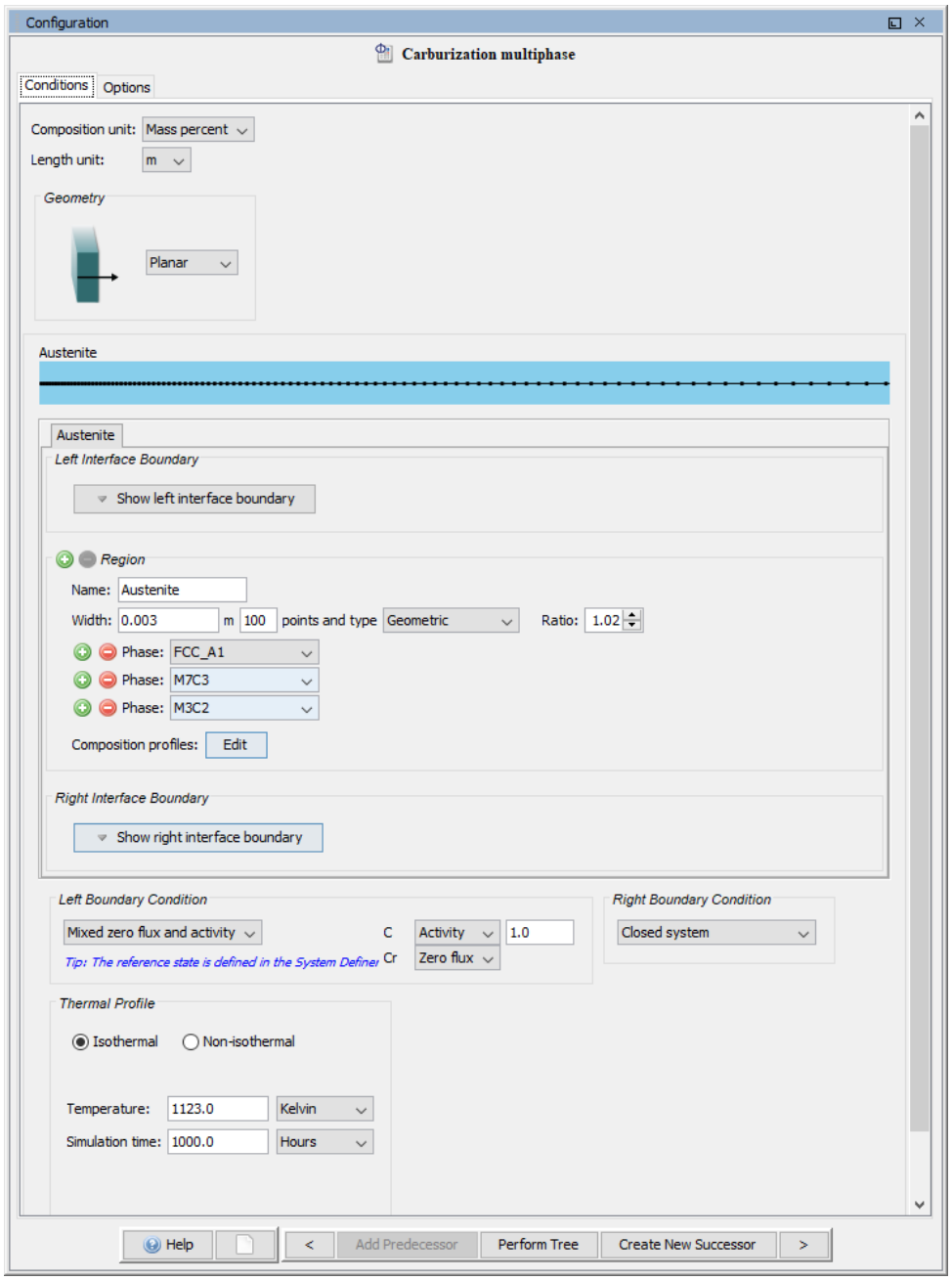
Working with diffusion simulations is an advanced topic. It is recommended you review the Diffusion Module (DICTRA) documentation and videos available or search for a specific topic.



1. Add a **Diffusion Calculator** node to the System Definer. If you used the **Diffusion Simulation** template, click the node to display the **Configuration** settings window.
2. In the Diffusion Calculator **Configuration** window, enter the settings described in Conditions Tab Settings and Options Tab Settings.
3. Once you have finished defining the Diffusion Calculator, you also choose settings on the Plot Renderer. Some additional settings are specific to the Diffusion Calculator Plot Renderer.

Conditions Tab Settings

The following Configuration window is from the *Graphical Mode Quick Start Guide*. It is using project example file *D_07: Diffusion Carburization Multiphase*.



These are the settings available from the **Conditions** tab. To edit the defaults for some settings, go to **Tools → Options → Graphical Mode → Diffusion**.

The Diffusion Module (DICTRA) in Console Mode has commands to perform some of the settings also available on the Diffusion Calculator. Where possible the name of the command is indicated and includes a link to the topic.

General

Composition Unit

Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Length Unit

Choose **m**, **µm** or **nm**.

Geometry

Choose **Planar**, **Spherical** or **Cylindrical**. For Cylindrical, also enter a value for the **First interface position** .

With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere. The highest coordinate (right boundary) is defined by the cylinder or sphere radius.

Region Settings



There should be one unique phase in each region.

Left and Right interface boundary

Toggle between hiding and showing the **Left interface boundary** or **Right interface boundary**.

Click the **Add quantity** or **Remove quantity** buttons as required to add a **Phase** and then enter a value for the **Driving force** as required. The default driving force is `1.0E-5`.

Name

Enter a **Name** for the region in the field. For example, enter `Austenite`. This name is automatically updated on the tab and above the grid points graphic. You can also double-click the tab to enter the name.

Width

Enter a numerical value in the **Width** field. The unit is the one selected for the **Length unit**.

Points

Enter a numerical value in the **points** field. The default is 50.

Type (of Grid)

Select a type of grid, **Linear**, **Geometric** or **Double geometric**.

Choose **Geometric** for a grid that yields a varying density of grid points in the region. Then enter a **Ratio** to determine the distribution. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.

Choose **Double geometric** to have a high number of grid points in the middle or at both ends of a region. Then specify two geometrical factors, the **Upper ratio** for the distribution in the lower (left) part of a region, and **Upper ratio** for the distribution in the upper (right) part of a region.

Phase

Choose a **Phase** from the list. The available options are defined in the System Definer. At least one phase that dissolves all system elements must be selected.

Click the **Add quantity** or **Remove quantity** buttons as required.

Composition Profile

Click **Edit** to open the **Initial Composition** window.

Select a **Dependent component** for which the composition does not need to be given. The available options depend on the phase description.

For each **Component** choose one of these options:

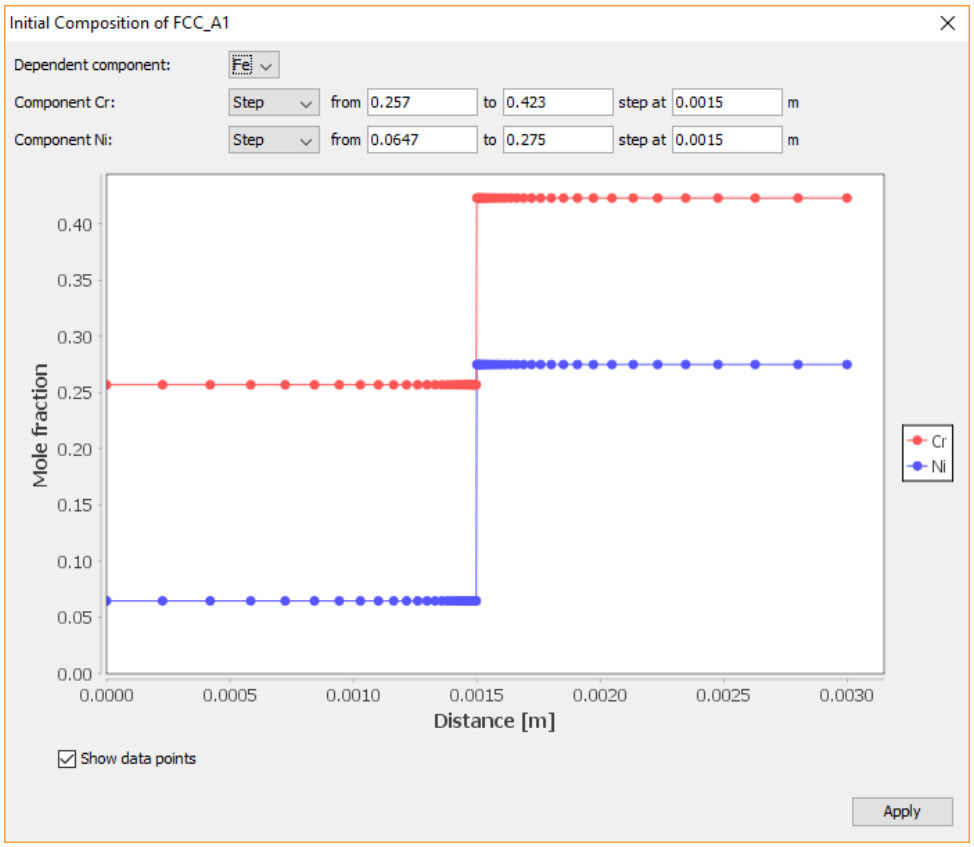
- **Linear**: Enter numerical values in the **from** and **to** fields.
- **Step**: Enter numerical values in the **from** , **to** , and **step at** fields. The unit is the same as the **Length unit** selected at the top of the Configuration window.
- **Function**: Enter a composition function in the field using SI units. The syntax to use for writing functions is a Python syntax (a programming language). Any valid Python expression that is a function of the distance variable *x* will work.
- 

  You can use the standard Jython math library but you must prefix these functions with the text "math" For example: `10 + math.sin(x*2)`. The Jython math library is available here: http://www.jython.org/docs/library/math.html.

  - The error function `erf(X)` is also available in the Jython math library and can be called with `math.erf(x)`.
  - Another useful function is the Heaviside step-function `hs(X)`. For example, `3+2hs(x-1e-4)` provides a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at 1e-4m=100mm.

Click **Apply** when you are done.

As you add these settings, the plot helps you visualize the region based on whether you use a **Linear**, **Step** or **Function** to define the components.



Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Examples D_06 and D_07 use boundary conditions, as described in Diffusion Module (DICTRA) Graphical Mode Examples.

The boundary condition settings are done on the **Diffusion Calculator**. The following describes the options available for the *Left boundary* and *Right boundary* conditions.

Closed system

By default it is a **Closed system**. Choose **Mixed zero flux and activity** or **Composition** if the system is not closed. Corresponds to a fix flux value, which is set to zero at all times. This is the default boundary condition.

Composition

Allows the user to set a fix composition at the boundary.



In Console Mode this is similar to the command STATE_VARIABLE_VALUE, but in Graphical Mode this condition is limited to setting a fixed composition.

Mixed zero flux and activity

The flux of selected components is either set to zero or a prescribed activity value.

For **Mixed zero flux and activity**, and for each independent element selected in the **Composition profile**, choose either **Zero flux** or **Activity** from the lists and enter a value in the field when **Activity** is selected. The reference state for the components are taken from the System Definer **Components** tab.

In the field for **Activity**, enter a formula that the software evaluates during the calculation.

The formula can be:

- A function of the variable TIME
- A constant

The formula must be written with these rules:

- A number must begin with a number (not a dot)
- A number must have a dot or an exponent (E)

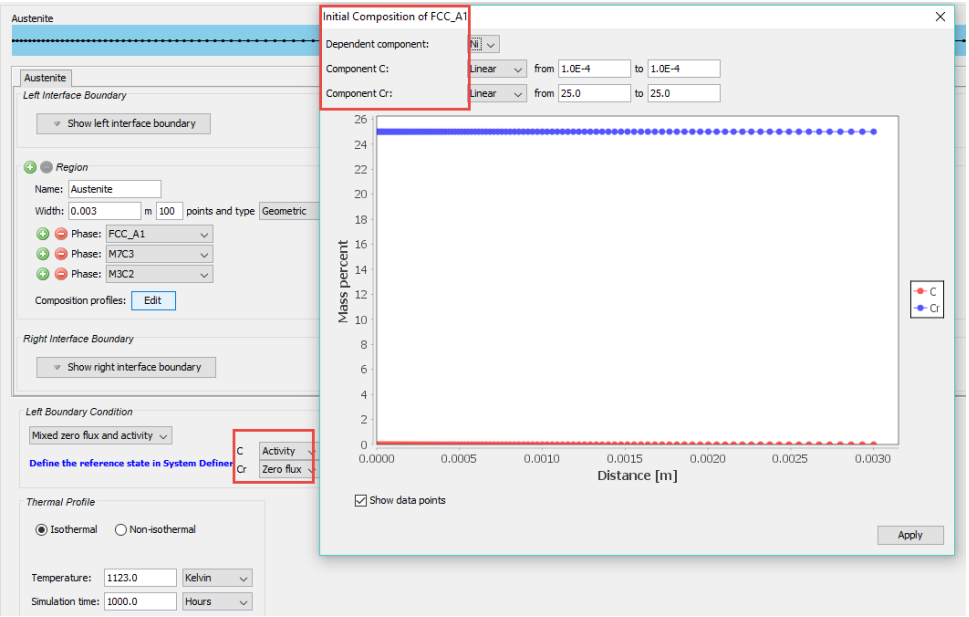
The operators + , - , * , / , ** (exponentiation) can be used and with any level of parenthesis.

As shown, the following operators must be followed by `()` i.e. open and closed parentheses:

- SQRT(X) is the square root
- EXP(X) is the exponential
- LOG(X) is the natural logarithm

- LOG10(X) is the base 10 logarithm
- SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)
- SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH(X)
- SIGN(X)
- ERF(X) is the error function

This image is from example *D_07: Diffusion Carburization Multiphase*.



Thermal Profile

Isothermal

Use an **Isothermal** calculation type to do a diffusion simulation at constant temperature. Choose a unit of measurement and enter a numerical value for the **Temperature** and **Simulation time**.

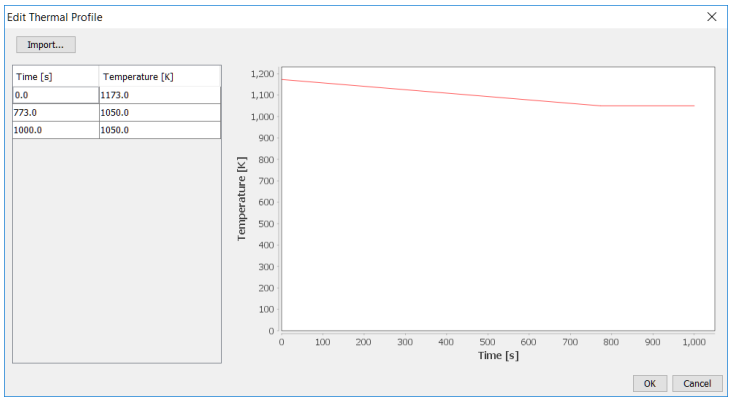
Non-isothermal

Use a **Non-isothermal** calculation type to do a diffusion simulation with a user-defined temperature profile. Select a **Temperature unit** and **Time unit** from the lists. Enter a numerical value for the **Simulation time**.

Click **Edit thermal profile** to enter thermal profile **Temperature** and **Time** coordinates into a table. A minimum of two points is required. You can also **Import** to add your own **Thermal profile** from a text file in ***.xls**, ***.xlsx**, or ***.csv** formats.

EDIT THERMAL PROFILE WINDOW

This image is from example *D_04: Diffusion Fe-C Moving Boundary Austenite to Ferrite*.



Options Tab Settings

The following settings are available on the **Options** tab for a Diffusion Calculator.

You can edit the defaults for some of these settings by going to **Tools → Options → Graphical Mode → Diffusion**. Also see Global Settings: Diffusion Calculator.

The Diffusion Module (DICTRA) in Console Mode has commands to perform some of the settings also available on the Diffusion Calculator. Where possible the name of the command is indicated and includes a link to the topic.

Simulation Conditions

DEFAULT SOLVER

Automatic or **Homogenization**.

Select **Homogenization** to define additional sections.

ABOUT THE HOMOGENIZATION SOLVER

The homogenization solver (called the homogenization model in Console Mode) is useful when you want to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point.

Time integration method

Automatic , **Trapezoidal** or **Euler backwards**.

The default is **Automatic** where the default degree of implicity corresponds to trapezoidal (0.5) for classic and Euler Backward (1.0) for the homogenization model. If large fluctuations occur in the profiles it may be necessary to use the more stable but less accurate *Euler backwards*.

Save results on file

Yes, **No** or **Every nth.** . Select **Every nth** to enter a value in the field.

This setting is determine if the results are to be saved on file during the course of the simulation.

- **Yes** to always save on file
- **No** to never save on file
- **Every nth.** to save every n^{th} time to file. Then enter an integer value ranging from 0 to 99.

Use forced starting values in equilibrium calculations

The default **Automatic** allows the software program to automatically use forced starting values to perform the equilibrium calculations. When a phase with an ordering contribution is entered into the simulation, for example the gamma-prime/fcc_l12 phase in Ni-base superalloys, forced starting values are automatically turned on. Or choose **Yes** or **No**.

Default driving force for phases allowed to form at interfaces

Enter a value in the field. The required driving force (evaluated as `DGM (ph)`) to be used for determining whether an inactive phase is stable. DGM is the variable for the driving force that is already divided by RT, and it is dimensionless. The default is `1E-5`.

▶ Suffixes

Timestep Control

Max Relative Error

Enter a value in the field. The default is `0.05`.

Max Absolute Error

Enter a value in the field. The default is `1.0E-5`.

Timestep

Enter values in the fields.



This value is always in seconds.

- **Initial**. What is used as the initial time step. The default is `1.0E-7`.
- **Smallest allowed**. The smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step. The default is `1.0E-7`.
- **Max % of simulation time**. The default is `10`.

Factor specifying the maximum increase in the time step taken from one time step to another

For example, if 2 is entered the maximum time step is twice as long as the previous time step taken.

Enter a value in the field. The default is 2.

The timestep is to be controlled by the phase interface displacement during the simulation

The default is **Automatic**. When a liquid phase is entered in a simulation this option is automatically turned on. Optionally choose **Yes** or **No** to set whether the time step is to be controlled by the phase interface displacement during the simulation.

Classic and Homogenization Model Settings

Classic Model Specific

Activity or Potential

Use the [**activity** or **potential**] of a component in order to find the correct tieline at the phase interface.

Determines whether the program should use the potential or the activity of a component in order to find the correct tie-line at the phase interface. The potential or the activity is varied by the program and is set in order to reduce the degrees of freedom at the local equilibrium.

Flux Balance Equation Accuracy

Required accuracy during the solution of the flux balance equations. The default is `1.0E-16`.

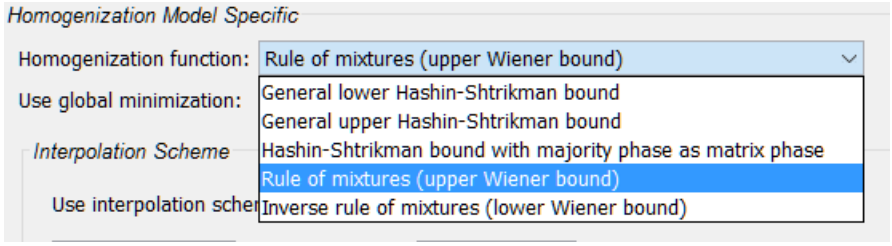
Homogenization Model Specific



This section is available when **Homogenization** is selected (or automatically selected) as the **Default solver**. These settings are available on the **Options** tab.

Homogenization Function

Several functions are available. The default is **Rule of mixtures (upper Wiener bound)**. See About the Homogenization Functions.


Homogenization Model Specific
Homogenization function:
Rule of mixtures (upper Wiener bound)
Use global minimization:
General lower Hashin-Shtrikman bound
General upper Hashin-Shtrikman bound
Hashin-Shtrikman bound with majority phase as matrix phase
Rule of mixtures (upper Wiener bound)
Inverse rule of mixtures (lower Wiener bound)
Interpolation Scheme
Use interpolation schem

Use global minimization

Select the check box for global minimization used in equilibrium calculations. In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.

Interpolation scheme

When the homogenization model is used, simulations are run using an implicit finite volume method to increase numerical stability. Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations. You can reduce simulation time with the **Use Interpolation scheme** check box. The check box is selected by default.

Discretization

[**Logarithmic** or **Linear**] discretization with *[number of]* steps in each dimension.

- For the linear discretization the scheme is not used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where composition span many orders of magnitude, the logarithmic discretization can be tried.
- Enter the number of steps in composition space. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization. The default is `10000` steps.

Memory to use

This is the fraction of free physical memory to be used by the interpolation scheme.

Select **Megabyte** or **Fraction of free** and then enter a value in the field.

About the Homogenization Functions

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase. For the general lower Hashin-Shtrikman bound the outermost shell consists of the phase with the most sluggish kinetics and vice versa for the general upper bound. The geometrical interpretation of the Hashin-Shtrikman bounds suggest further varieties of the bounds, viz. *Hashin-Shtrikman bound with prescribed matrix phase* and *Hashin-Shtrikman bound with majority phase as matrix phase*, where the outermost shell consist of a prescribed phase or the phase with highest local volume fraction, respectively.

The geometrical interpretation of the Wiener bounds are continuous layers of each phase either parallel with (upper bound) or orthogonal to (lower bound) the direction of diffusion.



The labyrinth factor functions (described below) are available in Console Mode and when using TC-Python.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with either the volume fraction (*Labyrinth factor f with prescribed matrix phase*), or the volume fraction squared (*Labyrinth factor f**2 with prescribed matrix phase*), of the matrix phase.



The varieties with excluded phases (described below) are available in Console Mode and when using TC-Python.

The varieties with excluded phases are useful in several respects. First, if a phase is modeled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as excluded causes the mobility of all components in that phase to be set to zero. Second, often there are some major matrix solid solution phases and some minor precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it produces a kinetic coefficient of zero. However, using *General lower Hashin-Shtrikman bound with excluded phase(s)* the excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Pause, Resume and Cancel Diffusion Calculations

Diffusion calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again.

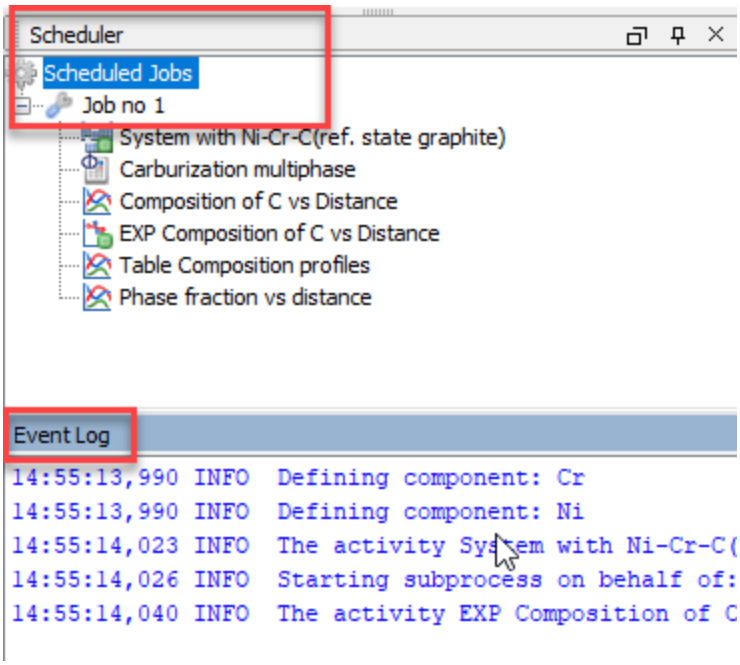
Graphical Mode

In Graphical Mode, you pause and resume when you are on the Diffusion Calculator **Configuration** window. When pausing a Diffusion Calculator calculation, you can make changes to the left and right boundary conditions and to the simulation time. This is useful, for example, when simulating carburization, where it is common to first have a step with high carbon activity in the furnace for the actual carburization, and then lower it and allow the carbon in the specimen to diffuse without further increased carbon content.

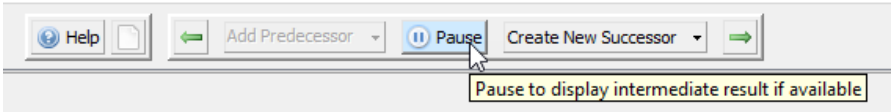
This is also available for the Precipitation Calculator (but not any other calculators). See Pause, Resume and Cancel Precipitation Calculations.

How to Pause and Resume a Job

1. Run the job (i.e. click **Perform Tree**). In the **Scheduler**, you can see the job listed and in the **Event Log** you can follow the progress of the calculation.

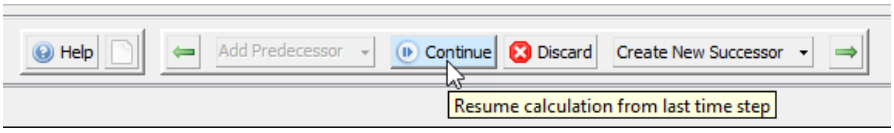


2. In the **Project** window, click the **Diffusion Calculator** node.
3. In the **Configuration** window at the bottom, click **Pause**. If there are intermediate results available these will be listed in the **Event Log**.



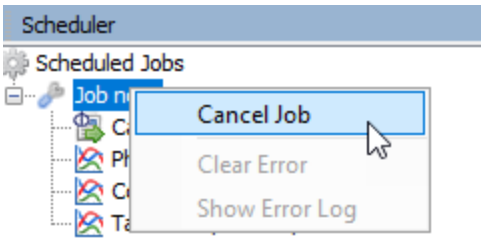
4. As required, make changes to the *Left Boundary Condition* and *Right Boundary Condition* settings and/or to the *Simulation time*. The rest of the **Configuration** window settings are grayed out and no other editing can be done while paused.
5. When ready, click **Continue** to resume your calculations from the last time step or click **Discard** to discard the calculation (then click **Yes** or **No** on the window that

opens).



How to Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



Console Mode

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To stop the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

Precipitation Calculator



The Precipitation Calculator is available with three elements if you do not have the additional Precipitation Module (TC-PRISMA) license. With the Add-on Module you can use all available elements. See Precipitation Module: Available Graphical Mode Features for more information.

A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use the **Precipitation Simulation** template.

Once you have added a Precipitation Calculator, the **Configuration** window has these settings tabs where there are many available conditions to set:

- **Conditions**: Set the conditions for your calculation that define the *Matrix phase* and *Precipitate phase*. Choose the *Calculation Type*.
- **Options**: Modify *Numerical Parameters* that determine how the conditions are calculated.

There are also unique settings available for this calculator once you add a Precipitation Calculator Plot Renderer.

Precipitation Module: Available Graphical Mode Features

The Precipitation Module, previously referred to as TC-PRISMA, is an Add-on Module to the core Thermo-Calc software. A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*.

Demonstration (Demo) Mode

Precipitation Simulation Template

A **Precipitation Simulation** template is available to all Thermo-Calc users.

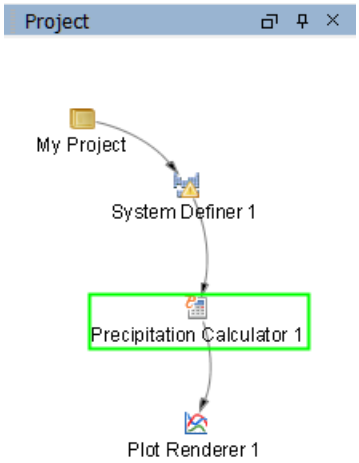


If you are accessing the Precipitation Module in Demo Mode, see Demonstration (Demo) Mode for what is available to you.

USING THE TEMPLATE

When you first open Thermo-Calc in Graphical Mode, on the **My Project** window, click the **Precipitation Simulation** button to add a *System Definer*, *Precipitation Calculator* and *Plot Renderer* to the **Project** tree.

Click the **Precipitation Simulation** button in the templates section to add these nodes to the Project.



Creating a Project from a Template

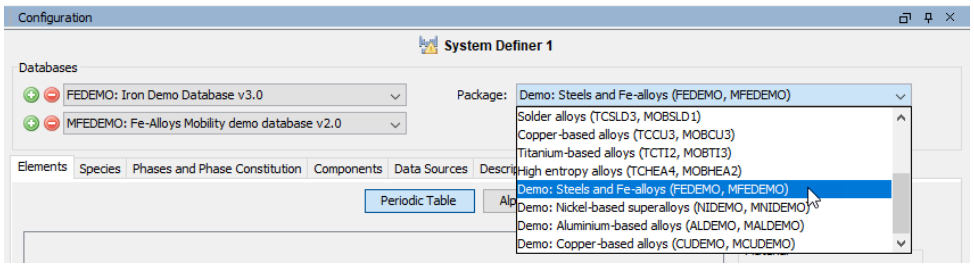
Precipitation Calculator

A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Precipitation Module simulation. If you have a Precipitation Module (TC-PRISMA) license you can run all the examples as the demonstration database packages are included with your installation. Select the database packages from the **System Definer** →**Configuration** window to run a simulation.

If you are using the Precipitation Module in Demo Mode, see Demonstration (Demo) Mode to learn more.



Demonstration (Demo) Mode

The Precipitation Module, and some examples, are available to all Thermo-Calc users but only for simulations of alloys with up to three elements. If you do not have a license for the Precipitation Module then you are in *Demonstration Mode* when using the Precipitation Calculator or Precipitation Simulation template.

PRECIPITATION SIMULATION TEMPLATE

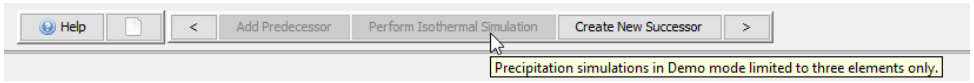
When you are in DEMO mode, in the **Templates** area this is indicated by the text under the logo.



PRECIPITATION CALCULATOR

If you are experimenting with the Precipitation Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define up to three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Precipitation Calculator, the **Perform** button is unavailable and the tooltip explains why. In this case one of the chosen elements needs to be removed and then the Perform button is made available.



Even if you have more than three elements, the Plot Renderer or Table Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Define the Precipitation Calculator

Precipitation Module: Available Graphical Mode Features

Working with precipitation simulations is an advanced topic. It is recommended you review the Precipitation Module (TC-PRISMA) documentation and videos available or search for a specific topic.

1. Add a **Precipitation Calculator** node to the System Definer. If you used the **Precipitation Simulation** template, click the node to display the **Configuration** settings window.
2. In the Precipitation Calculator **Configuration** window, enter the settings described in Conditions Tab Settings. Additional advanced options settings are also available and described Option Tab Settings.
3. Once you have finished defining the Precipitation Calculator, you also choose settings on the Plot Renderer. Some additional settings are specific to the Precipitation Calculator Plot Renderer.

Conditions Tab Settings

Below are details about the settings available from the **Conditions** tab on the calculator **Configuration** window.

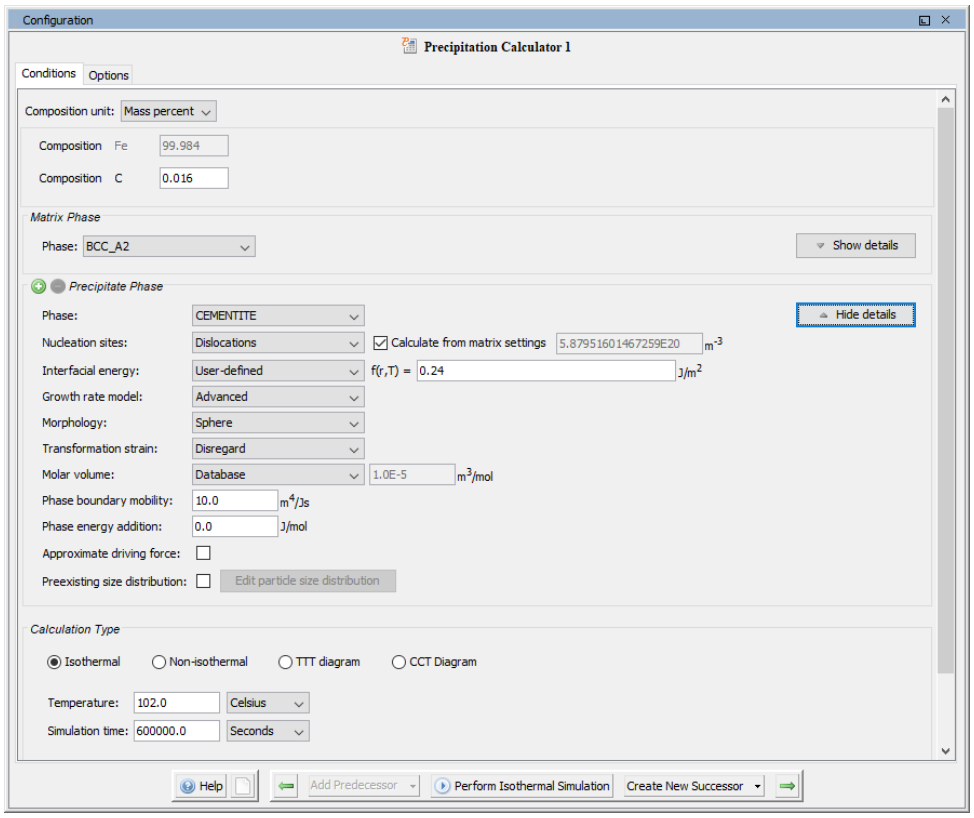


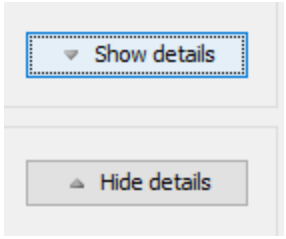
Figure 2: This is the Configuration window for example P_04_Precipitation_Fe-C_Cemetite.tcu. In this case, Show details is expanded to show the Precipitate Phase settings.



You can change these settings locally for a specific Precipitation Calculator or globally for some defaults in the **Options** settings. To open the Options window: From the main menu select **Tools → Options**. Click the **Graphical Mode** tab then click **Precipitation**.

Show or Hide Details

Click **Show details** (found to the right of the section) to view some of the additional settings listed below. You can also set the default to display in **Phase view mode** under **Tools → Options→Graphical Mode**, then click the **Precipitation** node.



COMPOSITION UNIT

Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

MATRIX PHASE

Phase



Only phases with kinetic data can be selected as the matrix phase. If the list is empty, go to the System Definer to confirm that both thermodynamic and kinetic databases are selected and defined.

Choose a **Phase** from the list. The list is based on the settings for the System Definer. When setting up a system, choose a matrix phase with kinetic data available in the database.

Elastic properties

Choose **Disregard** to ignore the elastic properties.

Default elastic constants for **Isotropic** or **Cubic** are based on the major element of the alloy system. The elastic properties can affect nucleation rate, nuclei size, and particle shape.

- For **Isotropic**, enter values for **Shear modulus** (in GPa) and **Poisson's ratio** as required.
- For **Cubic**, enter values for **c11**, **c12** and **c44** as required. c_{11}, c_{12}, c_{44} are the elastic constants.

Molar volume

Use the **Database** value (if the molar volume for the phase is defined in the thermodynamic database) or select **User-defined** to enter another value.

Grain size

Grain size is the "diameter" of a grain. The **Grain size** value changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the Precipitate Phase. Enter a numerical value and choose a unit from the list. The default is 1.0E-4 m.

Grain aspect ratio

For an elongated grain with a minor axis and a major axis, one may use the minor axis as grain size and the major/minor ratio as the grain aspect ratio to characterize the grain. The **Grain aspect ratio** value also changes the available nucleation sites when **Grain boundaries**,

Grain edges, or **Grain corners** is selected along with **Calculate from matrix settings** in the Precipitate Phase. Enter a numerical value. The default is 1.0.

Dislocation density

The **Dislocation density** value changes the available nucleation sites when **Dislocations** is selected along with **Calculate from matrix settings** in the Precipitate Phase. Enter a numerical value. The default is 5.0E12 m^{-3}.

Mobility enhancement prefactor

A parameter that multiplies to the mobility data from a database. This value scales the mobility by a constant amount. This can be useful, for example, when the material has a higher than normal vacancy concentration at the start of the precipitation simulation. (e.g. from a prior solutionizing and quenching treatment).

Mobility enhancement activation energy

A value that adds to the activation energy of mobility data from a database. This value scales the mobility by a temperature dependent amount. Similar usage as mobility enhancement prefactor.

PRECIPITATE PHASE

Phase

The phases available to choose have both thermodynamic and kinetic data. If the list is empty, go to the System Definer to confirm that both types of databases are selected and defined.

Choose a **Phase** from the list. The list is based on the System Definer settings.

Nucleation sites

The number of different nucleation sites is dependent on the shape and size of grains in the matrix. Grain size is the "diameter" of a grain. Choose one of the following from the list.

- **Bulk**, **Grain boundaries**, **Grain edges**, **Grain corners**, or **Dislocations**.
- For **Grain boundaries**, **Grain edges** and **Grain corners**, enter the **Wetting angle (0-90)** in addition to the matrix settings. **Wetting angle** defines the deviation from spherical shape (or dihedral angle).

Click to select the **Calculate from matrix settings** check box if you want to calculate the number density of sites from the matrix grain size or dislocation density.

To enter a specific value for the number of **Nucleation sites**, deselect the check box.

Interfacial energy

Choose **Calculated** to use the estimated value. To adjust the estimate, enter a different **prefactor** or choose **User-defined** to enter a value in J/m^2. For the User-defined option, you can also enter it as a function of radius (r) and temperature (T).

Growth rate model

Select **Simplified**, **General** , **Advanced**, **Paraeq** or **NPLE**. All models treat a particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Local equilibrium or paraequilibrium at the precipitate-matrix interface is assumed.

Morphology

Choose the particle shape: **Sphere** (default), **Cuboid**, **Plate** or **Needle**. Options are based on the **Elastic properties** selected for the **Matrix** phase:

- For **Cubic**, **Sphere**, **Plate** , **Needle** and **Cuboid** are available.
- For **Isotropic**, **Sphere**, **Plate** and **Needle** are available.

For **Plate** or **Needle**, select the **Calculate aspect ratio from elastic energy** check box or enter a numerical value in the **Aspect ratio** field to provide a constant aspect ratio.

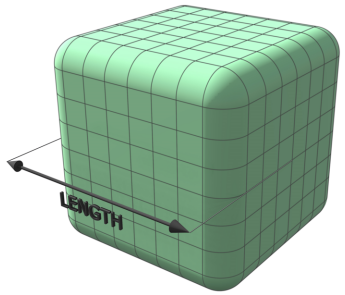


Figure 3: The cuboid shape is described by a supersphere. Cuboids have six faces, which form a convex polyhedron.

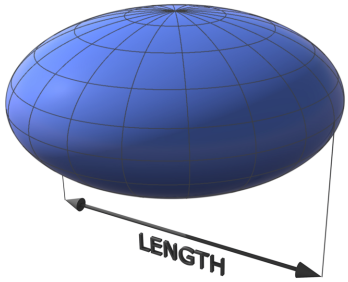


Figure 4: The plate is described as oblate spheroid. Oblate spheroids have rotational symmetry around an axis from pole to pole.

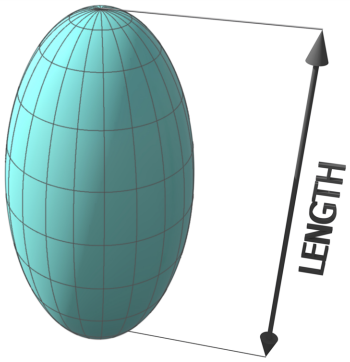


Figure 5: The needle shape is described as prolate spheroid. A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

Transformation strain

Choose **Disregard** to ignore the transformation strain. When **Isotropic** or **Cubic** is chosen in **Elastic properties** in Matrix Phase, you can also choose **Calculated from molar volume** to obtain a purely dilatational strain. If **Plate** or **Needle** is selected as the **Morphology**, you can alternatively choose **User-defined** and enter the properties for **ε11**, **ε12**, **ε13**, **ε22**, **ε23**, and

ε33.

Molar volume

Use the **Database** value (if the phase molar volume is defined in the thermodynamic database) or select **User-defined** to enter another value.

Phase boundary mobility

A parameter that accounts for interface-controlled growth. Only effective if a very small, positive value is used. Use with caution due to a tentative treatment.

Phase energy addition

An energy value that adds to the Gibbs free energy of the precipitate phase from a database.

Approximate driving force

Select the check box to include this if simulations with several compositions sets of the same phase create problems.

Preexisting size distribution

Select the check box to include this. Click **Edit particle size distribution** to open the **Preexisting Particle Size Distribution** window where you can edit the parameters and view a graph comparing the radius and number density for the selected component.

Press F1 and search for "Particle Size Distribution (PSD)" for detailed instructions.



See examples P_10 and P_11

CALCULATION TYPE

Isothermal

Use an **Isothermal** calculation type to do a precipitation simulation at constant temperature. Choose a unit of measurement and enter a numerical value for the **Temperature** and **Simulation time**.

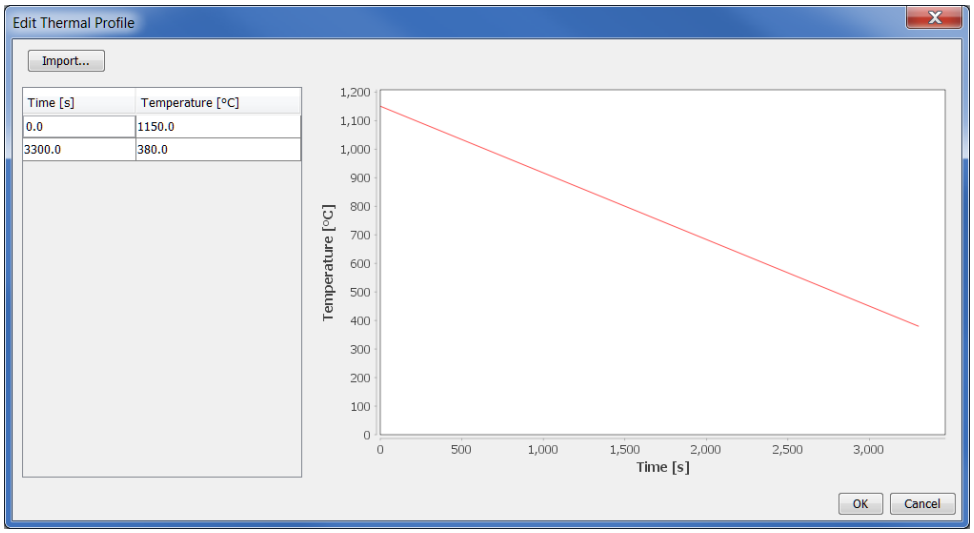


See examples P_01, P_02, P_04, P_05, P_08, and P_09.

Non-isothermal

Use a **Non-isothermal** calculation type to do a precipitation simulation with a user-defined temperature profile. Select a **Temperature unit** and **Time unit** from the lists. Enter a numerical value for the **Simulation time**.

Click **Edit thermal profile** to enter thermal profile **Temperature** and **Time** coordinates into a table. A minimum of two points is required. You can also **Import** to add your own **Thermal profile** from a text file in ***.xls**, ***.xlsx**, or ***.csv** formats.



See example P_06.

TTT diagram

Use a **TTT-diagram** to calculate the time-temperature-transformation (TTT) curve for the formation of the precipitate phase.

- **Temperature**: Enter **Min**, **Max**, and **Step** numerical values and choose a temperature **Unit**.
- **Max annealing time**: Enter a numerical value and choose a time **Unit**.
- **Stop criteria**: Choose **Volume fraction of phase** or **% of equilibrium fraction** and then enter a numerical value. For each temperature, the simulation stops when the stop criteria is fulfilled or if the maximum annealing time is reached, whichever happens first.

See example P_03.

CCT diagram

Use a **CCT-diagram** to calculate the continuous-cooling-transformation (CCT) curve for precipitation.

- **Temperature**: Enter **Min** and **Max** numerical values and choose a temperature **Unit**.
- **Cooling rate(s)**: Enter a range of values in the field, e.g. `.01 .1 1 10 100`. These values are equal to **K/s**, **°C/s** or **°F/s** per second based on the temperature **Unit** selected.
- **Stop criteria**: Enter a numerical value for the **Volume fraction of phase**. For each temperature, the simulation stops when the stop criteria is fulfilled.



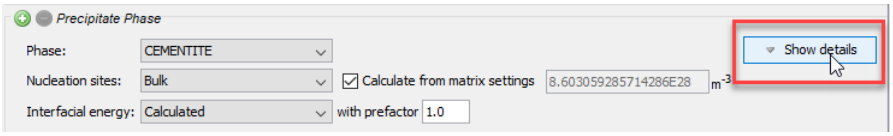
See example P_07.

Particle Size Distribution (PSD)

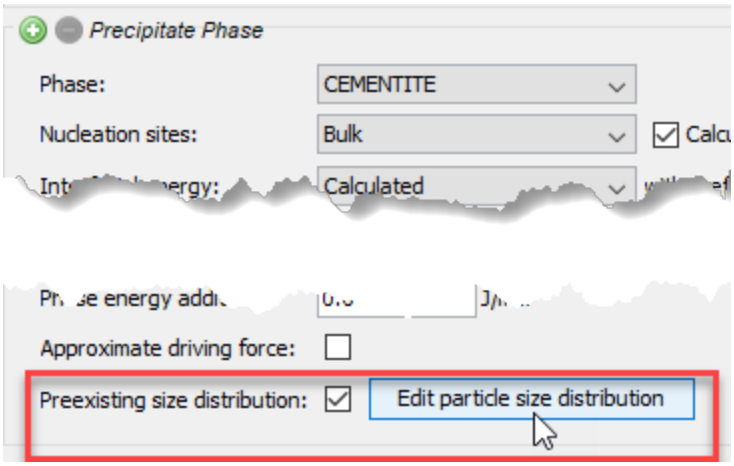
On the Precipitation Calculator you can set the pre-exisiting particle size distribution (PSD) parameters in the **Show details** section. The size distribution can be entered as a pre-defined distribution, by importing a file, or by manually entering information into a table.

Accessing the 'Pre-existing size distribution' Settings

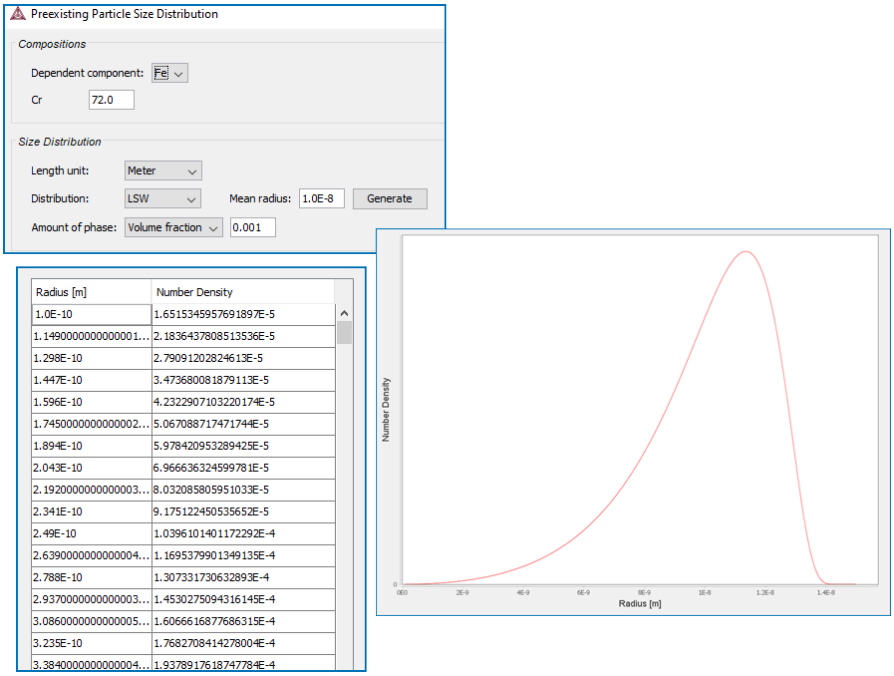
1. To the right of the **Precipitate Phase** settings fields, click **Show details**.



2. Click to select the **Preexisting size distribution** check box.

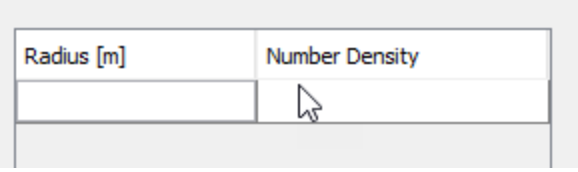


3. Click **Edit particle size distribution** to open the window as shown for example P_10.



DEFINING THE PREEXISTING SIZE DISTRIBUTION

1. Under **Compositions**, choose a **Dependent component** from the list and enter the composition for the other component.
2. Under **Size Distribution** define the following:
   a. Choose a **Length unit**: m, µm, or nm.
   b. Choose a **Distribution**: **LSW** (Lifshitz-Slyozov-Wagner), **Normal**, **Log normal** or **From file**. You can also manually enter numbers into the table instead of importing a file.



   c. For **LSW**, **Normal** and **Log normal**, enter a **Mean radius**.
   d. For **Normal** and **Log normal**, enter a value for the standard deviation (**Std**).
   e. For **From File**, click **Import** and navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.
   f. For all options, choose an **Amount of phase**: **Volume percent** or **Volume fraction** and then enter a number in the field.
   g. Once the **Distribution** is defined, click **Generate**.

Option Tab Settings

These settings are for the Precipitation Calculator and are located on the **Configuration** window → **Options** tab.

> You can change these settings locally for a specific Precipitation Calculator or globally in the **Options** settings. To open the Options window: From the main menu select **Tools → Options**. Click the **Graphical Mode** tab then click **Precipitation**.

NUMERICAL PARAMETERS

Click **Options** to go to these settings.

Max time step fraction

The maximum time step allowed for time integration as fraction of the simulation time. The default is 0.1.

No. of grid points over one order of magnitude in radius

Default number of grid points for every order of magnitude in size space. The default is 150.0.

Max no. of grid points over one order of magnitude in radius

The maximum allowed number of grid points in size space. The default is 200.0.

Min no. of grid points over one order of magnitude in radius

The minimum allowed number of grid points in size space. The default is 100.0.

Max relative volume fraction of subcritical particles allowed to dissolve in one time step

The portion of the volume fraction that can be ignored when determining the time step. The default is 0.01.

Max relative radius change

The maximum value allowed for relative radius change in one time step. The default is 0.01.

Relative radius change for avoiding class collision

Set a limit on the time step. The default is 0.5.

Max overall volume change

This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step. The default is 0.001.

Max relative change of nucleation rate in logarithmic scale

This parameter ensures accuracy for the evolution of effective nucleation rate. The default is 0.5.

Max relative change of critical radius

Used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step. The default is 0.1.

Min radius for a nucleus to be considered as a particle

The cut-off lower limit of precipitate radius. The default is 5.0E-10 m.

Max time step during heating stages

The upper limit of the time step that has been enforced in the heating stages. The default is 1.0 s.

Maximum relative solute composition change at each time step

Set a limit on the time step by controlling solute depletion or saturation, especially at the isothermal stage. The default is 0.01.

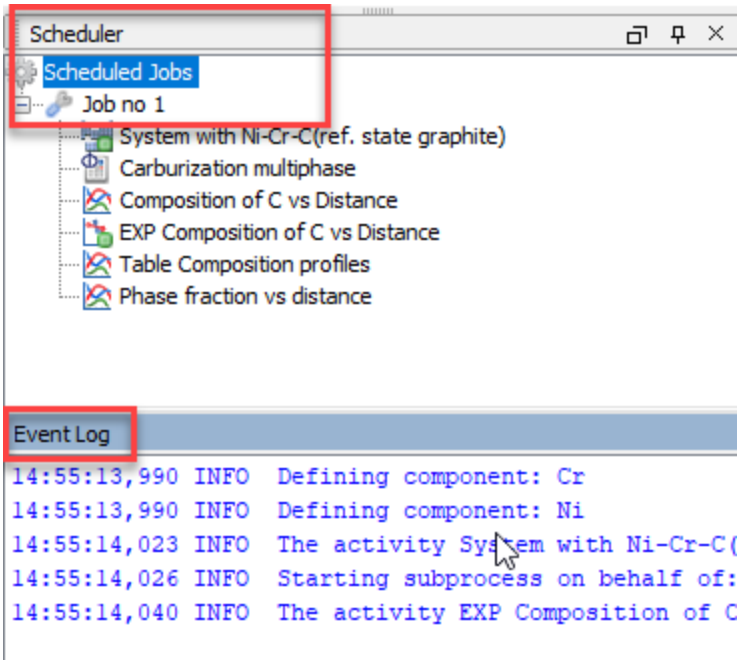
Pause, Resume and Cancel Precipitation Calculations

Precipitation calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again. You pause and resume from the Precipitation Calculator

Configuration window.

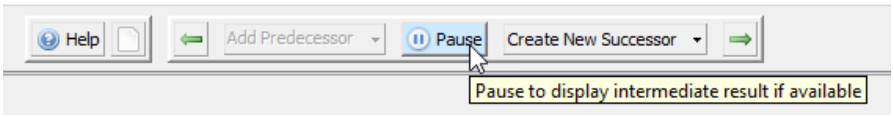
To Pause and Resume a Job

1. Run the job (i.e. click **Perform Tree**). In the **Scheduler**, you can see the job listed and in the **Event Log** you can follow the progress of the calculation.

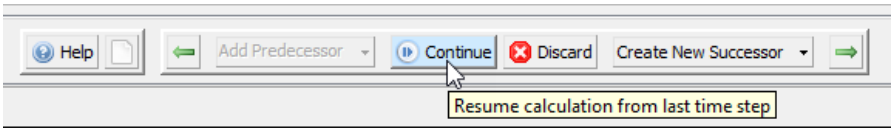


2. In the **Project** window, click the **Precipitation Calculator** node.

3. In the **Configuration** window at the bottom, click **Pause**. If there are intermediate results available these will be listed in the **Event Log**.

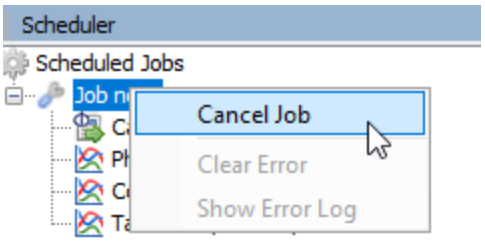


4. When ready, click **Continue** to resume your calculations from the last time step or click **Discard** to discard the calculation (then click **Yes** or **No** on the window that opens).



To Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



Plot Renderer

The Plot Renderer is where you define the settings and output results in a diagram that displays in the **Results** window. The available Plot Renderer settings are based on the System Definer and/or calculator activity node predecessors such as the Equilibrium, Scheil, Binary, Ternary, and Property Model Calculators. Setting availability is also determined by the calculation type as well as if you have the add-on Steel Model Library, or the Diffusion, Precipitation, or Process Metallurgy Modules. If you used any of the templates, the Plot Renderer is automatically added to the Project tree.

- Configuration Settings

There are additional details for more advanced settings and the Add-on Modules: Plotting Options, Diffusion Calculator Plot Renderer, and Precipitation Calculator Plot Renderer.

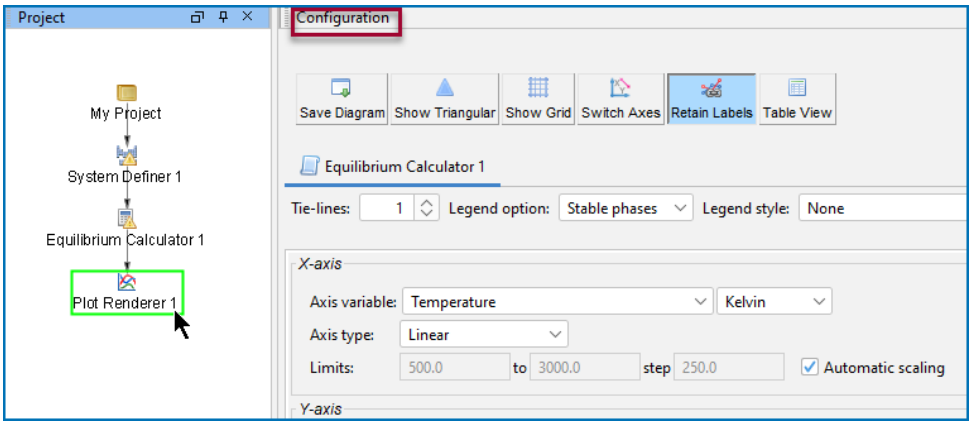
Plot Toolbar

Setting/Button	Description
Save Diagram 	Save the plot diagram. From the **Save** window, choose the file type–png (the default), jpg, ps, pdf, gif, svg, or emf. For PNG and JPG files you can also change the image quality. - Saving and Printing the Output (Graphical Mode)
Show Triangular 	Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
Show Grid 	Overlay a grid on the diagram.
Switch Axes 	Show the plotting X-axis variable on the diagram's Y-axis, and the Y-axis variable on the diagram's X-axis.
Retain Labels 	Toggle the default to keep labels displaying on the plot. By default labels are retained.
Table View 	Toggle to switch between displaying a Plot or the results of a Table in the **Results** window. This is available for single equilibrium or stepping calculations. When you click to toggle ON, click **Perform** to regenerate as a Table. When you click to toggle OFF, click **Perform** to regenerate the Plot. For example, set up the Plot Renderer and click **Perform** to display the Plot. Then click **Table View** and **Perform** to see the results in a Table format in the Results window. When toggled ON, click **Save table** to export the table data. Choose the **Decimal digits** and **Number format** (**Auto**, **Decimal**, or **Scientific**).

Setting/Button	Description
	Saving and Printing the Output (Graphical Mode)

Configuration Settings

Click the **Plot Renderer** node in the **Project** window to view the **Configuration** window. The settings available vary based on such choices as the Calculator and calculation type selected.



Working with Plots and Tables

For the Add-on Modules also see:

- Diffusion Calculator Plot Renderer
- Precipitation Calculator Plot Renderer

Examples of Calculation Type Differences

Grid

If you choose a **Grid** *Calculation Type*, select a **Plot type** and whether to **Interpolate** the data or not. With these calculation types you can choose to plot a **Heat map**, **Contour**, or **3D** diagram. See Heat Map, Contour, and 3D Plots.

For a **Grid** the *X*- and *Y*-axes always represent the quantities that define the calculation axes, but you need to set a variable for the *Z-axis* (the axis perpendicular to the plane defined by the X- and Y-axes).

Uncertainty

For an **Uncertainty** *Calculation Type*, you choose an **Axis type**: **Frequency**, **Histogram**, or **Normal probability**.

There are different axis types available such as **Linear**, **Logarithmic**, **Logarithmic 10**, and **Inverse**. Additional Plotting Modes are available.

Batch

For a **Batch** *Calculation Type*, the available options from the X- and Y- axes lists are based on the data file contents, i.e. if experimental data is included, then these are listed. See Working with Batch Calculations for details. Additional Plotting Modes are available.

Settings

The options along the top of the window are available depending on the calculation type.

Tie-lines

Select how many tie-lines to be plotted in the diagram. Every n^{th} number of tie-line is plotted, where *n* is the number set here. Consequently, the higher the number, the fewer the number of plotted tie-lines in the diagram.



This setting is not available if the Plot Renderer is a successor to an Equilibrium Calculator where only one axis is defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).

Legend option

Select whether the diagram's legend displays the **Stable phases**, the **Axis quantity**, or choose **Off** for no legend.

Legend style

You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for **Legend option**. Choose **None**, **All**, **Constitution description**, or **Ordering description**.

About Legend Styles

Filter

This is available with the **Property Model Calculator** and **Process Metallurgy Calculator**.

Use the **Filter** check box to add various filters to the plot or table based on the set up of the calculation. When selected, click the **Add quantity** and **Remove quantity** buttons to add filters. For example, enter a **Min** and **Max** and choose an axis variable such as **Ms Temperature** and the unit **Kelvin** to adjust the output in the Results window. Click **Perform** each time you add or remove a filter for the results to update.

Grouped mode or Flexible mode

Both are available with **Equilibrium Calculator** and **Property Model Calculator** > **One axis** *Calculation Type*. Flexible mode is also available with Property Model Calculator **Min/Max** calculations.

- Use **Flexible mode** to individually add and configure axes quantities and change the units or other associated settings one at a time.

- Use **Grouped mode** to add and configure groups of axis quantities at the same time and of the same type. For example, change units or settings in groups with similar settings like temperature units or axis types.

Plotting Modes

TTT Mode and CCT Mode (Steel Model Library)

These are available with a license for the Steel Model Library and when using the **Property Model Calculator**.

- Use **TTT mode** to make a TTT diagram from a One-axis calculation with temperature. The x- and y-axes are time and temperature, respectively. Time quantities (such as pearlite-start, bainite-start) are plotted as functions of temperature. Temperature quantities (such as Ms, M50) are independent of time and plotted as horizontal lines.

- Use **CCT mode** to make a CCT diagram from a One-axis calculation with Log10 (cooling rate [K/s]) from the CCT Diagram Property Model. The x- and y-axes are time and temperature, respectively. Result quantities defined as time-temperature pairs are identified and plotted. Cooling curves are also automatically added in the plot.

Plot Settings: TTT Mode and Plot Settings: CCT Mode

Statistical mode

Available with:

- **Property Model Calculator** > **Batch** or **Uncertainty** *Calculation Type*.
- **Process Metallurgy Calculator** > **Uncertainty** *Calculation Type*.

Use **Statistical mode** to select **Frequency** or **Normal probability** as the *Axis variable* and then the *Axis type* is set to **Histogram** or **Probability**, respectively.

Plotting Modes

Cross plot mode (Batch)

Available with **Property Model Calculator** > **Batch** *Calculation Type*.

Use **Cross plot mode** to plot the experimental data from a Batch calculation with the calculated result, e.g. you might be looking at liquidus temperature and now can plot both to compare the experimental data against the Thermo-Calc calculated results. You choose the experimental data value (which is read from the data file) as an X- or Y- Axis variable and then the calculated result as the other X- or Y- Axis variable.

Also use the **Show limits** and **Show calculation failures at value** check boxes with this mode.

- Working with Batch Calculations

Show limits (Batch)

This is available for the **Batch** calculation type, **Cross plot mode**.

Click the **Show limits** check box and then choose **RMS** (root mean squared), **Absolute**, or **Relative in % limits**. For **Absolute** or **Relative in %** enter a value in the field (the default is 15.0). A "perfect fit" line is added (solid line) to the plot and then the upper and lower limits shown on the plot are based on the type of limit selected.

- When **RMS** is selected, a "perfect fit" line is added (solid line) plus the upper and lower limits (dashed lines), which are calculated for the experimental data points (read from the data file). The RMS error value is shown in the plot legend. The upper and lower limits are then this calculated value plus and minus from the perfect fit line.

- When **Absolute** is selected, the value entered (e.g. the default is 15), then this is the plus or minus value from the perfect fit line.

- When **Relative in %** is selected, the value entered (e.g. the default is 15%), then this is the upper and lower limit that is plotted and this value is plus or minus percent from the perfect fit line as is calculated and shows in the plot legend.

Show calculation failures at value (Batch)

This is available for the **Batch** calculation type, **Cross plot mode**.

Click the **Show calculation failures at value** check box and enter a value in the field. Use this check box to include any values that failed in the calculation and you want to see these on the plot. The value entered in the field replaces the non-existing calculated value(s) and can be cross plotted against experimental results from that data file.

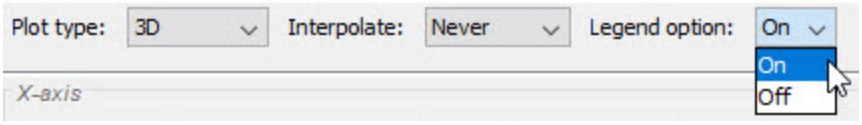
Plot type (Grid)

These settings are for a **Grid** *Calculation Type*.

Heat Map, Contour, and 3D Plots

- On a **Heat map** diagram, each Z-axis variable value in the grid is represented by a colour-coded area, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.

- On a **Contour** diagram, Z-axis variable values are traced with curves in the same way that height values are traced with curves on a topographical map. The colors used originate from the different data series.
- On a **3D** diagram, the 3D surface is created by Delaunay tesselation of the calculated data. The surface uses a cold to warm color map where red represents the highest Z-axis variable value and blue represents the lowest Z-axis variable value. The color map color legend can be turned on or off with the legend option.



Interpolate (Grid)

From the **Interpolate** list, choose to interpolate data **Never** (the default), **Once**, **Twice** or **3 times**. This means points are put in between calculated points in the grid and interpolated instead of calculated in the calculation engine.

Choose how many points of data to interpolate to improve curve smoothness – **Never**, **20x20**, **50x50**, or **100x100**. Try different settings for your own set of data.

Label decimal digits

Choose the number of decimal digits to display in the plot label. The default is **2**.

Label number format

Choose from **Auto** (the default), **Decimal** or **Scientific**.

Axis variable

Set the state variable you want plotted along the X-axis and the Y-axis.



If the stepping/mapping variables are changed in the Equilibrium Calculator that precedes the Plot Renderer, then the variables to be plotted along the diagram's X- and Y-axis are automatically updated to the appropriate quantities.

Axis type

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10** or **Inverse**.

Automatic scaling

The **Automatic scaling** check box is selected by default to allow the program to set the limits.

Limits

This setting is available when the **Automatic scaling** check box is cleared (the scaling is turned off).

Enter the lower and upper **Limits** of the variables to display on the axis. You can also determine the **step** size between the tick marks along each axis.



If the **Automatic scaling** is turned off (i.e. the check box is not selected) then it is important to enter a large enough number in the *step* field for the numerical values to display correctly on the axis. That is, if the step size is too small, the program ignores this setting and the axis labels will not be as expected.



For logarithmic axes, the step size is related to the exponent. For example, if the step entered is 1.0, then the exponent increases by one each time (10^{-9}, 10^{-8}, 10^{-7} and so forth).

Contour values and Use custom contour values (Z-axis, contour plots).

The **Use custom contour values** check box is available when **Contour** is selected as the **Plot type**. Select this check box to enter one or a series of numbers in the **Contour values** field. Numbers can only be separated by a space.

Add an axis and Remove this axis buttons

Use the **Add an axis** and **Remove this axis** buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the Z-axis.

- Plotting Options

Slag Property Options (Process Metallurgy)

For the **Process Metallurgy Calculator** when you are selecting axis variables on the Plot Renderer, there is the option to choose **Slag property**. The associated quantity that you select from the next drop-down list has these options to choose: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls** , or **Log10 (Sulphur capacity)**.

Also choose **In liquid slag only**, **In solid slag only** or **In all slag**.

- References and equations for these properties are described in Process Metallurgy Slag Properties.

Unit (Process Metallurgy)

For the **Process Metallurgy Calculator** select a **Unit** for the quantity to plot: **Tonne**, **Kilogram**, **Gram** or **Pound**

Plot Settings: CCT Mode

This mode is available with the Steel Model Library, which requires specific maintenance and database licenses. See About the Steel Model Library Property Models.

Use **CCT mode** to make a CCT diagram from a One-axis calculation with log10(cooling rate) from the CCT Diagram Property Model. The X- and Y-axes are time and temperature, respectively. Result quantities defined as time-temperature pairs are identified and plotted. Cooling curves are also automatically added in the plot.

The **CCT mode** is available for a **Plot Renderer** when it is a successor to a Property Model Calculator and a **One axis** *Calculation Type* is selected with **Log10(cooling rate [K/s])** as the axis quantity.

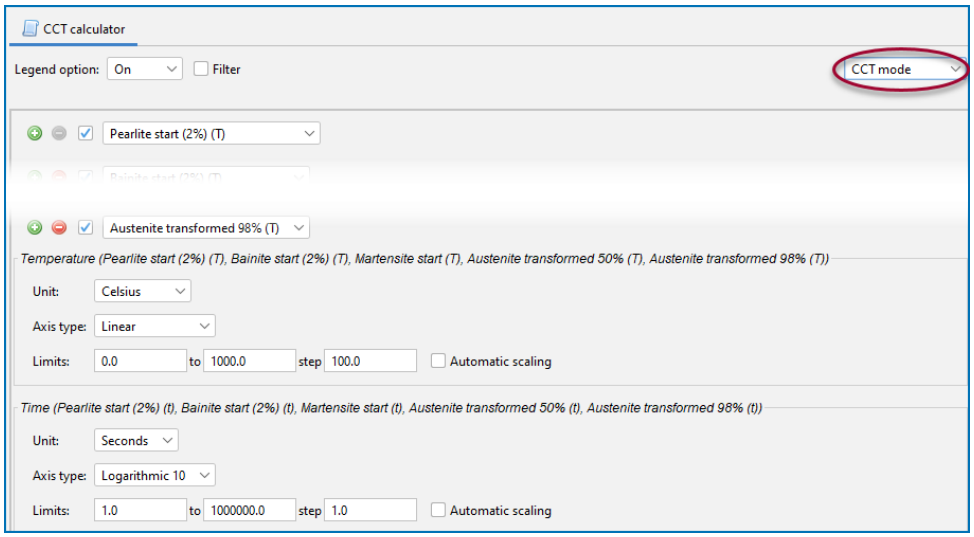
Then in general, it is available from the drop-down list in these situations:

- When you add the **Steel Library - CCT Template**, it is the default mode on the Plot Renderer (renamed CCT in the template).
- It is also available if a user-defined Property Model has both Time and Temperature quantities defined in a coupled manner, for example if you create your own Property Model with TC-Python. That is, if you select or create any model where the resulting combination of stepping-quantity and result-quantities has both time and temperature definitions.

Configuration Window Settings and Configuration Settings

Steel Library CCT Diagram Template

The settings example below uses Property Model example *PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu*. See PM_Fe_08: CCT Diagram Property Model.



CCT Mode on a Plot Renderer as a successor to a Property Model Calculator.

Plot Settings: TTT Mode

This mode is available with the Steel Model Library, which requires specific maintenance and database licenses. See About the Steel Model Library Property Models.

Use **TTT mode** to make a TTT diagram from a one-axis calculation with temperature. The X- and Y-axes are time and temperature, respectively. Temperature axis quantities (such as Ms, M50) are independent of time and plotted as horizontal lines.

The **TTT mode** is available for a **Plot Renderer** when it is a successor to a Property Model Calculator and a **One axis** *Calculation Type* is selected with **Temperature** as the axis quantity.

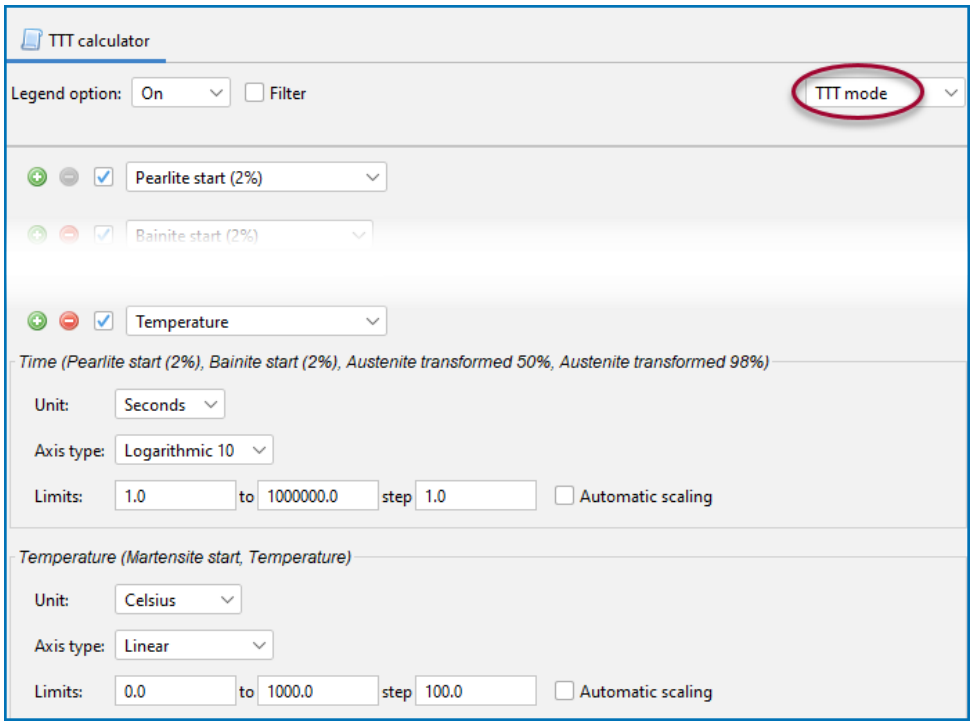
Then in general, it is available from the drop-down list in these situations:

- When you add the **Steel Library - TTT Template**, it is the default mode on the Plot Renderer (renamed TTT in the template).
- When you are using at least one of these Steel Property Models—**Martensite Temperatures**, **Pearlite**, or **Bainite** with a *One axis* calculation and when both time and temperature quantities are selected on the Plot Renderer—the TTT mode is available.
- If a user-defined Property Model has both Time and Temperature quantities defined in a coupled manner, for example if you create your own Property Model with TC-Python. That is, if you select or create any model where the resulting combination of stepping-quantity and result-quantities has both time and temperature definitions.

Configuration Window Settings and Configuration Settings

Steel Library TTT Diagram Template

The settings example below uses Property Model example *PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu*. See PM_Fe_06: TTT Diagram Property Model.



TTT Mode on a Plot Renderer as a successor to a Property Model Calculator.

Diffusion Calculator Plot Renderer

Conditions Tab Settings and Configuration Settings

The following is information about the settings available in both Simplified and Advanced mode for a Plot Renderer when it is a successor to a **Diffusion Calculator**.

Simplified Mode

When you open the Diffusion Calculator Plot Renderer, it defaults to **Simplified mode**. Use this mode to define the most common axis variables. The software automatically sets the correct **Plot condition** and **Independent variable**. Use the **Advanced mode** to have more flexibility.

When you click the **Switch to advanced mode** button, this expands the variable options available from both the X-axis and Y-axis lists. Otherwise the axis variables default to the most logical combination.

x-axis Variable

Select the variable for the *x*-axis: **Distance** or **Time**.

- For **Distance** also choose a unit (**m**, **µm**, or **nm**) and what region to include. The list contains the regions defined on the Diffusion Calculator or you can choose **All regions**.
- For **Time** choose a unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

y-axis Variable

Select the variable to plot on the *y*-axis. The available options are based on choices such as whether **Distance** or **Time** is chosen for the *x*-axis, whether isothermal or non-isothermal is selected, whether there is a homogenization solver, or if there is one or more regions.

Distance along the x-axis

If **Distance** is plotted along the x-axis, then by default the **Composition** is plotted along the *y*-axis.

- From the center list, choose the component to plot, or select **All**.
- From the next list, choose the unit to be **Mass percent**, **Mole percent**, **Mass fraction**, **Mole fraction**, or **u-fraction**.

Time along the x-axis (one region)

If **Time** is plotted along the x-axis, then choose the *y*-axis variable to plot plus the additional settings:

- **Total phase fraction**: **By volume** or **By mass**. Then select a phase from the list.
- **Total fraction of element**: **By mole** or **By mass**. Then select a component from the list.
- **Total fraction of element in phase**: **By mole** or **By mass**. Then select a component and a phase from the lists.
- For a non-isothermal thermal profile **Temperature** is available: **Kelvin**, **Celsius**, or **Fahrenheit**.

Distance along the x-axis (Homogenization)

If **Distance** is plotted along the x-axis and a Homogenization solver is being used, then choose **Composition** or **Phase fraction** to plot on the *y*-axis. Then select the applicable settings.

- Choose the component to plot, or select **All** and the unit **Mass percent**, **Mole percent**, **Mass fraction**, **Mole fraction**, or **u-fraction**.
- Choose **By mole** or **By mass** then select a component from the list.

Time along the x-axis (two or more regions)

If **Time** is plotted along the x-axis, then choose the *y*-axis variable to plot plus the additional settings:

- **Total phase fraction**: **By volume** or **By mass**. Then select a phase from the list.
- **Total fraction of element**: **By mole** or **By mass**. Then select a component from the list.

- **Total fraction of element in phase**: **By mole** or **By mass**. Then select a component and a phase from the lists.
- **Composition at interface**: **Mass percent**, **Mole percent**, **Mass fraction**, **Mole fraction**. Then choose a **Region** and whether it is **Upper** or **Lower** and a component.
- **Position of interface**: Choose a unit (**m**, **µm**, or **nm**) and the interface.
- **Velocity of interface**: Choose a unit (**m**, **µm**, or **nm**) and the interface.
- **Width of region**: Choose a unit (**m**, **µm**, or **nm**) and the interface.
- For a **Non-isothermal** profile, **Temperature** is available. Choose a unit **Kelvin**, **Celsius** or **Fahrenheit**.

Axis Type

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10** or **Inverse**.

Limits

Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** check box to allow the program to set the limits.

Time



An alternative **Time** setting is available in Advanced mode.

When the *x*-axis variable is **Distance**, choose a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**). Enter a numerical value.

Add and Remove Axes

Use the **Add an axis** and **Remove this axis** buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram).

Advanced Mode

Choose **Advanced mode** to access settings that enable you to manually select any combination of axis variables, **Plot condition** and **Independent variable**. Examples of advanced plot options are activity of a component at an interface, diffusivities, and diffusion

paths. Also user-defined functions can be used as plot variable where Console Mode syntax is used to define functions. In some cases, sensible default values are selected, but they can be changed according to your needs.

Plot Axis Settings in Advanced Mode

- If any plot axis variable of the type **Integral** is selected, then the plot condition is set to **Integral** and the Independent variable is set to **Time**.
- If a plot axis variable is set to **Time** then the plot condition is set to **Time** and the Independent variable is also set to **Time**.
- If a plot axis variable is set to **Distance** then the plot condition is set to **Distance** or **Interface** and the Independent variable is set to **Distance**.

Plot condition	Independent Variable settings based on the Plot condition
Time: Choose a unit (**Seconds**, **Minutes**, **Hours**, or **Days**). Enter a numerical value.	The default is **Distance**: Choose a **Global** or **Local** distance. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected. You can also choose **Time**, which requires no further settings.
Distance: Choose a specific **Region** from the list or use the default **All regions**.	The default is **Time** and there are no further settings. You can also choose a **Global** or **LocalDistance**. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected.
Interface: From the lists choose a **Region** and whether it is the **Upper** or **Lower** region.	The default is **Distance**: Choose a **Global** or **Local** distance. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected. You can also choose **Time**, which requires no further settings.
Integral	The default is **Time** and there are no further settings. You can also choose a **Global** or **LocalDistance**. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected.

Precipitation Calculator Plot Renderer

Conditions Tab Settings and Configuration Settings

The following is information about the settings available for a Plot Renderer when it is a successor to a **Precipitation Calculator**.

There are also specific settings related to non-isothermal simulations that are detailed in this topic.

Plot Settings

Legend option

Select whether the diagram's legend displays **On** or **Off**.

Axis variable

Set the state variable you want plotted along the X-axis and the Y-axis. The available variables in the list are based on how your system is set up.

Below are additional details related to the *Axis variable* chosen.

Separate Multimodal PSD

If you choose **Mean radius**, **Number density**, **Size distribution**, or **Number density distribution**, select the **Separate multimodal PSD** check box to enter settings for **Points**, **Excess kurtosis**, **Valley depth ratio** and **Minimum peak**.

See Non-Isothermal Simulations for definitions.

Yield Strength

If you choose **Yield strength**, you can further define the model. From the **Total yield strength** drop down list, select any or all the check boxes to plot the respective contributing elements to the yield strength. You can click **Configuration panel** to fine tune the model. These options are described for the Yield Strength Property Model Settings. The greyed out sections (e.g. the **Matrix** and **Precipitate** phases) are defined on the Precipitation Calculator and cannot be changed.

The P_01: Isothermal Precipitation of Al3Sc example demonstrates the use of this Yield Strength Model.

Axis type

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10** or **Inverse**.

Limits

Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** check box to allow the program to set the limits.

Unit (*Time X Axis*)

Choose a **Unit** : **Seconds**, **Hours**, or **Days**.

Add an axis and Remove this axis buttons

Use the Add an axis and Remove this axis buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the Z-axis.

Axis Variables

- **Mean radius**: Spherical radius of average volume of all particles for a specific phase and nucleation type, regardless of their actual shapes.
- **Critical radius**: Spherical radius of critical nuclei for a specific phase and nucleation type.
- **Yield strength**: To use the Yield Strength Property Model to calculate yield stress. For more information see About the Yield Strength Property Model.
- **Matrix composition**: Instantaneous compositions of the matrix phase.
- **Precipitate composition**: To track the instantaneous composition of precipitate particles. In particular, it is useful to distinguish different composition sets of the same phase (for example, FCC_A1#2 and FCC_A1#3). Further choose **Solutes** or **All**.
- **Number density**: Instantaneous number of particles per unit volume for a specific phase and nucleation type.
- **Size distribution**: Number of particles varying with their sizes per unit volume per unit length, for a specific phase and nucleation type, at a specific time.
- **Number density distribution**: Retrieve the number density (number of particles per unit volume) of precipitates distributed in different particle sizes.
- **Volume fraction**: Instantaneous volume fraction for a specific phase and nucleation type.
- **Nucleation rate**: Instantaneous number of nuclei per unit volume per unit time for a specific phase and nucleation type.
- **Normalized driving force**: Instantaneous nucleation driving force per unit mole of elements for a specific phase and nucleation type. It is normalized with RT and therefore, dimensionless.

- **Mean cubic factor**: Average cubic factor of cuboid particles. Available only when cuboid is selected as the **Morphology**.

The following settings area available as indicated when **Needle**, **Plate** or **Cuboid** are selected as the **Morphology** in the *Precipitate Phase* section on the Precipitation Calculator.

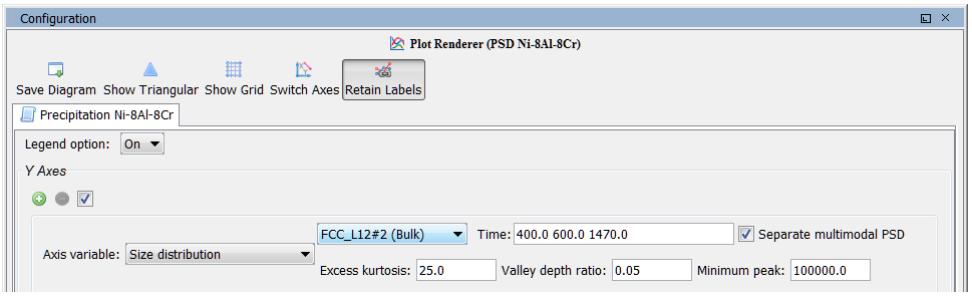
- **Cubic factor distribution**: Variation of cubic factor with particle size at a specific time. Available with a cuboid morphology.
- **Mean aspect ratio**: Average aspect ratio of non-spherical particles. Available with a needle or plate morphology. Note that this is always larger than 1, where 1 = a sphere.
- **Mean particle length**: Diameter of non-spherical particles along the longer axis. Available with a needle or plate morphology.
- **Aspect ratio distribution**: Variation of aspect ratio with particle size at a specific time. Available with a needle or plate morphology.

Non-Isothermal Simulations

When doing non-isothermal simulations it is common that particles grow in different generations. This results in multi-modal size distributions. To correctly estimate the properties of these different generations of particles you need to separate the peaks of multi-modal distributions.

Separate multimodal PSD

When the **Separate multimodal PSD** check box is selected on a Plot Renderer activity for the Precipitation Calculator, the size distribution is evaluated at the given time steps and checked for multi-modal peaks. These are separated and used to calculate the specified property.



It can be applied on the following plot properties:

- Mean radius
- Size distribution
- Number density
- Volume fraction

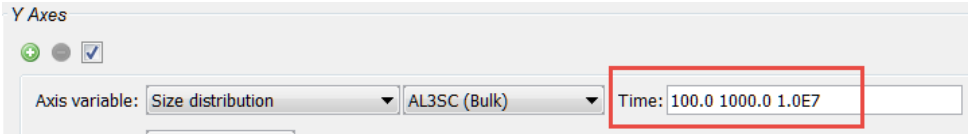
Points

This field is available when **Mean radius**, **Number density** or **Volume fraction** is selected as the **Axis variable**. Since the evaluation of multi-modality at each time step is costly, you can specify how many evaluation **Points** to use. The points are geometrically distributed over the time scale where nucleated particles are found. The default is 40 points.

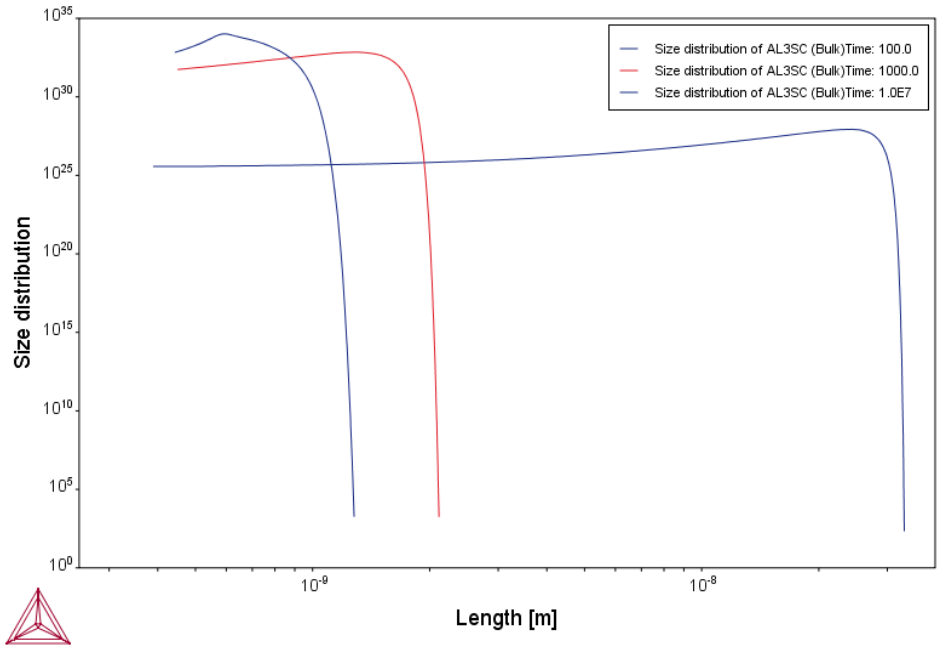
Time

This field is available when **Size distribution**or **Number density distribution** is selected as the **Axis variable**. Enter one or a series of numbers in the field, separated by a space.

For example, if you enter `100.0`, `1000.0` and `1.0E7` in the field:



When you click **Perform** the times are plotted:



Excess Kurtosis

The **Excess kurtosis** number specifies the sensitivity when the program evaluates whether a curve is bimodal or not. The evaluation process calculates the excess kurtosis of the given size distribution and compares it with the input value. If the value is lower than the given value, the distribution is split. The excess kurtosis is a statistical measure that measures how *peaked* and *how heavy tail* a distribution has. For the definition used see http://en.wikipedia.org/wiki/Kurtosis. The default is 25.0.

Minimum Separation Limit (Valley Depth Ratio)

The **Minimum Separation Limit** is a rough method to prevent that noise or wiggles are interpreted as different distributions. If a local minima is encountered above this value the following peak is not interpreted as a new distribution. The valley depth ratio is the ratio of the minimum separation limit to the peak value. The default is 0.01.

Minimum Peak

Any separated peak below the entered **Minimum peak** value is removed. The default is 100000.0.

Table Renderer

A **Table Renderer** visualizes calculation results in a table. Several Table Renderer activities (as well as Plot Renderer activities) can be shown in the Results window as different tabs.

You can add the Table Renderer directly (right-click a calculator node and select it from the **Create New Successor** menu) or use a variety of the available templates to automatically add the node. For example, the **Single Point Equilibrium** and **Quick Start** templates.

- For details about the templates, seeThe Quick Start Wizard and Templates and Creating a Project from a Template.

You can only successfully tabulate the results of a single equilibrium calculation or a stepping (i.e. property diagram) operation. The tabulated data from an equilibrium calculation is different from the tabulated data from a stepping calculation.

For the Plot Renderer, there is an option to use the Table View button to convert plots to table data for all calculation types and calculators. See Plot Renderer: Convert a Plot to a Table and Export the Data.

- The settings are described in the section Configuration Settings.

Results from an Equilibrium Calculation

The following tab shows the result of an equilibrium calculation (from example T_01: Calculating a Single-Point Equilibrium).

Table Renderer 1

System				
Moles	1.00000			
Mass	55.64392	[g]		
Temperature	1000.00000	[K]		
Total Gibbs Energy	-42140.55264	[J]		
Enthalpy	24707.16903	[J]		
Volume	7.29746E-6	[m3]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Fe	0.99537	0.99900	0.00619	-42277.77189
C	0.00463	0.00100	0.21818	-12658.35450
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.99609	55.59691	0.99711	Composition and constitution
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Fe	0.99928	0.99984		
C	0.00072	0.00016		
Constitution	$(Fe)_1 (C,VA)_3$			
	Constituent	*Site Fraction*		
Sublattice 1:				
	Fe	1.00000		
Sublattice 2:				
	VA	0.99976		
	C	0.00024		

For each stable phase listed, from the **Composition and constitution** menu you can select the information to view. In this example, the maximum amount of information is shown and includes details about both composition and constitution for **BCC_A2#1**.

The default for the Phase description detail can be changed globally. To open the Options window:From the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

Results from a Stepping Operation

The **Table Render 1** tab in the example shows the results of a stepping calculation (from example T_02: Stepping in Temperature in the Fe-C System).

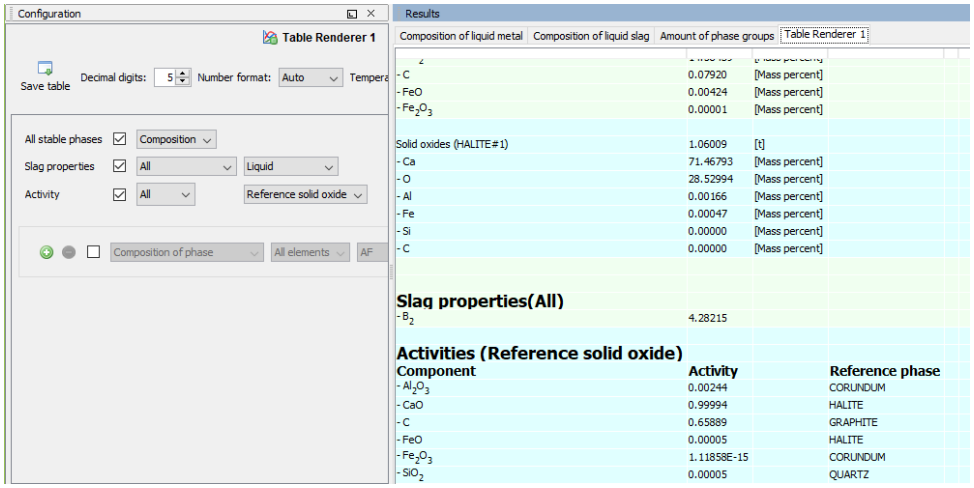
Results

Plot Renderer 1 | Table Renderer 1

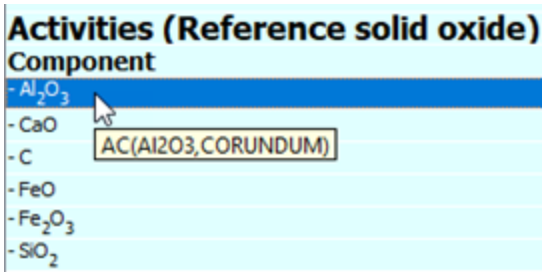
Temperature [K]	Amount of BCC_A2 [mol]	Amount of LIQUID [mol]	Amount of FCC_A1 [mol]	Amount of GRAPHITE [mol]
1000.00000	0.99609			0.00391
1010.00000	0.99618			0.00382
1011.17278	0.99620			0.00380
1011.17278	0.99620		0.00000E0	0.00380
1011.17278	0.87364		0.12636	0.00000E0
1011.17278	0.87364		0.12636	
1020.00000	0.86046		0.13954	
1030.00000	0.84331		0.15669	
1040.00000	0.82356		0.17644	
1050.00000	0.80082		0.19918	
1060.00000	0.77395		0.22605	
1070.00000	0.74180		0.25820	

Process Metallurgy Module Single Equilibrium

When you use a **Process Metallurgy Calculator**, there is a variety of additional information you can display in the table such as the **Slag properties** (see Process Metallurgy Slag Properties for equations and references) and the **Actitivies**.



For the activities in the table, you can hover over the Component and the syntax of the activity displays.



Yield Strength Property Model

The Yield Strength Property Model Settings is available with the Property Model Calculator. After defining the Model and adding a Table or Plot, the *Total yield strength* variable is available. The *Yield strength* variable is also accessible via a Table Renderer (or Plot Renderer) that is a successor to the Precipitation Calculator.

- About the Yield Strength Property Model

Results

Plot Renderer 1 | Table Renderer 1

Total yield strength	Mean radius Reppich model
102.55522	0.00000
102.55522	5.00000E-9
160.81151	1.00000E-8
256.04683	1.50000E-8
336.33393	2.00000E-8
407.06828	2.50000E-8
383.52273	3.00000E-8

Results

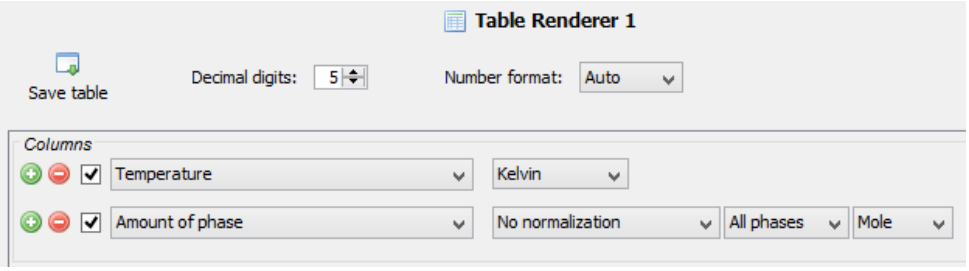
Plot Renderer 1 | Plot Renderer 2 | Table Renderer 1

Time [s]	Total yield strength
1.67530	14.96725
1.96032	14.96727
2.02728	14.96728
2.10831	14.96731
2.19545	14.96735
2.28983	14.96742
2.39233	14.96755

An example of the variable results when yield strength is chosen as the Axis variable for a Table Renderer that is a successor to the Property Model Calculator (top) or Precipitation Calculator (bottom).

Configuration Settings

The **Table Renderer** settings are done on the **Configuration** window. Depending on what calculator node the table is a successor to, you can have different settings available. For most tables, this is where you set the level of detail for the columns as shown in the figure.



Save the Table

To save all the data in a table as a plain text file (.txt), Hyper Text Marketup (.html), or Excel (.xls) format, in the **Configuration** window click **Save table** or in the **Results** window right-click in the table and select **Save As**.

To copy the data from a single cell of a table to the clipboard, right-click the cell and select **Copy**. To copy the whole table to the clipboard, select **Copy all**.

The data saved is what is shown in the **Table Renderer** tab on the **Results** window. If data is calculated but not displayed it is not saved.

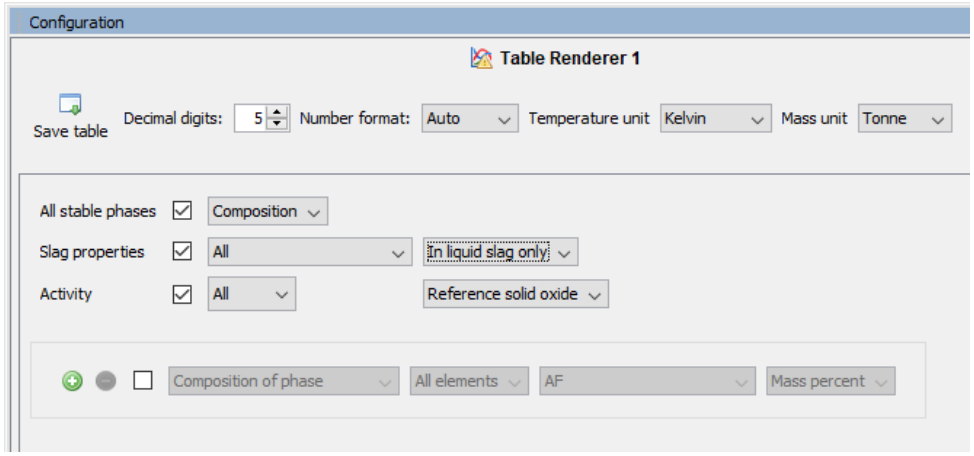
Number of Decimal Digits and Number Format

The table results can be presented in ordinary decimal number format or with normalized scientific notion. Choose **Scientific** or **Decimal** to increase or decrease the number of **Decimal digits** used in the table. The default is 5 digits. The **Number format** defaults to **Auto** to use the most appropriate format based on the tabulated data.

The defaults for these settings can be changed globally. From the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

Process Metallurgy Settings

For the **Process Metallurgy Calculator** there are additional settings available.



Choose a **Temperature unit**: **Kelvin**, **Celsius** or **Fahrenheit**.

Choose a **Mass unit** : **Tonne**, **Kilogram**, **Gram** or **Pound**.

Select the **All stable phases** check box and choose **Composition** or **Condensed** from the list.

Select the **Slag properties** check box and choose the associated quantity from the next drop-down list: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls** , or **Log10 (Sulphur capacity)**.

Also choose **In liquid slag only**, **In solid slag only** or **In all slag**.

Details, including references and equations, are described in Process Metallurgy Slag Properties.

Select the **Activity** check box then from the first list choose a component (or keep the default **All**). Then from the second drop-down list select **Reference solid oxide** or **Reference liquid slag**.

The activity is always given relative to a phase. The liquid slag is always the IONIQ_LIQ phase. The composition set of ION_LIQ depends on the calculation and the slag always contains a high amount of oxygen. The reference phase for the solid oxides depends on the components and it is always listed in the table.

Precipitation Calculator with Yield Strength

When you use a Precipitation Calculator**Precipitation Calculator** and choose **Yield strength** as an *Axis variable*, there are additional settings available.

If you choose **Yield strength**, you can further define the model. From the **Total yield strength** drop down list, select any or all the check boxes to plot the respective contributing elements to the yield strength. You can click **Configuration panel** to fine tune the model. These options are described for the Yield Strength Property Model Settings. The greyed out sections (e.g. the **Matrix** and **Precipitate** phases) are defined on the Precipitation Calculator and cannot be changed.

The P_01: Isothermal Precipitation of Al3Sc example demonstrates the use of this Yield Strength Model.

Experimental File Reader

The Experimental File Reader activity node is added as a predecessor from the top My Project node. This allows you to use (or "read") the data contained in an experimental data file (with the file extension `*.EXP`) and then plot the data on one or more Plot Renderers.

If you are a Console Mode user, this is the same concept as using the Experimental Data Files (*.POP, *.DOP)

The `EXP` file is a type of data file with information specifying a plotted diagram and it is written in the DATAPLOT graphical language. From this activity node you can plot the EXP file or save a copy of the file to another location.

Creating Activities and Successors and Plotting Experimental Data Files in the *DATPLOT User Guide* included with this documentation set.

How to Plot Using an Experimental Data File

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the *EXP file* field, enter the name of the EXP file to plot. Or click the **Select Exp file** button to navigate to a location on the computer to add the dataset.
3. Once the .EXP file is added, under **Dataset Selection** you can choose to include or exclude specific datasets. Use the **Select/Deslect all datasets** check box as required.
4. Right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.

   If the source EXP file is changed, you can also click the **Reload the selected EXP file from disk** button to refresh the data. If you want to save or export the loaded file, click the **Save EXP file** button, then navigate to where you want to save it and give it a file name.

5. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

General Property Models

Property Model Calculator

In this section:

About the Coarsening Property Model 196
About the Crack Susceptibility Coefficient Property Model 199
Driving Force Property Model Settings 208
About the Equilibrium with Freeze-in Temperature Property Model 209
Equilibrium Property Model Settings 216
About the Interfacial Energy Property Model 217
Liquid and Solidus Temperature Property Model Settings 219
Phase Transition Property Model Settings 221
About the T0 Temperature Property Model 223
About the Spinodal Property Model 226
About the Yield Strength Property Model 229

About the Coarsening Property Model

Coarsening is a Property Model available when using the Property Model Calculator in Thermo-Calc.

- Coarsening Property Model Settings

In the coarsening regime where the driving force is capillarity, the change of mean particle radius evolves according to the equation:

$$r^{-3} - r_0^{-3} = Kt$$

Following Morral and Purdy [1994, Morral], the rate constant of precipitating β phase in a multicomponent α phase is

$$K = \frac{8\sigma V_m^\beta}{9}\left[\left[c_i^\beta - c_i^\alpha\right]^T [M]^{-1}\left[c_k^\beta - c_k^\alpha\right]\right]^{-1}$$

The mobility matrix *M* is not the same as the mobilites that can be obtained directly from the Diffusion Module (DICTRA). The *M* matrix instead corresponds to the L'' matrix as defined by Andersson and Ågren [1992, Andersson].

Using the u-fractions that is defined as

$$u_k = \frac{x_k}{\sum\limits_{j \in S} x_j}$$

where the summation only is performed over the substitutional elements give the final equation for the coarsening rate coefficient.

$$K = \frac{8\sigma V_m^\beta}{9}\left[\left[u_i^\beta - u_i^\alpha\right]^T [L''^\alpha_{jk}]^{-1}\left[u_k^\beta - u_k^\alpha\right]\right]^{-1}$$

The interfacial energy σ is calculated using the extended Becker's model (that also is available as a separate Property Model Calculator model).

References

[1992, Andersson] J.-O. Andersson, J. Ågren, Models for numerical treatment of multicomponent diffusion in simple phases. J. Appl. Phys. 72, 1350–1355 (1992).

[1994, Morral] J. E. Morral, G. R. Purdy, Particle coarsening in binary and multicomponent alloys. Scr. Metall. Mater. 30, 905–908 (1994).

Coarsening Property Model Settings

About the Coarsening Property Model

For an example, see PM_G_02: Coarsening and Interfacial Energy.

Coarsening is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase.

The output using this Model is the coarsening rate coefficient [m^3/s] for the precipitate phase and the interfacial energy [J/m^2] between matrix and the precipitate phase.

This Model requires that the thermodynamic and kinetic databases used include descriptions of molar volume of the matrix and precipitates as well as mobilities for the matrix phase.

Configuration Settings

The settings are found on the Property Model Calculator when **Coarsening** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Matrix phase

Choose a **Matrix phase**.

Precipitate phase

Choose a **Precipitate phase** to calculate its coarsening rate. Click the **Add phase** button to add another Precipitate phase. Click the **Remove phase** button to remove a phase.

About the Crack Susceptibility Coefficient Property Model

The **Crack Susceptibility Coefficient** is a Property Model available when using the Property Model Calculator in Thermo-Calc. It is used to calculate the hot tearing tendency during solidification. The model is based on the publication by Yan and Lin [2006 Yan].

Hot tearing is one of the most common and serious defects encountered during the casting of, for example, aluminum alloys. In general, it is defined by the formation of a macroscopic fissure in a casting as a result of stress and the associated strain, generated during cooling, at a temperature above the non-equilibrium solidus.

Crack susceptibility is also referred to as solidification cracking, hot cracking, hot shortness, supersolidus cracking, and shrinkage brittleness [2006 Yan].



PM_G_07: Hot Crack Susceptibility

Input Parameters Theory and Background



The original model assumptions are from Clyne and Davis [1981 Clyne]. Later, the experimental hot cracking susceptibility was collected from several sources by Yan and Lin [2006 Yan] and given as a probability 0-100%. The CSC calculated with the current model cannot be compared by absolute values with the experimental number; instead it is best to compare the trends, to see if it is increasing or decreasing. The experimental values are therefore given with relative coordinates and do not map directly to the calculated plot axes.

- The input parameters are entered on the Configuration window for the Property Model Calculator and described in Crack Susceptibility Coefficient Property Model Settings.

The **Crack Susceptibility Coefficient** (CSC) was originally proposed by Clyne and Davies [1981, Clyne] to describe the effects of alloy composition on hot tearing. In Thermo-Calc, the CSC is calculated using Scheil and uses assumptions of cooling rates under the thermal conditions that the heat flow is proportional to $\frac{1}{\sqrt{time}}$.

The CSC is defined as $CSC = \frac{tV}{tR}$ where:

- tV is the time during solidification where the casting is vulnerable to cracking, and
- tR is the time available for the stress relief process.

The values for tV and tR are given by the thermal condition, the Scheil results, and the input parameters for the liquid fraction (defined on the **Configuration** window):

- Start of relaxation
- Transition to vulnerability
- Smallest for vulnerability

These liquid fraction parameters are elaborated on next using the results from a simulation using the latest version of the TCS Al-based Alloy Database (TCAL8) and the alloy Al-0.9Cu-10Mg-0.9Ni-12.2Si mass%.

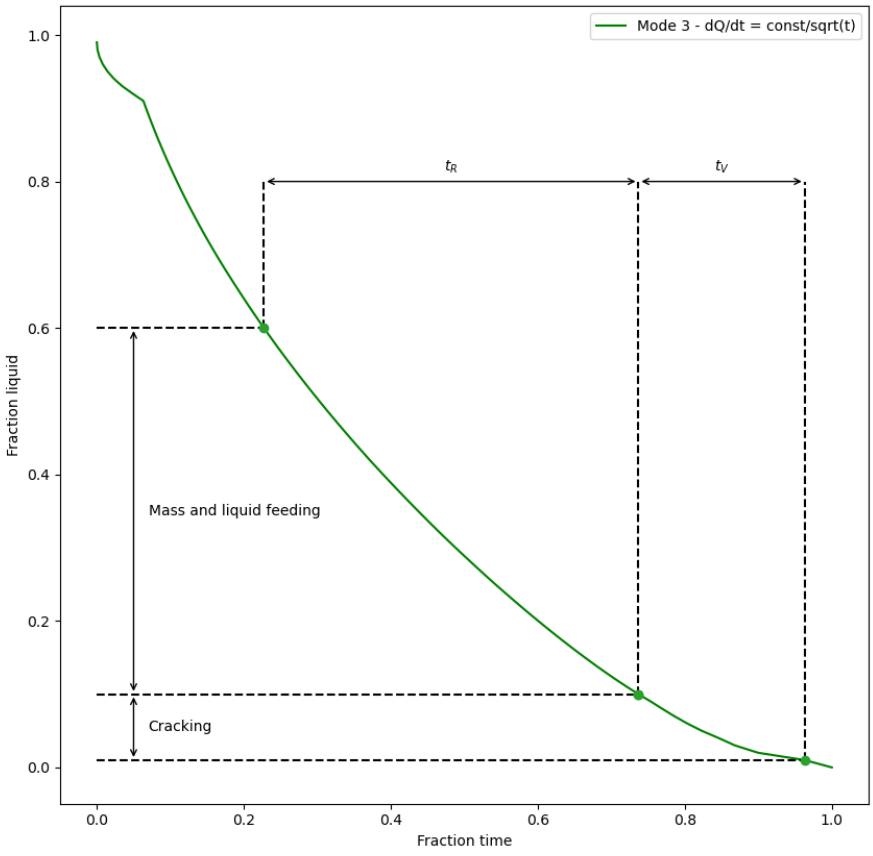


Figure 6: The results of the thermal condition in Mode 3, fraction of liquid, including the addition of lines and arrows to the plot for clarity. See the text for more detail.

Liquid Fraction Parameters

The **Crack Susceptibility Coefficient** Model is based on the concept of the existence of critical time periods during the solidification process when the structure is most vulnerable to cracking.

Clyne and Davies concluded that the mass and liquid feeding readily occurs at liquid volume fractions between about 0.6 and 0.1, so the time spent in these ranges was defined as time-relaxation (tR). At very low volume fractions of liquid, the material is too strong to crack. The authors chose a fraction of liquid between 0.1 and 0.01 as the vulnerable regime, and the time spent defined as tV. See Figure 6 for the results from a simulation using the TCAL8 and the alloy Al-0.9Cu-10Mg-0.9Ni-12.2Si mass%.

The Scheil simulation takes temperature steps and does not regard time at all. See Figure 7 for the typical Scheil results of amount of solid phases as function of temperature. The simulation is made with TCAL8 and the alloy Al-0.9Cu-10Mg-0.9Ni-12.2Si mass%.

A thermal condition is assumed to connect the amount of liquid fraction to fraction of time.

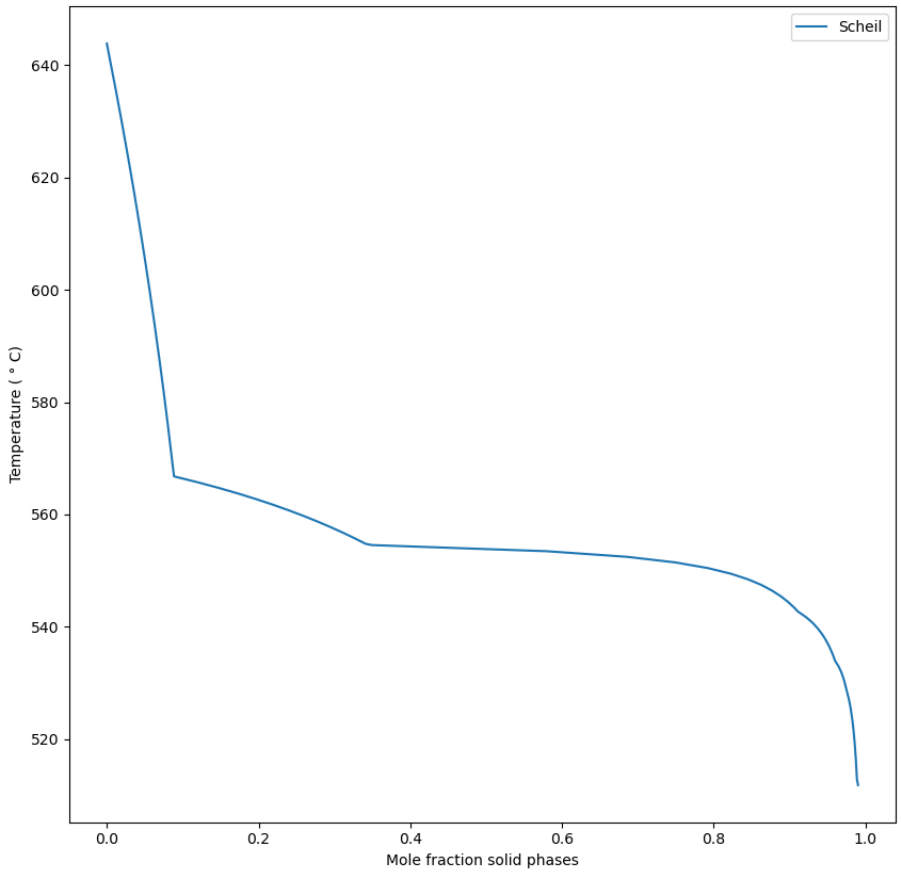


Figure 7: A Scheil simulation result of the mole fraction solid phases vs temperature (°C). See the text for more detail.

Following Clyne and Davies' approach, the cooling rates were then estimated under three different thermal conditions:

- Mode 1 with a constant cooling rate,
- Mode 2 with a constant heat flow, and
- Mode 3 with a heat flow proportional to the square root of time.

The crack index can then be obtained from the Scheil simulation results: fraction liquid vs T curve and the thermal condition.

1-fraction solid phases = fraction liquid phase.

Figure 8 can be thought of as the 'master curve' for the connection between fraction of liquid and fraction of time. The limits of the amount of liquid 0.01, 0.1, and 0.6 and the corresponding fraction time are shown for each thermal condition. In Figure 6 , which is a less cluttered plot, the time spent in the relaxation and in the vulnerable regions are marked with lines and arrows for a single thermal mode.

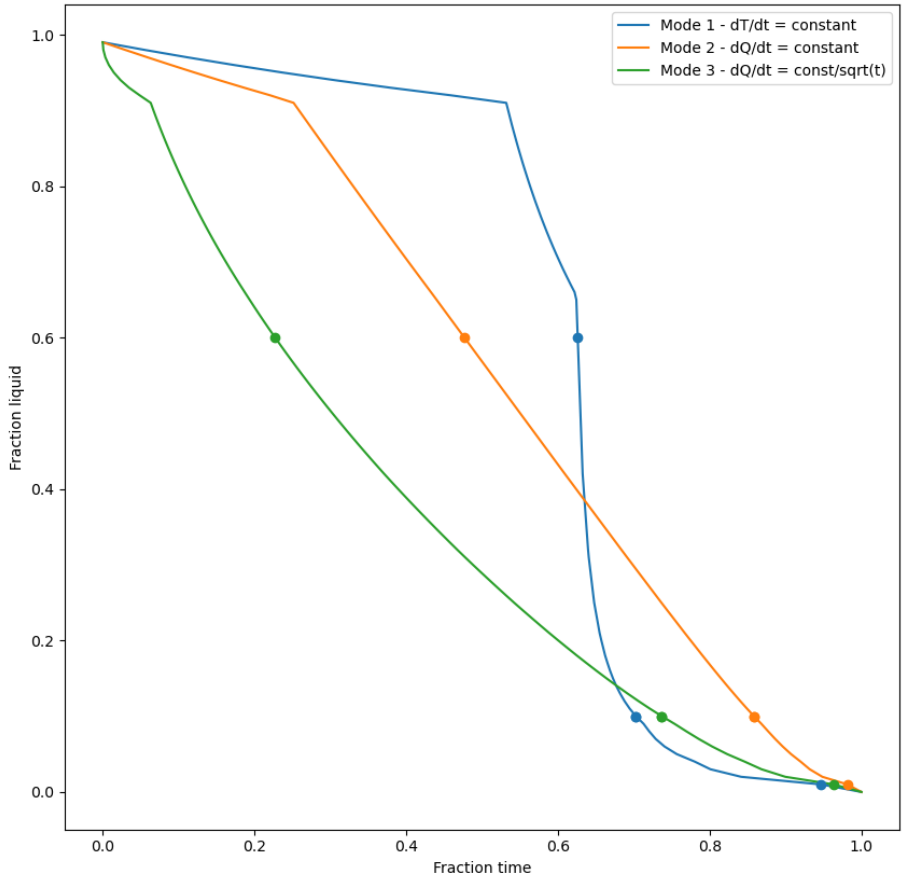


Figure 8: The results of the thermal condition in Modes 1-3, the fraction of time vs the fraction of liquid. See the text for more detail.

References

[1981 Clyne] T. W. Clyne and G. J. Davies, “The Influence of Composition on Solidification Cracking Susceptibility in Binary Alloy Systems,” Br. Foundrym., vol. 74, pp. 65–73, 1981.

[2006 Yan] X. Yan and J. C. Lin, “Prediction of hot tearing tendency for multicomponent aluminum alloys,” Metall. Mater. Trans. B, vol. 37, no. 6, pp. 913–918, Dec. 2006, doi: 10.1007/BF02735013.

Crack Susceptibility Coefficient Property Model Settings

For details about this more advanced model, see About the Crack Susceptibility Coefficient Property Model.

For an example, see PM_G_07: Hot Crack Susceptibility.

The **Crack Susceptibility Coefficient** is a Property Model available when using the Property Model Calculator in Thermo-Calc. The calculations use Scheil and assumptions of cooling rates under three different thermal conditions:

- Constant cooling rate, dT/dt = constant
- Constant heat flow, dQ/dt = constant
- Heat flow proportional to 1/sqrt(time)

Configuration Settings

These settings are found on the Property Model Calculator when **Crack Susceptibility Coefficient** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

Scheil and General Parameters

These parameters are the same as those used for the Scheil Calculator although some setting names are slightly different.

Scheil Start Temperature

Enter a **Scheil start temperature** for the Scheil simulation that is higher than the liquidus temperature of the alloy. Is given in the same unit as the temperature in the **Condition Definitions**.

Show Advanced Scheil Options

Click the **Show advanced Scheil options** check box to enter several settings related to Scheil calculations.

Temperature Step

Click the **Show advanced Scheil options** check box to view this setting. Enter a **Temperature step** for the Scheil simulation. Temperature step is given in the same unit as the temperature in the **Condition Definitions**.

Global Minimization

Click the **Show advanced Scheil options** check box to view this setting. By default the **Global minimization** check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.

Terminate at Fraction of Liquid Phase Amount

Click the **Show advanced Scheil options** check box to view this setting. Enter a value in field for **Terminate at fraction of liquid phase amount**. The value should not be larger than the setting **Liquid fraction: Smallest for vulnerability**.

Smallest Fraction

Click the **Show advanced Scheil options** check box to view this setting. The default **Smallest fraction** is 1.0E-12. This is the value assigned to constituents that are unstable.

This default setting is used as a start value in the Scheil Calculator. During simulation, and if there are convergence issues, the value can be decreased.

Liquid Phase

Click the **Show advanced Scheil options** check box to view this setting. The default in the list is the **LIQUID** phase already defined in the chosen database.

THERMAL MODE AND LIQUID FRACTION PARAMETERS



See About the Crack Susceptibility Coefficient Property Model for more background information about these parameters.

Thermal Mode

Select a **Thermal mode** for the solidification simulation:

- **Constant cooling rate, dT/dt = constant**
- **Constant heat flow, dQ/dt = constant**
- **Heat flow prop 1/sqrt(time)** (i.e. heat flow is proportional to $\frac{1}{\sqrt{time}}$)

Liquid Fraction for Start of Relaxation

Enter a value for the **Liquid fraction for start of relaxation**.

Liquid Fraction Transition to Vulnerability

Enter a value for the **Liquid fraction transition to vulnerability**.

Liquid Fraction Smallest to Vulnerability

Enter a value for the **Liquid fraction smallest to vulnerability**.

Driving Force Property Model Settings

Driving Force is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the thermodynamic driving force for a phase divided by RT.

For an example, see PM_G_03: Driving Force and Interfacial Energy.

Configuration Settings

The settings are found on the Property Model Calculator when **Driving force** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Matrix phase

Choose a **Matrix phase**, the single phase region to start in. Select 'Any phase' to use the phases that take part of the initial equilibrium or choose a specific phase.

Precipitate phase

Choose a **Precipitate phase** to calculate its driving force.

About the Equilibrium with Freeze-in Temperature Property Model

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at all other temperatures.

The electrical resistivity due to grain boundary (GB) phase scattering is evaluated as the scattering constant times the total volume fraction of the grain boundary phases. The default value for the constant has been found to be 4.83e-8 Ωm for aluminum alloys. The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.



For examples, see PM_G_10: Freeze-in Thermal Conductivity and PM_G_11: Freeze-in Electric Conductivity.

Equilibrium with Freeze-in Temperature Property Model Settings



This Property Model uses thermophysical properties that are included with some Thermo-Calc databases such as the TCS Al-based Alloy Database (TCAL), which is used in the two examples included with your installation. For more information about the availability and the theory, see About Thermophysical Properties Data Parameters, Electrical Resistivity Model, and Thermal Conductivity Model.

Equilibrium with Freeze-in Temperature Property Model Settings

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at all other temperatures.

For examples, see PM_G_10: Freeze-in Thermal Conductivity and PM_G_11: Freeze-in Electric Conductivity.

Configuration Settings

The settings are found on the Property Model Calculator when the **Equilibrium with Freeze-in Temperature** Model is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Freeze-in Temperature

Enter a Freeze-in Temperature value in the field. The units match those selected under Condition Definitions. This is the temperature where the equilibrium is calculated. The default is 623.15 K (350 °C).

Evaluate for Single Phase

Select this check box to evaluate the properties of a specific phase or deselect to evaluate the properties for the entire system.

Phase for Evaluation

This setting is available when the **Evaluate for a single phase** check box is selected. Select a **Phase for evaluation**.

Equilibrium Minimization Strategy

Select an **Equilibrium minimization strategy**.

The **Minimization strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed. The default uses the **Local minimization preferred** option.

With either the *Global* or *Local preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred** the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.



For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

Manual Settings GB (Grain Boundary) Phase Scattering

By default the automatic grain boundary (GB) phase scattering settings are used in the calculation. Automatic settings account for GB phase scattering with FCC_A1 as the matrix phase for Al-based alloys and HCP_A3 as matrix phase for Mg-based alloys.

Select the check box to enter user-defined settings **Account for GB scattering**, **Matrix phase**, and **GB phase scattering constant**.

Account for GB Scattering

This setting is available when the **Manual settings GB scattering** check box is selected.

Select the **Account for GB scattering** check box to evaluate as follows. The electrical resistivity due to grain boundary (GB) phase scattering is evaluated as the scattering constant times the total volume fraction of the grain boundary phases. The default value for the constant has been found to be 4.83e-8 Ωm for aluminum alloys. The contribution to thermal conductivity is assumed to be related to that of electrical resistivity, following the Wiedemann-Franz law.

Matrix Phase

This setting is available when the **Manual settings GB scattering** check box is selected.

Choose a **Matrix phase** to use for estimating the amount of grain boundary (GB) phases. The phases that are not matrix phase are assumed to be GB phases that contribute to the GB phase scattering.

GB Phase Scattering Constant

This setting is available when the **Manual settings GB scattering** check box is selected.

The default value for the **GB phase scattering constant** is found to be 4.83e-8 Ωm for aluminum alloys. This is a constant to evaluate electrical resistivity due to scattering at grain boundary phases.

The model evaluates the following properties:

- Electric resistivity (Ωm)
- Electric conductivity (S/m)
- Thermal conductivity (W/(mK))
- Thermal resistivity (mK/W)
- Thermal diffusivity (m^2/s)
- Molar volume (m^3/mol)
- Density (g/cm^3)
- Linear technical thermal expansion (1/K): Calculated as (L1-L0)/(T1-T0)/L0, where L0 is the length at a reference temperature T0. T0 is by default equal to room temperature
- Linear physical thermal expansion (1/K)
- Volumetric physical thermal expansion (1/K)

- Heat capacity (J/K)
- User-defined functions: Available when the **Define User Functions** check box is selected and the functions are defined.

Set Reference Temperature for Technical CTE

In the field, enter the **Reference temperature for technical CTE**, where CTE is the coefficient of thermal expansion. Typically room temperature is used as the default 293.15 K (20 °C).

Define User Functions

Select the **Define user functions** check box to enter up to two **User-defined functions**.

User-defined Functions (two fields)

Two fields are available when the **Define user functions** check box is selected. Enter functions using the Thermo-Calc syntax.



For an example, see T_07: User-Defined Functions.

Equilibrium Property Model Settings

Equilibrium is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the equilibrium for the given conditions.

> When you use this Model with the **Property Model Calculator**, it is the same calculation result as when you are using an **Equilibrium Calculator** with the **Single equilibrium** calculation type.

Configuration Settings

The settings are found on the Property Model Calculator when **Equilibrium** is selected under **General Models**.

> When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Define additional **Quantity Definitions** and **Function Definitions**. All quantities that normally can be obtained from an equilibrium calculation can also be obtained when plotting the results, as well as the defined functions.

About the Interfacial Energy Property Model

Interfacial Energy is a Property Model available when using the Property Model Calculator in Thermo-Calc.

- Interfacial Energy Property Model Settings

Interfacial energy is an important parameter used in precipitation simulations to calculate the rates of nucleation, growth/dissolution, and coarsening. The value of interfacial energy can vary dramatically (usually between 0.01 to 2.0 J/m^2).

The extended Becker's model functions to estimate coherent interfacial energy by using thermodynamic data from existing CALPHAD thermodynamic databases:

$$\sigma_c = \frac{n_s z_s}{N_A z_l} \Delta E_s$$

where σ_c is the coherent interfacial energy, n_s is the number of atoms per unit area at the interface, z_s is the number of cross bonds per atomat the interface, z_l is the coordination number of an atom within the bulk crystal lattice, and ΔE_s is the energy of solution in a multicomponent system involving the two phases being considered [1938, Becker].

Reference

[1938, Becker] R. Becker, Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen. Ann. Phys. 424, 128–140 (1938).

Interfacial Energy Property Model Settings

About the Interfacial Energy Property Model

For an example, see PM_G_02: Coarsening and Interfacial Energy.

Interfacial Energy is a Property Model available when using the Property Model Calculator in Thermo-Calc and is used to estimate the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. The approximation model is based on Becker's bond energy approach and is also available in Precipitation Module (TC-PRISMA).

In the actual calculation, the coefficients taken distinguish between only bcc and fcc structure for the (110) and (111) lattice plane, respectively.

For other planes and/or other phases, the estimate is approximate. In most situations, it is recommended to perform calibrations against some experimental data because the interfacial energy is dependent on so many factors that are ignored in the estimation, for example entropy, incoherency, orientation, and curvature, etc. Uncertainty factors must also be considered as thermodynamic data in CALPHAD databases are not always accurate.

Configuration Settings

The settings are found on the Property Model Calculator when **Interfacial energy** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Matrix phase

Choose a **Matrix phase** to calculate the interfacial energy [J/m^2].

Precipitate phase

Choose a **Precipitate phase** to calculate the interfacial energy [J/m^2].

Liquid and Solidus Temperature Property Model Settings

Liquidus and solidus temperature is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the liquid phase. If only the liquidus temperature is required, the calculation times are reduced.

Configuration Settings

The settings are found on the Property Model Calculator when **Liquidus and solidus temperature** is selected under **General Models**.



When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Only calculate liquidus temperature

Select the **Only calculate liquidus temperature** check box as required.

Liquid phase

Choose the **Liquid phase** of the system. This is a fallback choice. Normally this should be handled automatically, even if multiple liquid phases are present.

Upper temperature search limit

Upper temperature search limit: Initial temperature for the liquidus calculation. This needs to be in the fully liquid state.

Max. number of iterations

Max. number of iterations Maximum number of phase transformation iterations performed. The default is 10.

Global minimization

Global minimization for liquidus and **Global minimization for solidus**: Select one or both of these check boxes to find all phases present in the equilibria. However, note it significantly increases the calculation time.



Global minimization recommendation: First try to calculate without global minimization, then if inaccuracies occur, switch global minimization on. Problems mostly occur if many phases are present at a given temperature.

Suspend gas phase

Suspend gas phase: The occurrence of a gas phase may mislead the liquidus temperature determination. If the presence of the gas phase is absolutely required, you can activate it and then choose a user-defined phase.

Gas phase

Choose a **Gas phase** from the list.

Phase Transition Property Model Settings

Phase Transition is a Property Model available when using the Property Model Calculator in Thermo-Calc and by varying set conditions it calculates the point when a new phase may form. It is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the varied condition.

For an example, see PM_G_01: Phase Transition.

Configuration Settings

The settings are found on the Property Model Calculator when **Phase transition** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Matrix Phase

Select the **Matrix phase**, the single phase region to start in. Select **Any phase** to use the phases that take part of the initial equilibrium or choose a specific phase.

Phase to Form

For the new **Phase to form**, select **Any phase** or choose a specific phase.

Condition to Vary

Choose a composition or temperature **Condition to vary** when calculating the phase transition.

Search Direction

For the composition or temperature condition being varied, choose the **Search direction** to be in a **Positive**, **Negative**, or **Positive and Negative** direction.



The start value (given in *Condition Definitions*) and phase transition point need to be within these limits, otherwise the model returns *Not a Number* as result. For example, a start temperature is 1100 K then the limits need to be outside these, e.g. 500-1500.

About the T_0 Temperature Property Model

T-Zero Temperature is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the so-called T_0 line.

The T_0 temperature is defined as the temperature where two phases of identical chemical composition have the same molar Gibbs free energy. This temperature is an important quantity in the field of diffusionless phase transformations, e.g. martensitic transformation, since it is the upper limit where diffusionless phase transformations can occur.

With this Model up to two root solutions can be found. When searching for the root you can vary the condition of temperature or element composition in units of mass percent (e.g. mass percent Fe, mole percent Fe, and so forth). When **Temperature** is the varied condition, the root(s) equal the T_0 temperature(s).



For an example, see PM_G_09: T-Zero Temperature

- The input parameters are entered on the Configuration window for the Property Model Calculator and described in T0 Temperature Property Model Settings.

T_0 Temperature Property Model Settings

About the T0 Temperature Property Model

For an example, see PM_G_09: T-Zero Temperature

T-Zero Temperature is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the so-called T_0 line. In other words, it finds the root(s) where the two selected phases have equal Gibbs energy.

All other phases are suspended and up to two roots can be found.

Configuration Settings

These settings are found on the Property Model Calculator when **T-Zero Temperature** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

First Phase

From the **First phase** list select the applicable phase you want to search for the evaluation of Gibbs energy.

Second Phase

From the **Second phase** list select the applicable phase you want to search for the evaluation of Gibbs energy.

Condition to Vary

From the **Condition to vary** list select an option to vary when searching for the root. Up to two roots can be found. These options are **Temperature** or those based on the **Composition** (e.g. Fe, Cr, and so forth) and **Composition unit** (i.e. Mass percent, Mole percent, Mass fraction, or Mole fraction).



When **Temperature** is the varied condition, the root(s) equal the T_0 temperature(s).

Manual Search Limits

The **Manual search limits** check box is not selected by default and this sets automatic search limits.

Select the check box to enter user-defined search limits in the fields. Enter the **Lower condition limit** and **Upper condition limit**. Then in the **Steps when estimating root(s)** field, enter the number of steps in a linear grid when estimating the position(s) of the root(s).

About the Spinodal Property Model

Spinodal is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the spinodal line.

The spinodal is defined by the condition where the second derivative of Gibbs free energy is zero (d2G/dx2 = 0). The locus of these points is known as the *spinodal curve*.

With this Model up to two spinodal solutions can be found. When searching for the spinodal you can vary the temperature or a composition in mass percent, mole percent, mass fraction, or mole fraction (e.g. mass percent Fe, mole percent Fe, and so forth).

When within the miscibility gap, but above the spinodal curve, phase transformation occur by classical nucleation and growth of the spinodal phase. When within the miscibility gap, but below the spinodal curve, the phase transformation occur by spinodal decomposition of the spinodal phase.

- The input parameters are entered on the Configuration window for the Property Model Calculator and described in Spinodal Property Model Settings.

For an example, see PM_G_08: Spinodal.

The microstructure evolution of spinodal decompositon can be calculated with the phase field method. For some background information you can read more about it in chapter 2 of this doctoral thesis: T. Barkar, “Modelling phase separation in Fe-Cr alloys: A continuum approach,” PhD thesis, KTH Royal Institute of Technology, 2018, http://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-235394.

Spinodal Property Model Settings

About the Spinodal Property Model

For an example, see PM_G_08: Spinodal.

Spinodal is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the spinodal line.

Configuration Settings

These settings are found on the Property Model Calculator when **Spinodal** is selected under **General Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

Spinodal Phase

From the **Spinodal phase** list select the applicable phase you want to search for the spinodal.

Condition to Vary

From the **Condition to vary** list select an option to vary when searching for the spinodal. Up to two spinodals can be found. These options are **Temperature** or those based on the **Composition** (e.g. Fe, Cr, and so forth) and **Composition unit** (i.e. Mass percent, Mole percent, Mass fraction, or Mole fraction).

Manual Search Limits

The **Manual search limits** check box is not selected by default and this sets automatic search limits.

Select the check box to enter user-defined search limits in the fields. Enter the **Lower condition limit** and **Upper condition limit**. Then enter the number of steps when estimating the position(s) of the spinodal(s)in the **Steps when estimating spinodal** field.

About the Yield Strength Property Model

The settings for these contributions are found on the Property Model Calculator when the Yield Strength Property Model Settings is selected under **General Models**.

Yield strength is also available as a variable when working with Plots and Tables that are successors to the **Precipitation Calculator**.

The **Yield Strength** Model is a general model to estimate the yield stress of a material that considers these contributions to the overall yield stress of the material:

- Intrinsic strength (σ_i) for the pure elements,
- Grain boundary strengthening (σ_{gb}),
- Solid solution strengthening (σ_{ss}),
- Precipitation strengthening (σ_p), and
- A user set, constant strength contribution (σ_c).

The temperature (T) is used to evaluate the equilibrium state of the system, and the resulting compositions and phase fractions are subsequently used in the evaluation of mechanical properties. Below follows a short summary for each of the contributions.

Intrinsic Strength

Intrinsic strength, σ_i, is the base strength as evaluated from linear combination of the pure elements' strength. If data is missing for one or more elements a message displays in the software to indicate this.

Constant Addition of Strength

The parameter σ_c is set by the user as a constant strength addition to the material.

Grain Boundary Strengthening

The **grain boundary strengthening**, σ_{gb}, is the contribution to the total strength stemming from the grain boundary's ability to hinder dislocation movement described by the Hall-Petch relation [2004, Hansen].

The parameters you enter are the Hall-Petch constant, k_{h-p} in MPa μm$^{1/2}$, and the average grain diameter in μm.

Solid Solution Strengthening

 PM_G_06: Yield Strength HEA

The **solution strengthening**, σ_{ss}, is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. For the solid solution strengthening the option of evaluating the strength at any temperature is available. The result is normalized with respect to the sum of all mole fractions for FCC, BCC and HCP. This option uses the phase fractions and compositions calculated at the overall equilibrium temperature. The model by Walbrühl et al. [2017, Walbruhl] is implemented.

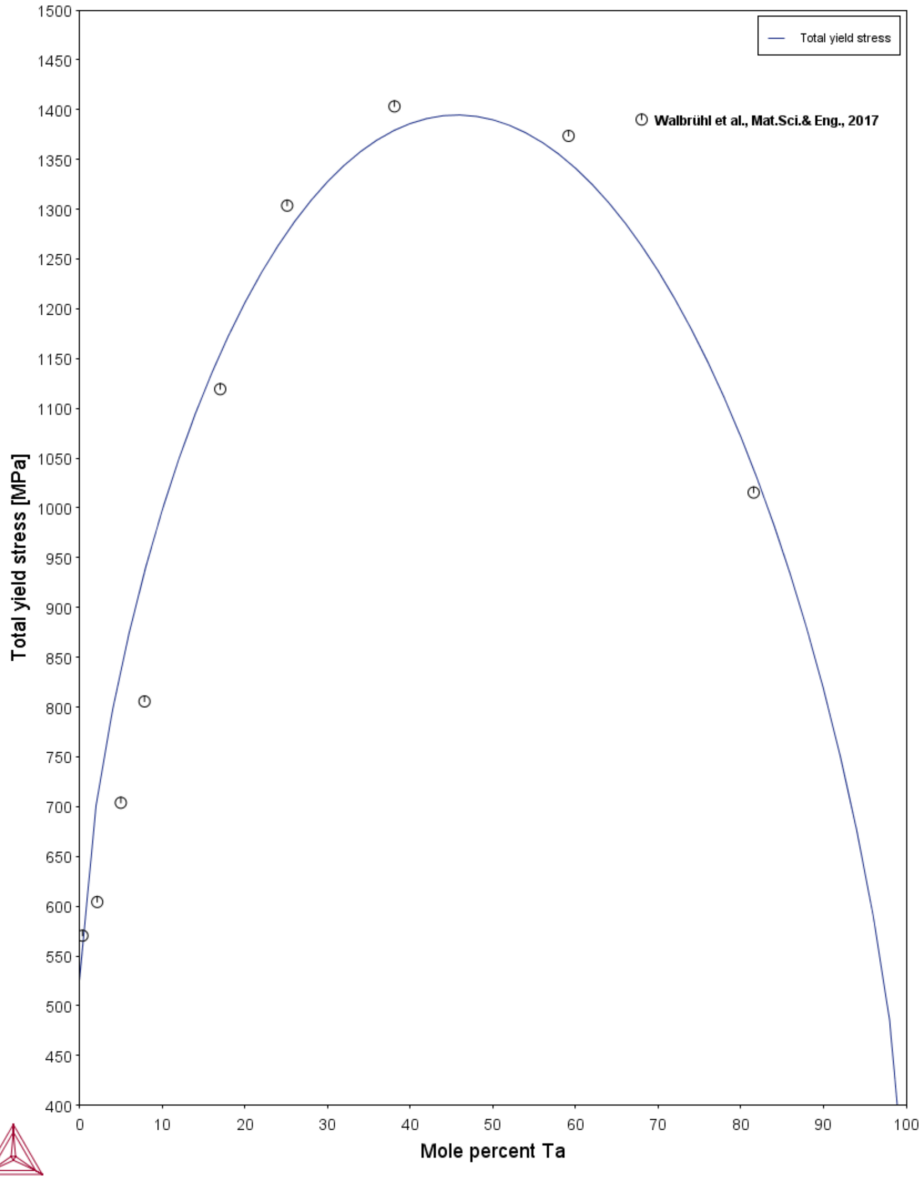


Figure 9: Yield strength vs Ta-content for the binary high entropy Mo-Ta alloy.

Precipitation Strengthening

The **precipitation strengthening**, σ_p, is the contribution to total strength due to precipitation of a secondary phase, e.g. gamma prime in Ni-base alloys or Al_3Sc precipitates in Al-base alloys. This model is available for any number of precipitating phases. The total particle strength is calculated by the square mean of the individual particle strength contributions:

$$\sqrt{\sigma_{p1}^2 + \sigma_{p2}^2 + \ldots + \sigma_{pn}^2}$$

The Simplified model (general), Seidman model (Al-base) and Reppich model (Ni-based) are available to estimate the precipitation strengthening contribution.

Simplified Model (General)

PM_G_04: Yield Strength

The **simplified model** is based on the work by Zander et al. [2008, Zander] and considers the general mechanisms of cutting and looping without regard to any detailed dislocation mechanisms. The default parameters are, however, optimized against experimental data for the Al-0.3wt%Sc alloy described by Seidman et al. [2002, Seidman].

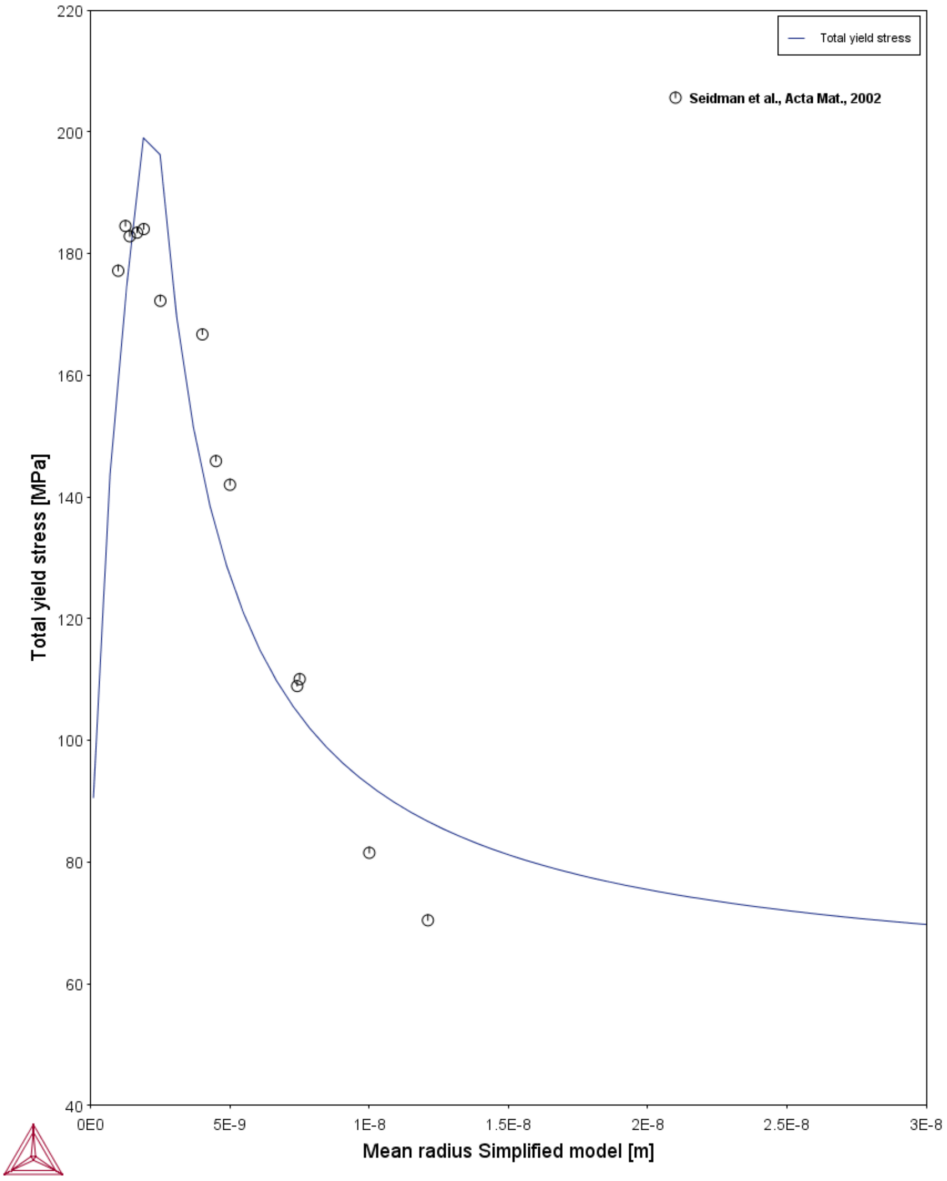


Figure 10: Yield strength Property Model plot example using the 'Simplified model' as described in the text.

Seidman Model (Al-base)

PM_G_04: Yield Strength

The **Seidman model (Al-base)** by Seidman et al. [4] considers several contributions to the overall precipitation strengthening - ordering, coherency stresses, shear modulus mismatch, and Orowan looping. The Seidman model is suitable for Al-base alloys with a low volume fraction of spherical precipitates. In example **PM_G_04_Yield_Strength**, the simplified and Seidman models are compared to experimental data on the increase in yield strength due to precipitation hardening. Although the experimental set up was designed to eliminate grain boundary and solid solution strengthening, these are also included by optimizing of model parameters.

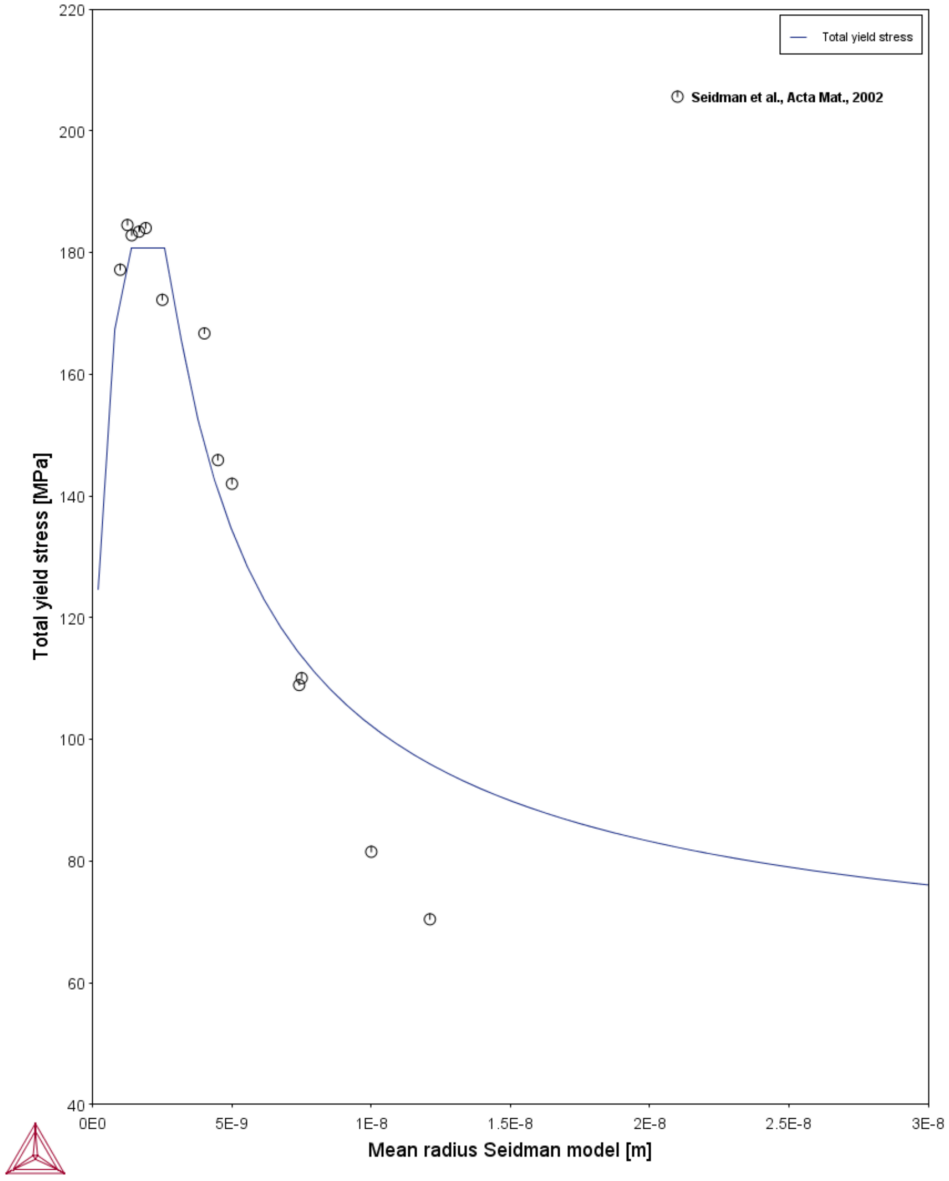


Figure 11: Yield Strength Property Model plot example using the 'Seidman model' as described in the text [2002, Seidman].

Reppich Model (Ni-base)

PM_G_05: Yield Strength NiAlCr

The **Reppich model (Ni-base)** by Reppich et al. [1982a, Reppich] considers both weak and strong coupling of dislocation as they propagate through an ordered secondary phase and is thus suitable for Ni-base alloys with relatively high volume fractions of gamma prime or gamma double prime.

The Reppich model is not valid for very small values of volume fraction precipitate and precipitate radius.

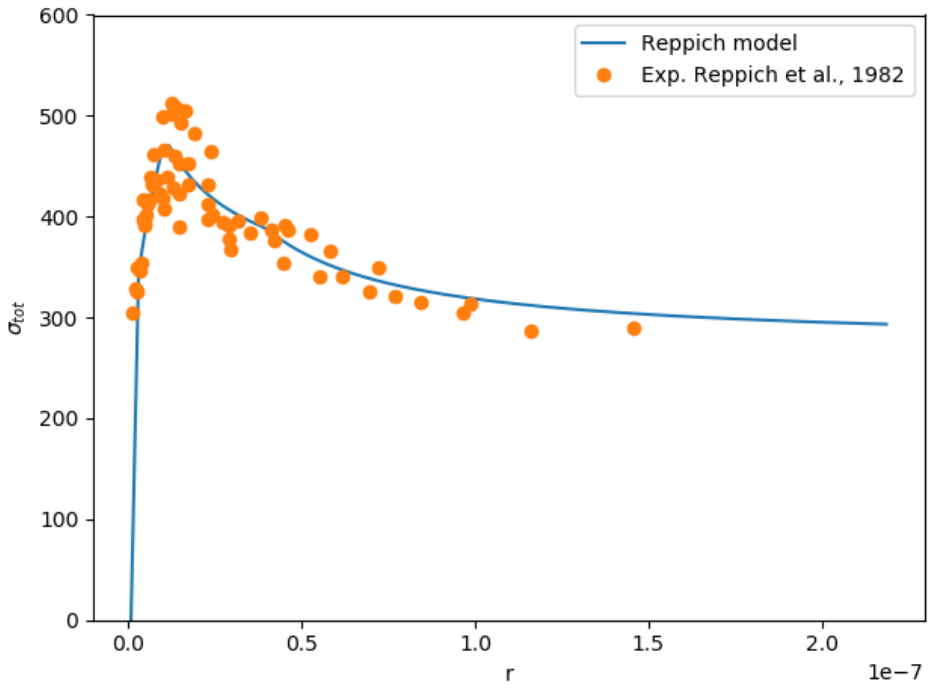


Figure 12: Reppich model plotted with results and experimental data for PE16 [1982b, Reppich], all data is normalized with the square root of the volume fraction of precipitate.

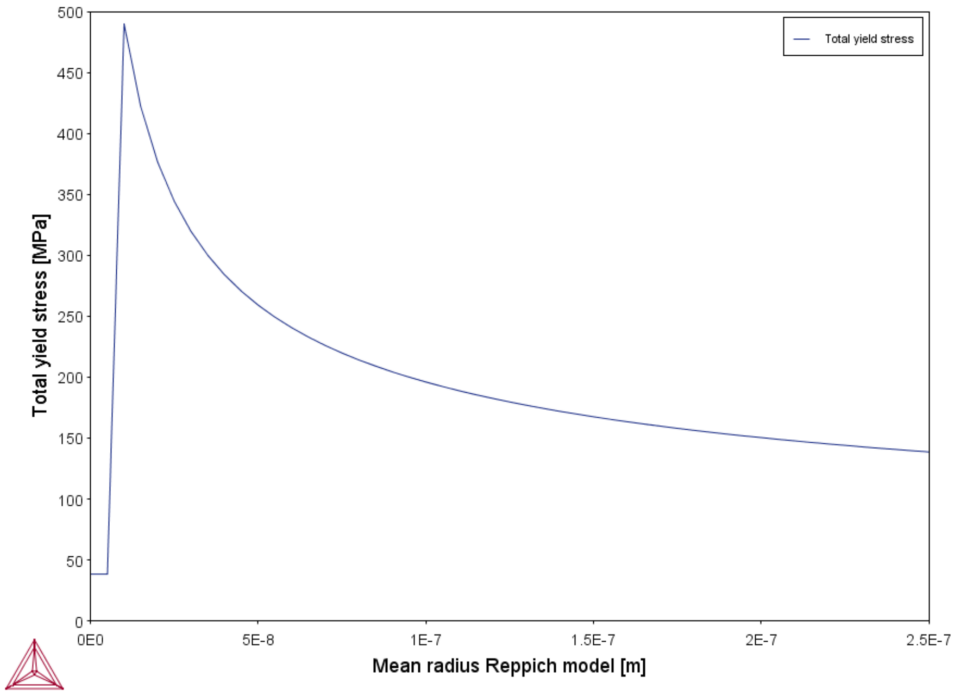


Figure 13: Reppich model yield strength vs mean precipitate radius for Ni-10Cr-10Al.

References

[1982a, Reppich] Reppich, B. "Some new aspects concerning particle hardening mechanisms in γ’ precipitating Ni-base alloys—I. Theoretical concept," Acta Metall. 30, 87–94 (1982).

[1982b, Reppich] Reppich, B., Schepp, P. & Wehner, G. "Some new aspects concerning particle hardening mechanisms in γ’ precipitating nickel-base alloys—II. Experiments," Acta Metall. 30, 95–104 (1982).

[2002, Seidman] Seidman, D. N., Marquis, E. A. & Dunand, D. C. "Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys," Acta Mater. 50, 4021–4035 (2002).

[2004, Hansen] Hansen, N. "Hall–Petch relation and boundary strengthening," Scr. Mater. 51, 801–806 (2004).

[2008, Zander] Zander, J. & Sandström, R. "One parameter model for strength properties of hardenable aluminium alloys," Mater. Des. 29, 1540–1548 (2008).

[2017, Walbruhl] Walbruhl, M., Linder, D., Ågren, J. & Borgenstam, A. "Modelling of solid solution strengthening in multicomponent alloys," Mater. Sci. Eng. A 700, 301–311 (2017).

Yield Strength Property Model Settings

About the Yield Strength Property Model

The **Yield Strength** Model is available with the Property Model Calculator and calculates yield stress.

Yield strength is also available as a variable when working with Plots and Tables that are successors to the **Precipitation Calculator**.

The Yield Strength Model returns the yield strength at room temperature for the specified material using the equilibrium values calculated at temperature *T*. The Model is defined by further setting these contributions:

- Intrinsic strength (σ_i) contribution
- Solid solution strengthening (σ_{ss})
- Grain boundary strengthening (σ_{gb})
- Precipitation strengthening (σ_p)
- Constant strength addition (σ_c)

For examples using the Property Model Calculator, see PM_G_04: Yield Strength, PM_G_05: Yield Strength NiAlCr, and PM_G_06: Yield Strength HEA.

For an example when it is available as an axis variable with the Precipitation Calculator, see P_01: Isothermal Precipitation of Al3Sc.

Configuration Settings

The settings for these contributions are found on the Property Model Calculator when the **Yield Strength** Model is selected under **General Models**.

There are settings described elsewhere when **Yield Strength** is selected as an axis variable for a Plot Renderer or Table Renderer that are successors to the **Precipitation Calculator**.



When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

General Model Settings

Composition unit

Choose a unit: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Condition Definitions

Choose a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a value for the **Temperature** and **Composition** for each component.

The values entered in *Condition Definitions* are used as the start values for the different calculation types.

Yield Strength Model Settings

Matrix

Matrix: Choose a **Matrix** phase.

Solid solution strengthening evaluation temperature

Click to select the **Solid solution strengthening evaluation temperature** check box to further define this model.

Then enter a **Solid solution strengthening temperature** in the field. The unit of temperature is the same as that selected above under *Condition Definitions*.



If no temperature is entered, room temperature is used.

Grain boundary strengthening

Click to select the **Grain boundary strengthening** check box to include calculated grain boundary strengthening (σ_{gb}). Then enter the following settings.

Grain size: The grain diameter in µm.

Select the **User defined Hall-Petch coefficient** check box to enter the **Hall-Pletch coefficient**: k_{h-p} in MPa µm$^{1/2}$.

Precipitation strengthening

Click to select the **Precipitation strengthening** check box to include calculated precipitation strengthening (σ_p). Then enter the following settings.

Select a **Precipitate** from the list. Use the **Add** and **Remove** buttons to add and remove additional precipitate phases.

The Precipitation Module (TC-PRISMA) has additional advanced functionality when you are working with the Precipitation Calculator and add a Plot Renderer or Table Renderer with **Yield strength** as a plot variable.

The precipitation strengthening contribution (σ_p) is calculated by one of these models:

Select a **Precipitation strengthening model** from the list:

- **Simplified model (general)**
- **Seidman model (Al-base)**: Preferentially used for Al-based alloys.
- **Reppich model (Ni-base)**: Preferentially used for Ni-based alloys.

The Reppich model is not valid for very small values of volume fraction precipitate and precipitate radius.

For the **Simplified model (general)**, enter values in the fields for the following. The default values of kp and r_c are optimized against experiments for Al-Sc.

- **Mean radius Simplified model**: The precipitate mean radius. The unit is meter (m).
- **kp**: The prefactor for the simplified model, which adjusts the overall height of the yield strength curve.
- **Critical radius** r_c, which determines the mean precipitate radius where transition between cutting and looping occurs. The unit is meter (m).

For the **Seidman model (Al-base)**, enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Seidman model**: The precipitate mean radius. The unit is meter (m).
- **Anti-phase boundary energy**: γ_{apb}, which is the average anti-phase boundary energy for the precipitate phase. The unit is Jm^{-2}.
- **m**: A Seidman exponent, it is a constant in the expression for strengthening by modulus mismatch.
- **alpha**: A Seidman prefactor. It is a fitting constant in the expression for coherency strengthening.

For the **Reppich model (Ni-base)**, enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Reppich model**: The precipitate mean radius. The unit is meter (m).
- **Anti-phase boundary energy**: γ_{apb}, which is the average anti-phase boundary energy for the precipitate phase. The unit is Jm^{-2}.
- **w**: A parameter that accounts for elastic repulsion between strongly coupled dislocations.
- **A**: Numerical factor reflecting particle morphology (0.72 for spherical).

Constant strength addition

Enter a value for the **Constant strength addition**, σ_c. The unit is MPa.

Equilibrium minimization strategy

Select an **Equilibrium minimization strategy**.

The **Minimization strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed. The default uses the **Global test preferred** option.

With either the *Global* or *Local preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred** the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.



For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

Calculation Type Settings

Calculation Type

Choose a calculation type: **Single** (no axes), **One axis**, **Grid**, **Min/Max**, **Uncertainty**, or **Batch**.

- Select **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Results** window.

  Equilibrium Property Model Settings

- Select **One axis** to vary a quantity on the X-axis.
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.
- The **Min/Max** calculation evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log.
- The **Uncertainty** calculation evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Renderer activity.
- The **Batch** calculation allows for high throughput calculations with Property Models. Data can be read from a file, such as a spreadsheet, rather than, for example, having a fixed grid or random values. Results from these batch calculations can then be compared to experimental values (as long as this data is included), using the Cross plot mode on the Plot Renderer.

Axis Definition

For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.

Grid Definition Settings

Grid Definitions

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.



For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour*, or *3D* diagram.

- Heat Map, Contour, and 3D Plots

Min/Max Definitions

For the **Min/Max** calculation type, click to select the applicable check boxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under *Condition Definitions* for the respective quantity.

Enter numerical values in the Δ**Min/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the **Event Log**.

Sampling of Data from Gaussian Distributions

For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

- About the Uncertainty Calculations

Sampling Parameters

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

- About the Uncertainty Calculations

Steel Model Library Property Models

Property Model Calculator

In this section:

About the Bainite Property Model 251
About the CCT Diagram Property Model 255
About the Critical Transformation Temperatures Property Model 263
About the Martensite Fractions Property Model 267
About the Martensite Temperatures Property Model 270
About the Pearlite Property Model 274
About the TTT Diagram Property Model 279

About the Bainite Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The **Bainite** Property Model, available when using the Property Model Calculator in Thermo-Calc, describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. In this Model, bainite is modeled as ferrite or a ferrite-cementite mixture.

For a given austenite composition, the bainite start temperature, WB_S, is calculated following Leach et al. [2018] (see Eqs. 8 and 9 and Table 1 in the paper). At WB_S, the driving force for ferrite to precipitate out of austenite under the “para” condition (i.e. no partitioning of substitutional elements, carbon in equilibrium) is balanced by a barrier, which is modeled as a function of composition.

At a temperature below WB_S, there is a net driving force (over the barrier) for the growth of bainitic ferrite. The steady-state lengthening rate of ferrite plate is calculated based on the method from Leach et al. [2019] with modifications. In the Bainite Model, unlike in [2019 Leach], local equilibrium of carbon at the ferrite/austenite is sought, and a finite interfacial friction term is added to the dissipation terms. Otherwise the two methods are both based on a driving-force–dissipation balance and the Zener-Hillert equation, with a unique lengthening rate determined by maximizing it with respect to radius of curvature at the plate tip.

The Bainite Model also considers the case where cementite (under the “para” condition) can precipitate on the ferrite/austenite interface and grow into ferrite, forming a ferrite-cementite mixture. The formation of para-cementite usually accelerates lengthening, by enlarging the driving force of transformation while reducing carbon partitioning from bainite to austenite. Carbon partitioning to austenite vanishes if para-cementite forms in bainite to its maximum fraction allowed by mass balance.

Thickening of bainitic plates is usually much slower than lengthening. In the Bainite Model, it is assumed that whenever there is a positive driving force of precipitating para-cementite on the ferrite/austenite interface, the final state of the bainite transformation should be a mixture of ferrite and cementite, with austenite being completely transformed. Otherwise, the final state is a ferrite-austenite mixture with no cementite but a finite fraction of retained austenite (incomplete transformation).

The overall kinetics of bainite transformation is calculated in the extended-volume approach devised by Cahn [1956] and generalized for ellipsoids. Both grain boundary (GB) nucleation and volume nucleation are considered, the former being very temperature-sensitive, the latter temperature-insensitive. This is used to model the kinks at about 350 °C in the TTT diagrams of some medium- and high-carbon steels—At higher temperatures GB nucleation is predominant, whereas at lower temperatures it is effectively suppressed, and volume nucleation becomes significant.



For an example of the Bainite Model, see PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite



The input parameters are entered on the Configuration window for the Property Model Calculator. There are also additional axis variables available on the Plot Renderer. See Bainite Property Model Settings for details.

References

[1956 Cahn] J. W. Cahn, “The kinetics of grain boundary nucleated reactions”, Acta Metallurgica 4, 449–459 (1956).

[2018 Leach] L. Leach, P. Kolmskog, L. Höglund, M. Hillert, and A. Borgenstam, “Critical driving forces for formation of bainite”, Metallurgical and Materials Transactions A 49, 4509–4520 (2018).

[2019 Leach] L. Leach, J. Ågren, L. Höglund, and A. Borgenstam, “Diffusion-controlled lengthening rates of bainitic ferrite a part of the Steel Genome”, Metallurgical and Materials Transactions A 50, 2613–2618 (2019)

Bainite Property Model Settings

The **Bainite** Property Model, available when using the Property Model Calculator in Thermo-Calc, describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. In this Model, bainite is modeled as ferrite or a ferrite-cementite mixture.

Considered elements: Fe, C, Mn, Si, Cr, Ni, Mo. Other elements in the system are neglected for bainite by mass percent.

About the Bainite Property Model

For an example, see PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite.

Configuration Settings

These settings are found on the Property Model Calculator when **Bainite** is selected under **Steel Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

Austenite Composition From

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide or ferrite, before pearlite starts to form in austenite. But the Model only considers the effect of other phase(s) on austenite composition.

Austentizing Temperature

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under Condition Definitions.

Grain Size

Enter the **Grain size** of the austenite in micrometers (µm). The default is 100 µm.

Plot Renderer Settings

- Plot Renderer and Configuration Settings
- Steel Library TTT Diagram Template and Plot Settings: TTT Mode

When setting up your calculation on the Plot Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- Start time (2% bainite)
- Half time (50% bainite)
- Finish time (98% bainite)
- Lengthening rate
- Bainite start temperature
- Cementite fraction in bainite
- Retained austenite fraction

About the CCT Diagram Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The **CCT Diagram** Property Model, available when using the Property Model Calculator in Thermo-Calc, can be used to calculate a Continuous-Cooling-Transformation (CCT) diagram, with a *One-axis* calculation on Log10(cooling rate[K/s]). This Model calculates the kinetics of concurrent transformation of austenite into pearlite, bainite, and martensite. The algorithms and parameters for pearlite, bainite, and martensite are the same as in their individual Property Models (Pearlite, Bainite, Martensite Temperatures, and Martensite Fractions), but the competitive occupation of prior austenite grain boundaries and bulk volume is handled in the **CCT Diagram** Property Model.

For an example, see PM_Fe_08: CCT Diagram Property Model.

The input parameters are entered on the Configuration window for the Property Model Calculator. There are also additional axis variables available on the Plot Renderer.

CCT Diagram Property Model Settings

The **CCT Diagram** Property Model, available when using the Property Model Calculator in Thermo-Calc, calculates the concurrent transformations to pearlite, bainite, and martensite under continuous cooling conditions and is used to construct a continuous-cooling-transformation (CCT) diagram.

- About the CCT Diagram Property Model

For an example, see PM_Fe_08: CCT Diagram Property Model.

Configuration Settings

These settings are found on the Property Model Calculator when **CCT Diagram** is selected under **Steel Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

- For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

Austenite Composition From

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide or ferrite, before pearlite starts to form in austenite. But the Model only considers the effect of other phase(s) on austenite composition.

Austentizing Temperature

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under Condition Definitions.

Grain Size

Enter the **Grain size** of the austenite in micrometers (μm). The default is 100 μm.

Start Temperature

Enter a **Start temperature**, which is the temperature at time zero where cooling starts.

End Temperature

Enter an **End temperature**, which is the lowest temperature where cooling stops. Cooling may also stop before reaching this temperature if austenite has fully transformed (>98%).

Log10(cooling rate [K/s])

Enter a **Log10(cooling rate [K/s])** , which is the 10-base logarithm of cooling rate in K/s.



The unit must be Kelvin per second, and it does NOT follow the unit selection in the GUI. This is the *Axis Quantity* if a CCT diagram is to be constructed.

Calculation Setting

Select **Quick** (the default), **Accurate**, or **Custom** to balance accuracy and calculation time. Choose **Custom** to define the numerical settings yourself, which are otherwise set in the background when **Quick** or **Accurate** is selected. See the separate section below about the details for the **Custom** settings.

Quick Calculation Setting

Quick is used for a relatively quick and rough calculation to reveal the general feature of a CCT diagram. Interpolation is used when necessary, in order to avoid calculating the growth rates and nucleation rates of pearlite and bainite at every time step. Pearlite mode is Parapearlite for its simplicity. Calculation time may vary between 30 minutes and several hours.

Accurate Calculation Setting

Accurate evaluates the growth rates and nucleation rates at every time step accurately (without interpolation). The time step control is also tighter than when using the **Quick** setting. Pearlite mode is Optimal Pearlite, but its rate calculation becomes slower if austenite contains many alloying elements. Calculation time may vary between several hours and tens of hours.

Details about the Quick and Accurate Calculation Settings

When you choose **Quick** or **Accurate** as the calculation setting, the following is what is automatically set in the background for each of the sections. These sections are visible to you and also can be edited when **Custom** is chosen:

Setting	Quick	Accurate
Pearlite check box	check box selected (yes)	check box selected (yes)
Bainite check box	check box selected (yes)	check box selected (yes)
Martensite check box	check box selected (yes)	check box selected (yes)

Setting	Quick	Accurate
Pearlite criterion	Maximize growth rate	Maximize growth rate
Pearlite mode	Para-pearlite	Optimal pearlite
Use interpolation when necessary check box	check box selected (yes)	check box NOT selected (no)
Interpolation error tolerance	0.1	(does not apply)
Maximum phase fraction change (absolute) in a time step	0.005	0.005
Maximum phase fraction change (relative) in a time step	0.05	0.05
Error tolerance for austenite fraction	1E-3	1E-4

Custom Calculation Setting

The following settings are available when **Custom** is selected as the *Calculation Setting*. Otherwise these settings are handled in the background as described above for when **Quick** or **Accurate** is selected.

Pearlite/Bainite/Martensite check boxes

By default the **Pearlite**, **Bainite**, and **Martensite** check boxes are selected. Click to deselect as required to exclude it from the CCT Diagram calculation.

Pearlite Criterion

This setting is available when the **Pearlite** check box is selected.

Select an option from the **Pearlite criterion** list to determine the pearlite growth condition.

For **Maximize growth rate**, pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives maximal growth rate and minimal lamellar spacing. This is the default criterion.

For **Maximize Gibbs energy dissipation rate**, Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives a

smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.

Pearlite Mode

This setting is available when the **Pearlite** check box is selected.

This setting is to determine how substitutional alloying elements partition between ferrite and cementite in pearlite. Select an option from the **Pearlite mode** list.

For **Optimal pearlite**, the partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.

For **Para-pearlite**, ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.

For **Ortho-pearlite**, ferrite and cementite are in ortho-equilibrium.

Use Interpolation When Necessary

If the **Use interpolation when necessary** check box is selected, and depending on alloy composition and temperature, if the code determines that an interpolation is necessary, then a composition grid (TTT diagram) or composition-temperature grid (CCT diagram) is generated and refined as needed. The growth rates and nucleation rates of pearlite and bainite, as functions of composition (TTT diagram) or composition and temperature (CCT diagram), are determined by interpolation (if sufficiently accurate). This is intended to avoid direct calculations of pearlite and bainite rates for every time step, which is usually time-consuming.



For a good usage of interpolation grid, cooling rates should not be too few. Otherwise it may be possible that grid calculations are more than actually needed during the cooling trajectories, causing a waste of calculation time. Also, the interpolation grid is only for a one alloy composition with varying cooling rate. Varying other quantities than cooling rate may lead to erroneous results.

Interpolation Error Tolerance

This setting is available when the **Use interpolation when necessary** check box is selected.

The growth and nucleation rates of pearlite and bainite, if determined from interpolation, are accepted only when the relative interpolation error estimated is below the value entered here. A large number implies few grid points necessary (shorter calculation time) and lower accuracy, and a small number implies the opposite.

Maximum Phase Fraction Change (Absolute/Relative) in a Time Step

The **Maximum phase fraction change (absolute) in a time step** and **Maximum phase fraction change (relative) in a time step** settings are used to control time step size during time integration.

The phase fraction (X) of pearlite and bainite cannot change more than `atol + X * rtol` during a time step, where `atol` and `rtol` are the absolute and relative maximum change, respectively. If the change is too large, the new time step is rejected, and time integration is retried with a smaller time step.

Error Tolerance for Austenite Fraction

The **Error tolerance for austenite fraction** setting is used to control the accuracy for austenite fraction during time integration. Finite time steps cause an error in austenite volume fraction. When the error is larger than the tolerance, time integration is backed up and retried with a smaller time step.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer, the following axis variables result quantities are available for the conditions defined on the Property Model Calculator.

Each quantity is defined in both time and temperature:

- Pearlite start (2%), time (t) and temperature (T)
- Bainite start (2%), time (t) and temperature (T)
- Martensite start, time (t) and temperature (T)
- Austenite transformed 50%, time (t) and temperature (T)
- Austenite transformed 98%, time (t) and temperature (T)

The **CCT mode** on the Plot Renderer the time-temperature pairs are automatically identified and arranged in the plot to give a CCT diagram. Selected cooling curves are also given in the CCT Mode.

About the Critical Transformation Temperatures Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Critical Transformation Temperatures is a Property Model available when using the Property Model Calculator in Thermo-Calc. Use it to calculate critical transformation temperatures for steels under equilibrium conditions.

For an example, see PM_Fe_04: Critical Temperatures.

This Property Model can output the transformation temperatures for the following:

- Liquidus: First austenite or ferrite transformation from the liquid
- Solidus: Liquid fully transformed to solid
- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)
- A4: Delta-ferrite (BCC_A2) transforms to austenite (FCC_A1)
- Acem: Austenite (FCC_A1) transforms to cementite. Requires that the **Suspend graphite** check box is selected on the Configuration window, which it is by default.
- Agraph: Austenite (FCC_A1) transforms to graphite. Requires that the **Suspend graphite** check box is NOT selected on the Configuration window, i.e. graphite is not suspended.

The input parameters are entered on the Configuration window for the Property Model Calculator and described in Critical Transformation Temperatures Property Model Settings.

Critical Transformation Temperatures Property Model Settings

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

- About the Critical Transformation Temperatures Property Model

For an example, see PM_Fe_04: Critical Temperatures.

Critical Transformation Temperatures is a Property Model available when using the Property Model Calculator in Thermo-Calc. Use it to calculate critical transformation temperatures for steels under equilibrium conditions.

Configuration Settings

These settings are found on the Property Model Calculator when **Critical Transformation Temperatures** is selected under **Steel Models**.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

- For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

Calculate Solidus and Liquidus

Select the **Calculate solidus and liquidus** check box to calculate these temperatures.

Calculate Ax Temperatures

Select the **Calculate Ax temperatures** check box to calculate A0, A1, A3, Acem, and Agraph temperatures. Typically, only one temperature of A3, Acem, and Agraph exists. See below for additional details about these temperatures.

- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)
- A4: Delta-ferrite (BCC_A2) transforms to austenite (FCC_A1)
- Acem: Austenite (FCC_A1) transforms to cementite (requires that the **Suspend graphite** check box is selected, which it is by default)
- Agraph: Austenite (FCC_A1) transforms to graphite (requires that the **Suspend graphite** check box is NOT selected, i.e. graphite is not suspended)

Suspend Graphite

By default the **Suspend graphite** check box is selected and suspends the graphite phase. Click to clear the check box as needed to enable the graphite.

Suspend Gas

By default the **Suspend gas** check box is selected and suspends the gas phase. Click to clear the check box as needed.

Manual Temperature Search Limits

By default the temperature search limits are automatically defined. Select the **Manual temperature search limits** check box to manually change the limits for the **Lower temperature search limit**, **Upper temperature search limit**, and **Max temperature step**. Is

given in the same unit as the temperature in the **Condition Definitions**.

Lower and Upper Temperature Search Limits

These settings are available when the **Manual temperature search limits** check box is selected.

In the **Lower temperature search limit** and **Upper temperature search limit** fields enter temperature values to search the lower and upper limits of transformation temperatures.

Max Temperature Step

This setting is available when the **Manual temperature search limits** check box is selected.

In the **Max temperature step** field, enter the largest temperature step. This is most often reduced when changes in driving force or the amount of the phases indicate a phase transformation at a shorter temperature step.

About the Martensite Fractions Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The **Martensite Fractions** Property Model is a Property Model available when using the Property Model Calculator in Thermo-Calc. It calculates fraction of athermal martensite based on an analytical equation derived in Huyan et al. [2016, Huyan]. It is assumed that the first forming martensite morphology is the only forming one. The first morphology is determined based on the Ms-temperatures of all morphologies.

For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing.

- The input parameters are entered on the Configuration window for the Property Model Calculator and described in Martensite Fractions Property Model Settings.

Reference

[2016, Huyan] F. Huyan, P. Hedström, L. Höglund, A. Borgenstam, A Thermodynamic-Based Model to Predict the Fraction of Martensite in Steels. Metall. Mater. Trans. A. 47, 4404–4410 (2016).

Martensite Fractions Property Model Settings

The **Martensite Fractions** Property Model is a Property Model available when using the Property Model Calculator in Thermo-Calc.

- About the Martensite Fractions Property Model

Configuration Settings

The settings are found on the Property Model Calculator when **Martensite Fractions** is selected under **Steel Models**.



For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing.



When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Intercritical Annealing

From the **Intercritical annealing** list select **No** if the specified composition is used directly or select **Yes** to assume intercritical annealing. For **Yes**, an equilibrium calculation is performed at the specified temperature and the composition of the austenite phase is used for the martensite temperature calculation.

Annealing Temperature

This setting is available when **Yes** is selected from the **Intercritical annealing** list.

Enter an **Annealing temperature** in the field. The unit is the same as that selected under Condition Definitions.

Grain Size [µm]

In the **Grain size [µm]** field enter the grain size of the austenite phase in µm. By default 100 µm is set. The Ms temperature and thus the martensite fractions change for significantly smaller grain sizes.

Parent Phase Gibbs Energy Addition

In the **Parent phase Gibbs energy addition [J/mol]** field enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is 0 J/mol.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- **Total martensite percentage**
- **Retained austenite percentage**

About the Martensite Temperatures Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The **Martensite Temperatures** is a Property Model available when using the Property Model Calculator in Thermo-Calc. The Model calculates the martensite start temperature (Ms) based on modeling the transformation barrier with fitted analytical equations. It is based on Stormvinter et al. [2012, Stormvinter] with subsequent update and extension by Gulapura Hanumantharaju [2017, Gulapura] and Thermo-Calc internal assessment. The partitionless equilibrium temperature T_0 is calculated using the thermodynamic database. The Model also gives temperatures corresponding to 50%, 90%, and 99% transformations.

Martensite fractions are calculated with the same algorithm as in the **Martensite Fractions** Property Model.

For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing and PM_Fe_02: Fe-Mn Martensite Morphologies.

- The input parameters are entered on the Configuration window for the Property Model Calculator and described in Martensite Temperatures Property Model Settings.

References

[2012, Stormvinter] A. Stormvinter, A. Borgenstam, J. Ågren, Thermodynamically Based Prediction of the Martensite Start Temperature for Commercial Steels. Metall. Mater. Trans. A. 43, 3870–3879 (2012).

[2017, Gulapura] A. K. Gulapura Hanumantharaju, Master's thesis, KTH Royal Institute of Technology (2017).

Martensite Temperatures Property Model Settings

Martensite Temperatures is a Property Model available when using the Property Model Calculator in Thermo-Calc. It calculates the martensite start (Ms) temperature based on modeling of the transformation barrier. Martensite half and finish temperatures are also given according to the Martensite Fractions Property Model.

- About the Martensite Temperatures Property Model

Configuration Settings

The settings are found on the Property Model Calculator when **Martensite Temperatures** is selected under **Steel Models**.

For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing and PM_Fe_02: Fe-Mn Martensite Morphologies.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Intercritical Annealing

From the **Intercritical annealing** list select **No** if the specified composition is used directly or select **Yes** to assume intercritical annealing. For **Yes**, an equilibrium calculation is performed at the specified temperature and the composition of the austenite phase is used for the martensite temperature calculation.

Annealing Temperature

This setting is available when **Yes** is selected from the **Intercritical annealing** list.

Enter an **Annealing temperature** in the field. The unit is the same as that selected under Condition Definitions.

Grain Size [µm]

In the **Grain size [µm]** field enter the grain size of the austenite phase in µm. By default 100 µm is set. The Ms temperature and thus the martensite fractions change for significantly smaller grain sizes.

Parent Phase Gibbs Energy Addition

In the **Parent phase Gibbs energy addition [J/mol]** field enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is 0 J/mol.

Plot Renderer Settings

- Plot Renderer and Configuration Settings
- Steel Library TTT Diagram Template and Plot Settings: TTT Mode

When setting up your calculation on the Plot Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- **Ms**: Martensite start temperature
- **Lath Ms**: Martensite start temperature of lath alpha or alpha-prime martensite
- **Plate Ms**: Martensite start temperature of plate alpha or alpha-prime martensite
- **Epsilon Ms**: Martensite start temperature of epsilon martensite

- **M50**: 50% martensite temperature
- **M90**: 90% martensite temperature
- **M99**: 99% martensite temperature

About the Pearlite Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The **Pearlite** Property Model [2020, Yan] is available when using the Property Model Calculator in Thermo-Calc and is part of the Steel Model Library. It calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.

For an example see PM_Fe_03: Fe-C-Mn Pearlite.

The **Pearlite** Model describes the thermodynamics and kinetics of pearlite formation from austenite. It is assumed that the overall composition of pearlite is the same as the austenite composition, and growth rate is constant over time. Growth rate and lamellar spacing of pearlite are determined by a criterion where either growth rate or Gibbs energy dissipation rate is maximized. The Model considers Gibbs energy dissipation due to formation of ferrite-cementite interface in pearlite, finite austenite-pearlite interfacial mobility, solute drag, and diffusion of elements within austenite and along austenite-pearlite interface.

Divergent pearlite, of which growth rate and lamellar spacing change with time, is not considered. This Model only considers the transformation from FCC_A1 phase to pearlite consisting of BCC_A2 and CEMENTITE_D011 (for TCFE9 this is CEMENTITE). Pearlite with other phases is not implemented.

Pearlite is assumed to nucleate on austenite grain boundaries. Grain boundary nucleation rate is modeled as a function of composition and temperature. The isothermal transformation kinetics follows Cahn [1956, Cahn]. Start, half, and finish times are taken as 2%, 50%, and 98% transformation, respectively.

Austenite composition can be taken either as the nominal composition or from an equilibrium calculation at an austenitization temperature. The latter option can be useful when austenite coexists with other phase(s), e.g. primary carbide or ferrite, before pearlite starts to form in austenite. But the Model only considers the effect of other phase(s) on austenite composition.

Model parameters have been determined from published data of maximal growth rate, minimal lamellar spacing, partition coefficients, and isothermal transformation kinetics in ternary and multicomponent systems.



The input parameters are entered on the Configuration window for the Property Model Calculator and described in Pearlite Property Model Settings.



The included elements in the Pearlite Property Model are Fe (dependent element), C, Mn, Cr, Mo, W, Si, Al, Ni, Co. Other elements are neglected by weight percent.

References

[1956, Cahn] J. W. Cahn, The kinetics of grain boundary nucleated reactions. Acta Metall. 4, 449–459 (1956).

[2020, Yan] J.-Y. Yan, J. Ågren, J. Jeppsson, Pearlite in Multicomponent Steels: Phenomenological Steady-State Modeling. Metall. Mater. Trans. A. 51, 1978–2001 (2020).

Pearlite Property Model Settings

The **Pearlite** Property Model [2020, Yan] is available when using the Property Model Calculator in Thermo-Calc and is part of the Steel Model Library. It calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.

The included elements in the Pearlite Property Model are Fe (dependent element), C, Mn, Cr, Mo, W, Si, Al, Ni, Co. Other elements are neglected by weight percent.

About the Pearlite Property Model

Configuration Settings

The settings are found on the Property Model Calculator when **Pearlite** is selected under **Steel Models**.

For an example see PM_Fe_03: Fe-C-Mn Pearlite.

When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

Austenite Composition From

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide or ferrite, before pearlite starts to form in austenite. But the Model only considers the effect of other phase(s) on austenite composition.

Austentizing Temperature

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under Condition Definitions.

Pearlite Criterion

Select an option from the **Pearlite criterion** list to determine the pearlite growth condition.

For **Maximize growth rate**, pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives maximal growth rate and minimal lamellar spacing. This is the default criterion.

For **Maximize Gibbs energy dissipation rate**, Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives a smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.

Pearlite Mode

This setting is to determine how substitutional alloying elements partition between ferrite and cementite in pearlite. Select an option from the **Pearlite mode** list.

For **Optimal pearlite**, the partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.

For **Para-pearlite**, ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.

For **Ortho-pearlite**, ferrite and cementite are in ortho-equilibrium.

Grain Size [µm]

In the **Grain size [µm]** field enter the austenite grain size in µm. By default 100 µm is set.

Plot Renderer Settings

- Plot Renderer and Configuration Settings
- Steel Library TTT Diagram Template and Plot Settings: TTT Mode

When setting up your calculation on the Plot Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- Growth rate
- Lamellar spacing
- Cementite molar fraction in pearlite
- Driving force of pearlite formation
- Start time (2% pearlite)
- Half time (50% pearlite)
- Finish time (98% pearlite)

About the TTT Diagram Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The **TTT Diagram** Property Model, available when using the Property Model Calculator, can be used to calculate a Time-Temperature-Transformation (TTT) diagram, with a *One-axis* calculation on Temperature. The Model calculates the isothermal kinetics of concurrent transformation of austenite into pearlite, bainite, and martensite. The algorithms and parameters for pearlite, bainite, and martensite are the same as in the individual Property Models (Pearlite, Bainite, Martensite Temperatures, and Martensite Fractions), but the competitive occupation of prior austenite grain boundaries and bulk volume is handled in the **TTT Diagram** Property Model.

If the reaction temperature is below martensite-start temperature (Ms), it is assumed that a fraction of (athermal) martensite according to the calculation forms instantaneously at time zero, prior to the formation of bainite and/or pearlite. Otherwise austenite transforms to bainite and/or pearlite.

For an example see PM_Fe_06: TTT Diagram Property Model

The input parameters are entered on the Configuration window for the Property Model Calculator. There are also additional axis variables available on the Plot Renderer.

TTT Diagram Property Model Settings

The **TTT Diagram** Property Model, available when using the Property Model Calculator in Thermo-Calc, calculates the concurrent transformations to pearlite, bainite, and martensite under isothermal conditions and is used to construct a time-temperature-transformation (TTT) diagram.

- About the TTT Diagram Property Model

For an example see PM_Fe_06: TTT Diagram Property Model

Configuration Settings

These settings are found on the Property Model Calculator when **TTT Diagram** is selected under **Steel Models**.

> When working in the Configuration window, click the **Description** tab for more information about the Model. When the Property Model is not encrypted, or it is a user-defined Property Model, there is also a **Python code** tab that displays the related code.

- For details about the Condition Definitions and Calculation Type settings, see Configuration Window Settings

Austenite Composition From

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide or ferrite, before pearlite starts to form in austenite. But the Model only considers the effect of other phase(s) on austenite composition.

Austentizing Temperature

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under Condition Definitions.

Grain Size

Enter the **Grain size** of the austenite in micrometers (µm). The default is 100 µm.

Calculation Setting

Select **Quick** (the default), **Accurate**, or **Custom** to balance accuracy and calculation time. Choose **Custom** to define the numerical settings yourself, which are otherwise set in the background when **Quick** or **Accurate** is selected. See the separate section below about the details for the **Custom** settings.

Quick Calculation Setting

Quick is used for a relatively quick and rough calculation to reveal the general feature of a TTT diagram. Interpolation is used when necessary, in order to avoid calculating the growth rates and nucleation rates of pearlite and bainite at every time step. Pearlite mode is Parapearlite for its simplicity. Recommended temperature interval: 50-100K. Each temperature can take several minutes.

Accurate Calculation Setting

Accurate evaluates the growth rates and nucleation rates at every time step accurately (without interpolation). The time step control is also tighter than when using the **Quick** setting. Pearlite mode is Optimal Pearlite, but its rate calculation becomes slower if austenite contains many alloying elements. Recommended temperature interval: 20-50K or even lower. Calculating the whole TTT diagram may take several hours.

Details about the Quick and Accurate Calculation Settings

When you choose **Quick** or **Accurate** as the calculation setting, the following is what is automatically set in the background for each of the sections. These sections are visible to you and also can be edited when **Custom** is chosen:

Setting	Quick	Accurate
Pearlite check box	check box selected (yes)	check box selected (yes)
Bainite check box	check box selected (yes)	check box selected (yes)
Martensite check box	check box selected (yes)	check box selected (yes)
Pearlite criterion	Maximize growth rate	Maximize growth rate
Pearlite mode	Para-pearlite	Optimal pearlite
Use interpolation when necessary check box	check box selected (yes)	check box NOT selected (no)
Interpolation error tolerance	0.1	(does not apply)
Maximum phase fraction change (absolute) in a time step	0.005	0.005
Maximum phase fraction change (relative) in a time step	0.05	0.05

Setting	Quick	Accurate
Error tolerance for austenite fraction	1E-3	1E-4

Custom Calculation Setting

The following settings are available when **Custom** is selected as the *Calculation Setting*. Otherwise these settings are handled in the background as described above for when **Quick** or **Accurate** is selected.

Pearlite/Bainite/Martensite check boxes

By default the **Pearlite**, **Bainite**, and **Martensite** check boxes are selected. Click to deselect as required to exclude it from the TTT Diagram calculation.

Pearlite Criterion

This setting is available when the **Pearlite** check box is selected.

Select an option from the **Pearlite criterion** list to determine the pearlite growth condition.

For **Maximize growth rate**, pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives maximal growth rate and minimal lamellar spacing. This is the default criterion.

For **Maximize Gibbs energy dissipation rate**, Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives a smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.

Pearlite Mode

This setting is available when the **Pearlite** check box is selected.

This setting is to determine how substitutional alloying elements partition between ferrite and cementite in pearlite. Select an option from the **Pearlite mode** list.

For **Optimal pearlite**, the partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.

For **Para-pearlite**, ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.

For **Ortho-pearlite**, ferrite and cementite are in ortho-equilibrium.

Use Interpolation When Necessary

If the **Use interpolation when necessary** check box is selected, and depending on alloy composition and temperature, if the code determines that an interpolation is necessary, then a composition grid (TTT diagram) or composition-temperature grid (CCT diagram) is generated and refined as needed. The growth rates and nucleation rates of pearlite and bainite, as functions of composition (TTT diagram) or composition and temperature (CCT diagram), are determined by interpolation (if sufficiently accurate). This is intended to avoid direct calculations of pearlite and bainite rates for every time step, which is usually time-consuming.

Interpolation Error Tolerance

This setting is available when the **Use interpolation when necessary** check box is selected.

The growth and nucleation rates of pearlite and bainite, if determined from interpolation, are accepted only when the relative interpolation error estimated is below the value entered here. A large number implies few grid points necessary (shorter calculation time) and lower accuracy, and a small number implies the opposite.

Maximum Phase Fraction Change (Absolute/Relative) in a Time Step

The **Maximum phase fraction change (absolute) in a time step** and **Maximum phase fraction change (relative) in a time step** settings are used to control time step size during time integration.

The phase fraction (X) of pearlite and bainite cannot change more than `atol + X * rtol` during a time step, where `atol` and `rtol` are the absolute and relative maximum change, respectively. If the change is too large, the new time step is rejected, and time integration is retried with a smaller time step.

Error Tolerance for Austenite Fraction

The **Error tolerance for austenite fraction** setting is used to control the accuracy for austenite fraction during time integration. Finite time steps cause an error in austenite volume fraction. When the error is larger than the tolerance, time integration is backed up and retried with a smaller time step.

Plot Renderer Settings

- Plot Renderer and Configuration Settings
- Steel Library TTT Diagram Template and Plot Settings: TTT Mode

When setting up your calculation on the Plot Renderer, the following result quantities are available for the conditions defined on the Property Model Calculator.

- Pearlite start (2%)
- Bainite start (2%)
- Austenite transformed 50%
- Austenite transformed 98%
- Martensite start
- Martensite 50%
- Martensite 98%

The Pearlite start (2%), Bainite start (2%), Austenite transformed 50%, and Austenite transformed 98% are time quantities. Martensite start, Martensite 50%, and Martensite 98% are temperature quantities.

In the TTT Mode of a Plot Renderer, the three temperature quantities for martensite are plotted as horizontal lines because they are independent of time. The other time quantities are plotted as functions of temperature.

The Process Metallurgy Module

Process Metallurgy Module Examples Collection

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About the Process Metallurgy Module

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

The Process Metallurgy Module is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Process Metallurgy Calculator*. The Add-on Module is designed to model reactions that occur in metallurgical processes. Although primarily used in steelmaking and steel refining processes—such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy, and so forth—applications are not limited to steelmaking.

There are two main branches of calculations possible: **Equilibrium** and **Process simulation**. Equilibrium calculations do not consider any kinetics, the process simulation includes reaction kinetics.

In general, for both types, the main difference compared to using a standard Equilibrium Calculator is that it is easy to handle the different materials present in a metallurgical process. The materials used in the process can be pre-defined, saved and used for the equilibrium calculations. Metallic materials can be defined in element weight percent, oxide materials in weight percent of oxide components, the gas phase in volume percent of gas components and its amount can be defined in normal cubic meters, and so forth. In principle this can be done in a standard Equilibrium Calculator. However, it is much easier when using the Process Metallurgy Calculator as this is designed for this specific purpose.

When using the **Equilibrium** branch of calculations, both isothermal and adiabatic calculations are possible. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction, meaning that the temperature changes as a result of exothermal or endothermal reactions taking place.

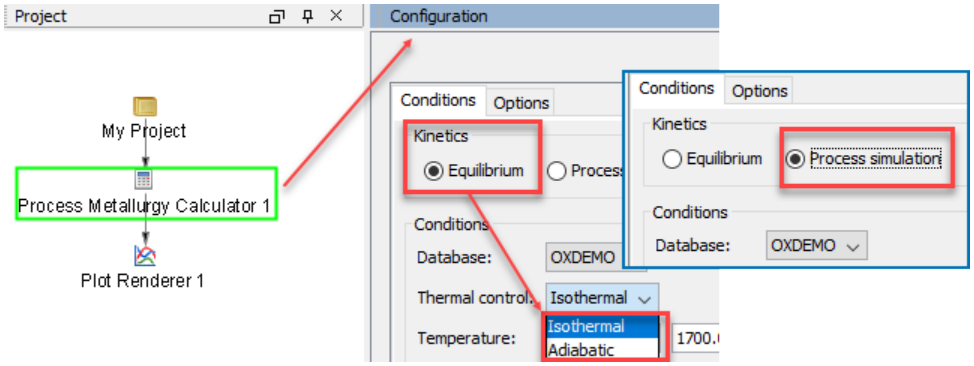
For a **Process simulation** branch of calculation, the reaction kinetics of the process are considered. This is done by dividing the system into zones. Typically one would have one steel zone containing liquid metal and a slag zone containing liquid oxide (slag). The kinetic model assumes that only a fraction of the steel zone reacts with a fraction of the slag zone per time step. This reacting fraction of the whole system is termed the reaction zone (in literature it has become known as Effective Equilibrium Reaction Zone or EERZ).

You can use the Process Metallurgy Module to calculate the following:

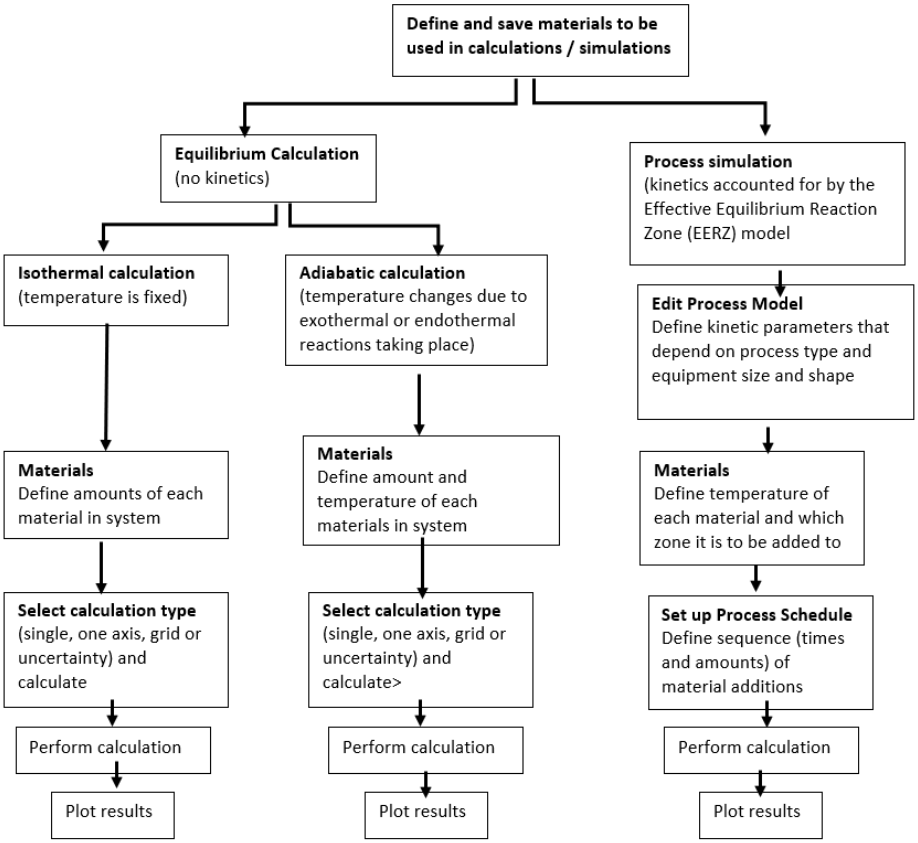
- The equilibrium between custom-defined steels, slags, and gasses.
- The equilibrium between other metallic and non-metallic phases.
- Desulfurization, dephosphorization, and decarburization.
- Any partition coefficient, for example the partitioning of sulfur between the liquid steel and slag phase.
- Slag characteristics, such as slag basicity or sulfur capacity.
- The fraction of liquid and solid in the slag.
- The temperature change in an adiabatic process.
- Kinetics of the reaction between phases. Typically this is the reaction between a liquid metal and slag phase, but it could also be the reaction between a solid oxide and slag (simulation of refractory wear) or between a solid metal and liquid metal (simulation of dissolution of alloy), etc.

Setting Up a Process Metallurgy Simulation

The following basic steps need to be carried out to set up calculations in the **Process Metallurgy Calculator**. There are three branches of simulation to choose from on the **Configuration** window when setting up the simulation an isothermal equilibrium calculation, an adiabatic equilibrium calculation, and a process simulation.



Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.



The three branches of simulations available for the Process Metallurgy Calculator (1) an isothermal equilibrium calculation, (2) an adiabatic equilibrium calculation, and (3) a process simulation.

Equilibrium Simulations

Two **Equilibrium** simulation types are available: **Isothermal** and **Adiabatic**. In general for the equilibrium simulation, the three most common material groups—*Steel*, *Slag*, and *Gas* are automatically included with the default composition input types that are relevant to each material group. You can add materials and save your material compositions directly from the Process Metallurgy Calculator and quickly access these for other simulations. For example, you might want to predefine compositions of steels, ferro-alloys, slags, and slag additions. The overall composition of the steel and slag is then obtained by adding amounts of these predefined materials.

Each group of materials is automatically added to the similar group where it is defined. You can manage these groups using the *Material Manager* (see Working with the Material Manager).

For adiabatic calculations, the selection of material type (steel, slag, gas) has an influence on the calculation. For isothermal calculations, the results are identical.

The reason the selection of materials for adiabatic calculations has an influence is because there are different strategies to calculate the enthalpy of the materials at the temperature at which these are added. Therefore, defining FeO as a *steel* containing 50at% Fe and 50at% O or as a *slag* with 50at% Fe and 50at% O or as *slag* with 100% FeO, all result in different enthalpies assigned to the component FeO, which in turn results in different equilibrium temperatures.

- Defining the Equilibrium Simulation
- Equilibrium Simulation: Conditions Tab
- Adiabatic Calculations: Material Enthalpy

Process Simulations

When you choose to do a **Process simulation** it includes the reaction kinetics. Using the EERZ (Effective Equilibrium Reaction Zone) model, you can first define your materials as you do with an **Equilibrium** simulation. You also need to define the **Process model** where you define the kinetic parameters of the simulation by setting up reaction zones, reaction rates, heat transfer coefficients, and so forth. You also need to define the **Process schedule** where the sequence and amounts of added materials are defined.

- Defining the Process Simulation
- Process Simulation: Conditions Tab

Calculation Types

The calculations available for an **Equilibrium** simulation, for both isothermic and adiabatic calculations, are *Single* equilibrium, *One axis*, *Grid*, and *Uncertainty*. After adding a **Plot Renderer** or **Table Renderer**, you can choose a variety of quantities, including slag properties such as Bells ratio and B2, to output results that provide useful visual representations of the steelmaking systems being analyzed.

- Process Metallurgy Calculator and Defining the Equilibrium Simulation



You can find several learning resources on the Process Metallurgy page of our website (or in Thermo-Calc, go to **Help → Thermo-Calc website**). You can also subscribe to the Thermo-Calc newsletter to be kept up-to-date about upcoming releases, training, examples, videos and much more.

Working with the Process Metallurgy Module

Working with the **Process Metallurgy Calculator** allows you to easily define complex metallurgical reactions. The calculator streamlines how you set up these steel and slag systems but there are details about various inputs and outputs that are different from other calculators. This topic is a general collection of information related to the Process Metallurgy Module and is intended to help you better understand how to interpret and make choices when you are setting up your steelmaking simulation.

Database Dependency



It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

Material Manager

For information about saving and deleting materials used with the Process Metallurgy Calculator, see Working with the Material Manager. Also see the next section.

Working with Material Groups (Steel, Slag, and Gas)

- For more details about these fields, see Defining the Equilibrium Simulation.
- For information about saving and deleting materials, see Working with the Material Manager.

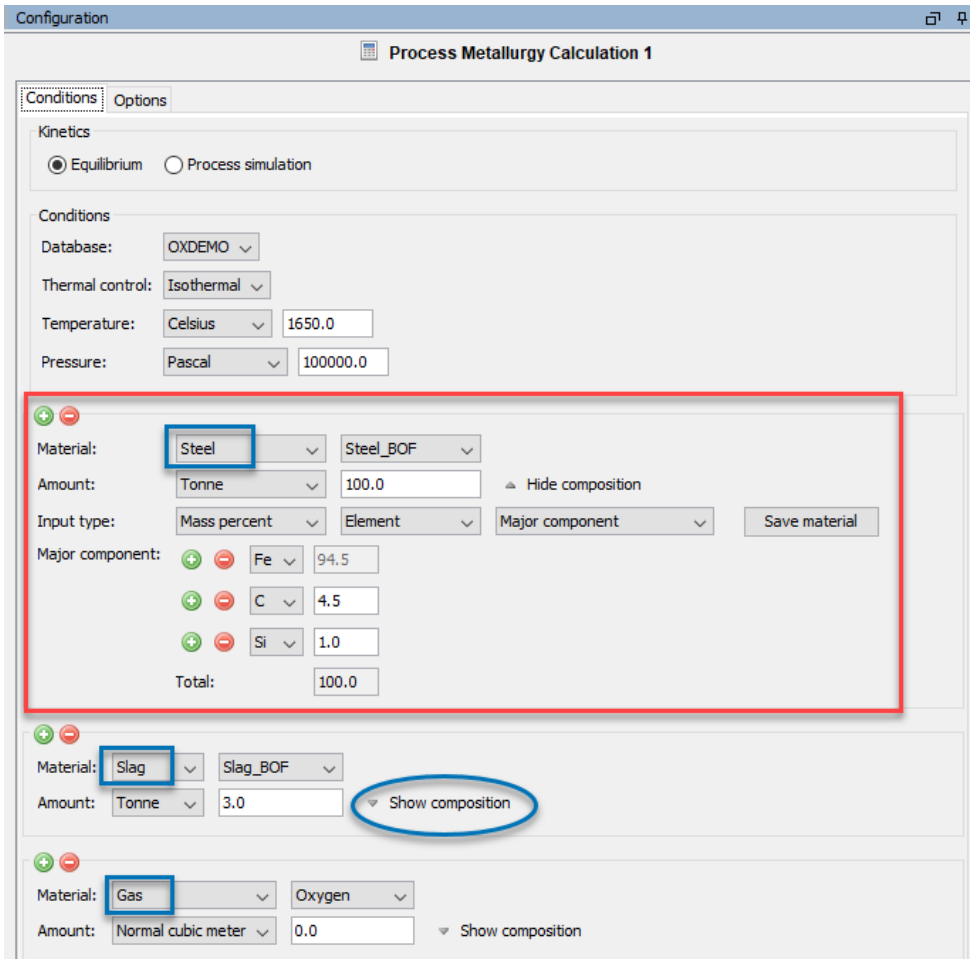
There are three groups to define: **Steel** (or another user-defined **Metal** group), **Slag**, and **Gas**.



It is recommended you open the PMET_01: Basic Oxygen Furnace (BOF) example to follow along with the descriptions.

Open the example project file(s) from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_01_Basic_Oxygen_Furnace.tcu**. Choose a, b, or c versions of the example based on whether you have a license for the TCOX database.

In the image below, the red-highlighted area is where the Steel material group is defined. The drop-down menu that displays *Steel_BOF* shows a user-defined material. This can be defined and then saved to the material library.

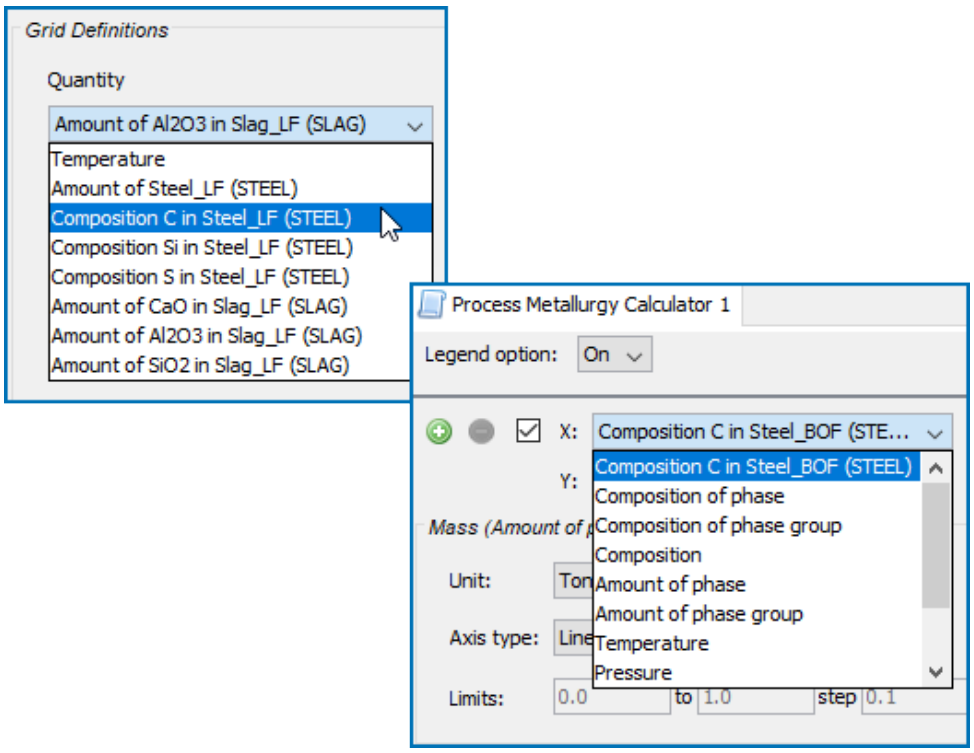


The three material group areas on the Process Metallurgy Calculator where you can define components and save materials. You can create your own material groups using the Material Manager.

When you click **Show composition** next to any material group, additional fields display to give composition and input type where you can further define each material group. You can remove materials and add and remove material groups using the *Material Manager* (available on the **Configuration** window → **Options** tab).

In the example, click **Show composition** next to the **Slag** and **Gas** groups to see how the *Slag_BOF* and *Oxygen* materials are defined.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group. In this example, the *Steel_BOF* material was defined first and then named at the end. It is now available in the lists wherever you select the **Steel** material or need to choose quantities to plot.



After defining and saving a material composition, the named material is available for selection in a variety of places such as when choosing quantities on the calculator and defining axis variables on the Plot Renderer.



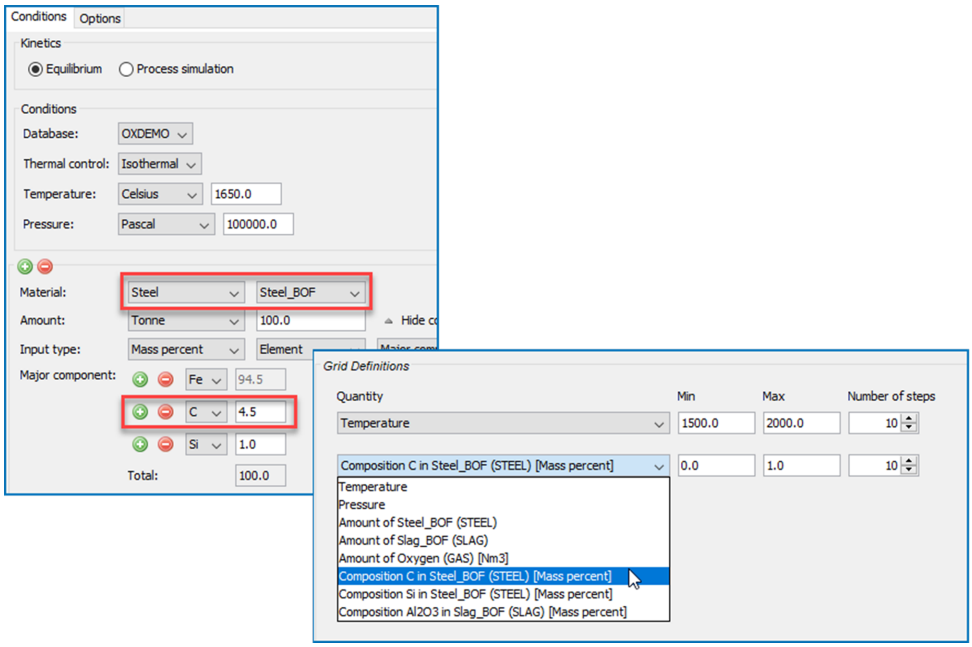
To add one or more material groups click the green add button. Click the red minus button to remove a material group. The new material inherits the default settings of that group.

Understanding the Grid Definitions Quantities and How These Relate to the Composition

When you choose a **One axis** or **Grid** *Calculation Type*, you also choose a **Quantity** under the *Grid Definitions*. The relationship between these quantities and how the material group composition is defined as follows.

The following uses **Composition of C in Steel_LF (STEEL)** as an example quantity for a **One axis** calculation.

Under *Grid Definitions*, the availability of the **Quantity** in the list is based on the material (**Steel_BOF**) that is defined and saved for the **Steel** group (or any user-defined metal, slag, or gas group).

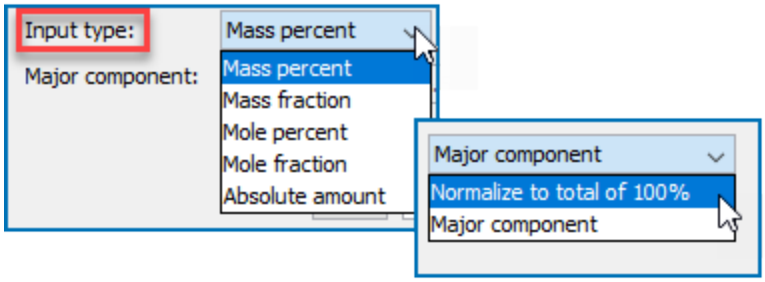


Defining the Material Composition

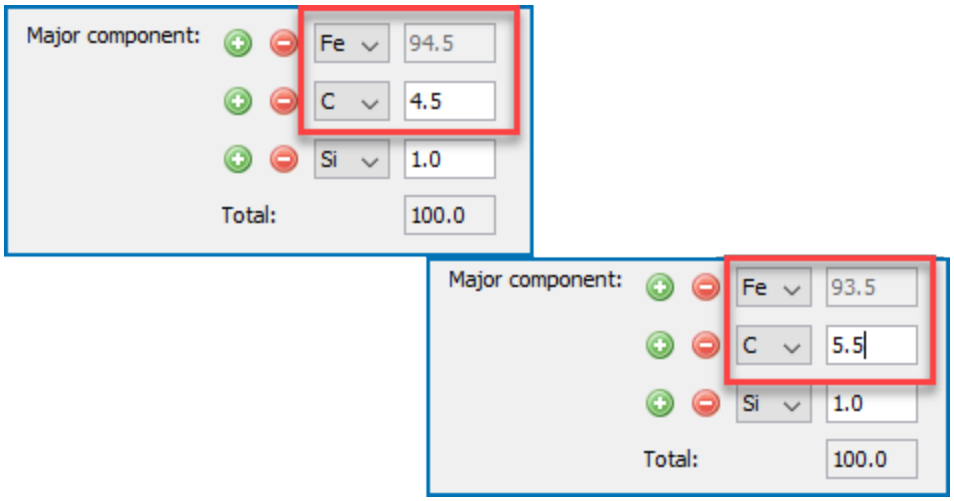
When you choose the **Input type** for a steel the composition of the elements can be set up using a combination of settings starting with **Mass**- or **Mole percent**, **Mass**- or **Mole fraction**, or **Absolute amount**. Then you further choose to define the composition using either the **Major component** or **Normalize to total of 100%** options.



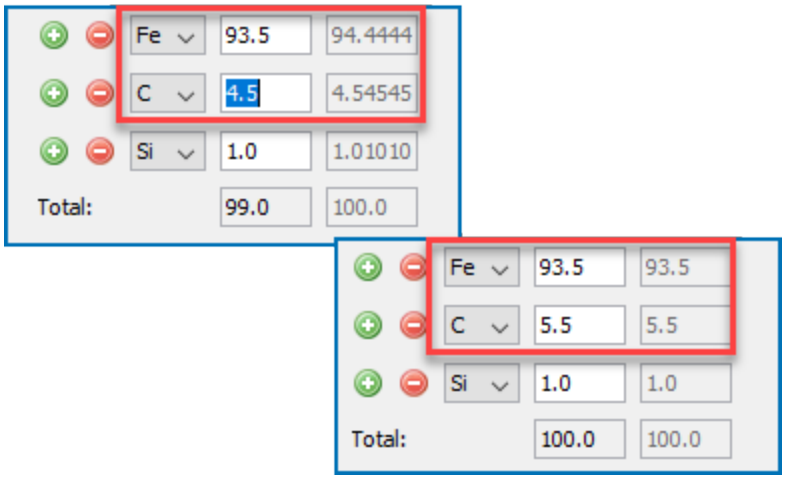
The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.



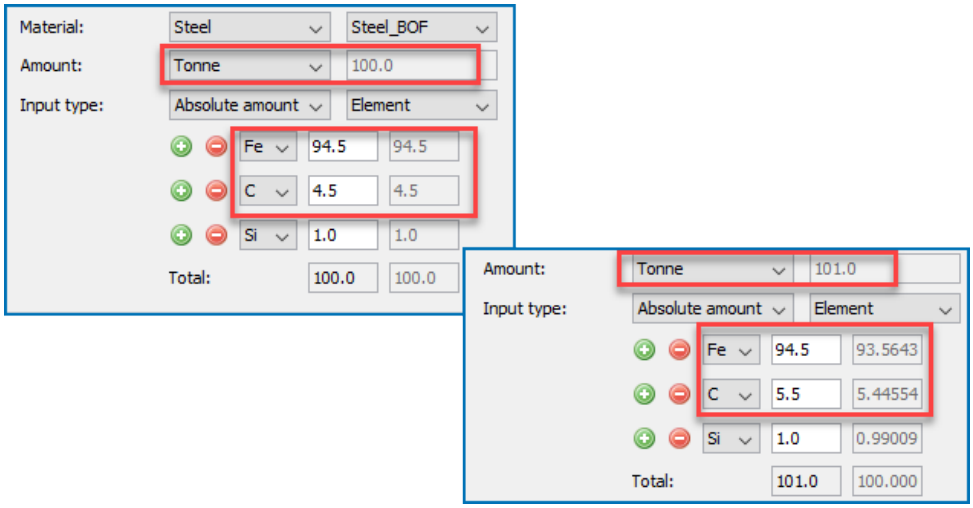
When you use **Major component**, as you add other components or adjust the composition, the major one is adjusted to be the rest of the composition.



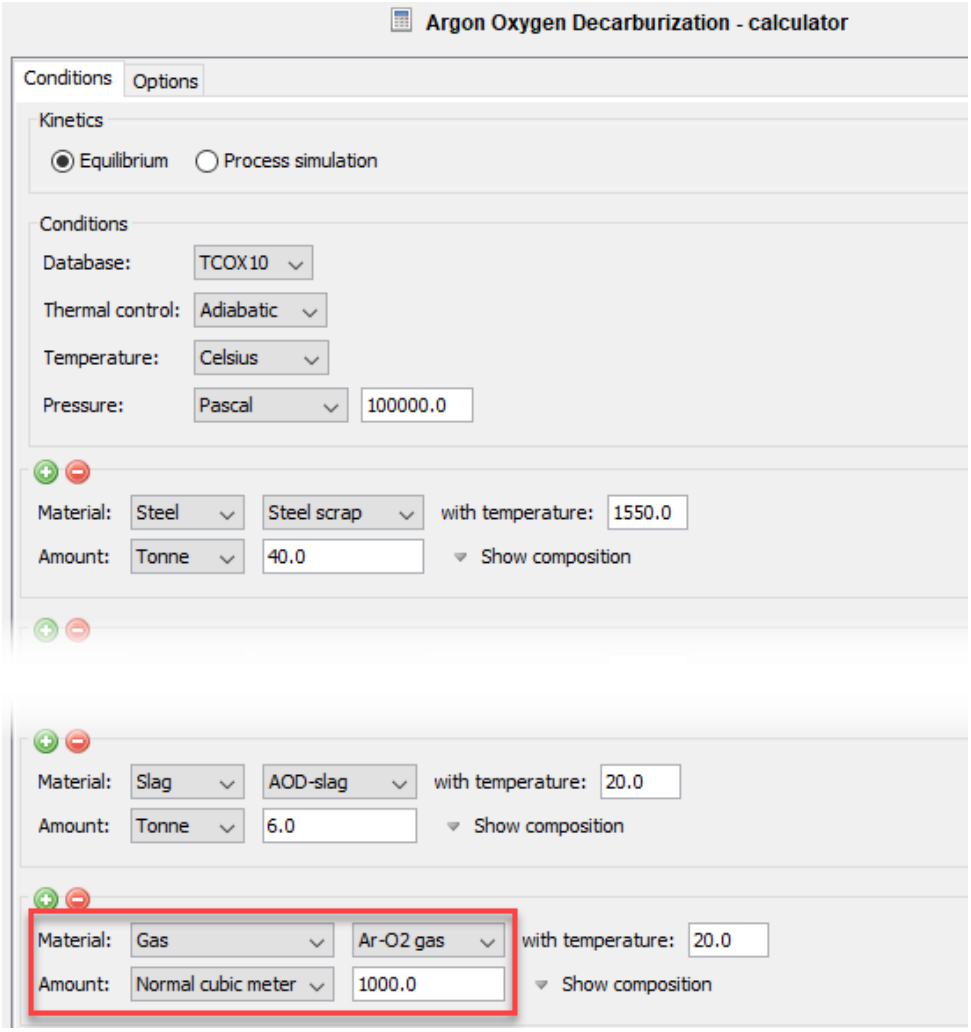
When you use **Normalize to total of 100%**, the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100%.



Sometimes its preferable to use input of amount of each component **Amount** by weight (**Tonne**, **Kilogram**, **Gram**, or **Pound**), it can useful to choose **Absolute amount** as the **Input type**. In this case, the total amount of material automatically adjusts the total.



For the **Gas** component, if you choose **Normal cubic meter** as the **Amount**, then beside regular mass units, the amount of gas can also be provided in Nm^3.

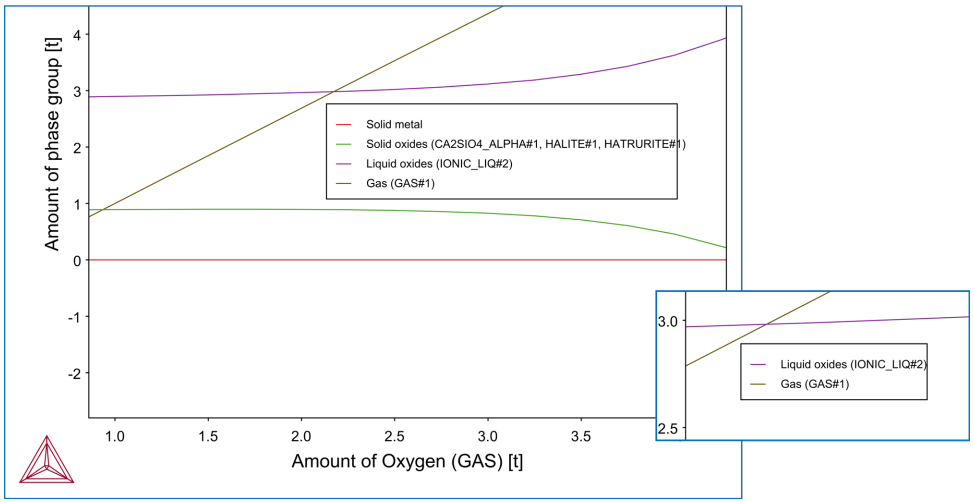


Phase Groups

The phases that are plotted after you run a simulation are grouped together on the plot to make the interpretation of the results easier.

Phases of similar type are bundled together in the groups *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides*, and *gas*. Except for the gas phase, all the groups can have more than one phase. This grouping is particularly useful for liquid metal and liquid oxide because they are both described by the same phase, IONIQ_LIQUID, and because there is typically two or more compositions sets of IONIQ_LIQUID. This is also useful for solid oxides, because a large number of phases can be stable, making the interpretation of results difficult without this grouping.

The term *oxides* in the Process Metallurgy Module can also mean carbides, sulfides, and fluorides.



Example of the plot labels with the phases grouped together. As you zoom in, only the phases that you can see are listed in the label, making it easier to examine the results.

Slag Property Quantities

The slag properties describe the capability of a slag to take up sulfur from the metal melt. The Process Metallurgy Module defines so-called phase groups. These contain all phases of a certain kind, for example all solid slag or all slag phases. The component composition of such a phase group is calculated by weighting the component composition of each phase with their fraction in the group.

This allows to calculate slag properties for the phase groups, for example for the overall slag.

On the Plot Renderer (for axis quantities) and Table Renderer there is an option to choose or define the **Slag property**. The associated quantity that you select has these options: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls** , or **Log10 (Sulphur capacity)**.

- Details, including references and equations, are described in Process Metallurgy Slag Properties.

Adiabatic Calculations

When setting up the Process Metallurgy Calculator under the **Equilibrium Kinetics** branch, you choose the thermal control to be either **Isothermal** or **Adiabatic**. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction. The adiabatic process is implemented by an isenthalpic process with constant pressure (i.e. H=const), which is equivalent.

- Adiabatic Calculations: Material Enthalpy

Gas Volume Units

Beside regular mass units, the amount of gas can also be provided in Normal cubic meter (Nm^3). The applied reference conditions are 1013.25 hPa and 15.0 °C (according to ISO 2533).



There are slightly deviating definitions present in the industry, which need to be converted for precise results. For most applications of the Process Metallurgy Module this difference has a minor influence.

Calculation of Component Compositions

The composition of all ionic phases is provided as elemental as well as component composition (i.e. Fe2O3, FeO, CaO, …). In order to provide a representation similar to that usually used in the industry, the content of S is provided as elemental content and the content of P is given as component content of P2O5. This is a simplification because P and S can also be present as sulphates and phosphates in the slag and can bind to different metal cations. This can cause deviations in the overall component composition if the content of S and P is high in the phases. In doubt, the elemental composition can be used, it will always be exactly correct.

For non-ionic phases such as ALABANDITE, always the elemental composition will be shown only. This is also true if the IONIC_LIQ composition cannot be described by components only due to constraints of the overall composition (for example if the material has been oxidized completely and forces a certain composition of the ionic liquid slag).

Definition of Partial Pressure of Oxygen

The oxygen partial pressure in the gas phase is calculated with the following formula:

$$p_{O_2} = p \cdot AC(O_2, GAS)$$

In the formula, *p* describes the total system pressure and *AC* the activity of oxygen in the gas phase.

Activities of Slag Components

The chemical activity of each component *AC(COMPONENT, REFERENCE_PHASE)* is available either with reference to the liquid or the solid slag phase. It can only be calculated for components being present in the thermodynamic database.

Process Schedule

When you are working with the **Process simulation** branch you set up a process schedule. There are some useful details about this described in Working with the Process Schedule.

Dynamic Time Stepping

The nature of a **Process simulation** requires a dynamic choice of the time step lengths. To understand this better, see About Dynamic Time Stepping. These settings are done on the Options Tab.

Pressure-Dependent Calculations

It is possible to apply variable pressure during process metallurgical calculations, which is relevant in various processes such as Vacuum Oxygen Decarburization (VOD) or Ruhrstahl-Heraeus (RH). See About Pressure-Dependent Calculations.

Working with the Process Schedule

- Defining the Process Simulation
- Process Simulation: Process Schedule Tab
- About Dynamic Time Stepping

Materials and heat can be added at any time in any amount. They can be either added to a:

- bulk zone (such as steel, slag, etc.), or
- reaction zone (interface between two bulk zones).

These types of materials are used in the process schedule set up:

- Material addition (in tonne, kilogram, etc.)
- Continuous material addition (in kilogram per minute, etc.)
- Thermal / electrical power (i.e. a continuous heat addition in MW)

A material addition is typically used to model some event like emptying a bucket into the melt. A continuous material addition is instead used to model a continuous material feeding into the melt, such as wire feeding. Finally, heat can be added or removed during a time step and this is defined as power.

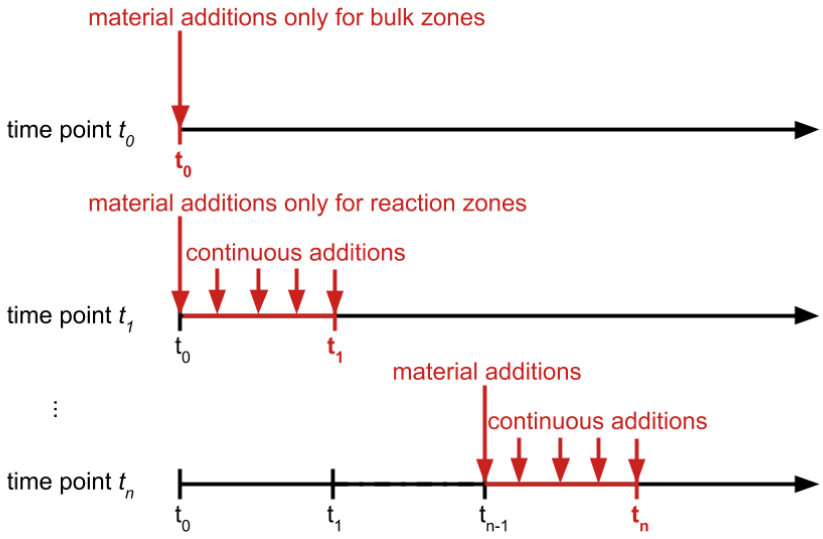


Figure 14: A process schedule additions scheme.

Generally the addition of materials and heat is modeled in the process simulations for any time point t_n as follows:

- Material additions happen immediately after the previous time point t_{n-1}, i.e. at the beginning of the time step.
- Continuous material and heat additions (power) are conceptually happening during the complete time step between t_{n-1} and t_n.

The data presented in the results is always referring to the time point, i.e. to the end of the time step. This means that reactions and heat transfer have happened between adding materials and heat at the beginning of the time step and the end of the time step. If for example a strongly cooling material is added, a possibly quite large heating of the zone might have happened until the end of the time step.

The first two time points are different:

- The first time point t_0 at *t=0* does not represent a time step, instead only a mixing and equilibrium reaction of the material additions in each bulk zone is taking place. There are no reaction zones existing at this time point.
- The second time point t_1 represents the first time step in the simulation where the different bulk zones react between each other via the reaction zones. Nevertheless it is conceptually identical to any other time point.

Working with the Material Manager

The Material Manager is only available for the Process Metallurgy Calculator.

Use the *Material Manager* to create and delete groups of materials and delete materials you have saved directly from the **Process Metallurgy Calculator**. It is useful for frequently used materials.

Material groups created in the Material Manager now appear in all of the Process Metallurgy Calculator dropdown lists, and these are also globally removed. Deleted group data directories are moved to the computer's trash/bin.

A material saved in any of the material configuration panels is now directly accessible globally in the Process Metallurgy Calculator Configuration window. When a material is removed in the Material Manager panel it is globally removed from the Process Metallurgy Calculator.

The settings are available on the **Configuration** window Options Tab.

Saving a Material

This is done directly from the **Process Metallurgy Calculator** → **Configuration** window.

1. Add the Process Metallurgy Calculator to **My Project** directly (right-click and select it from the **Create New Activity** menu) or use the available Process Metallurgy template.
2. On the **Configuration** window, next to the **Material** group you want to define, for example **Steel** (or another user-defined metal group), **Slag** or **Gas**. Click **Show composition**.
3. Enter the composition and the **Major component** of the material you want to save for future use. You can alternatively select **Normalize to total of 100%** and enter the percentages for each element.
4. Click **Save material**.
5. In the window that opens, enter a **Material name**. Click **OK**.

   When you go to the *Material Manager*, you can select this saved material from the applicable list if you need to delete it.



It is not possible to rename a saved material—you need to recreate/redefine the material and save it again with the new name.

Deleting a Material

This is done with the *Material Manager*, located on the **Configuration** window, **Options** tab.

1. After Saving a Material, go to the *Material Manager*.
2. Select the **Material** group associated to the material saved previously, for example, **Steel** (or another user-defined metal group), **Slag** or **Gas**.
3. From the **Material** list, select the material you want to delete and click **Delete material**.
4. In the window that opens, click **Yes** to delete the material and **No** to cancel.

Creating a Material Group

This is done with the *Material Manager*, located on the **Configuration** window, **Options** tab.

1. Go to the *Material Manager*.
2. Click **Create group**.
3. In the window that opens, select the **Material group type** (**Metal**, **Slag** or **Gas**) you want to create.
4. Enter a **Material group name**. The new group is now available to select from the **Material group** list.

Deleting a Material Group

This is done with the *Material Manager*, located on the **Configuration** window, **Options** tab.

1. Go to the *Material Manager*.
2. From the **Material group** list, select the group you want to delete and click **Delete group**.
3. In the window that opens, click **Yes** or **No**.

About Dynamic Time Stepping

- Defining the Process Simulation
- Working with the Process Schedule
- Options Tab

The nature of a process simulation requires a dynamic choice of the time step lengths. On the one hand the simulation needs to capture very fast changes of temperature and composition, for example after addition of cold material. On the other hand it should calculate processes that take several hours in reality within an appropriate calculation time.

The time step control algorithm is primarily controlling the change of the temperature in each zone (including the reaction zones) such that it stays below a specified limit but is always as large as possible.

The dynamic time stepping can be switched off by choosing a very large maximum allowed temperature change per step (such as 1.0e6 K). In this case the maximum time step is always used, however this is only recommended in special situations.

If a temperature change is too large, the algorithm reverts the time step and returns to the previous time point in order to try a smaller time step. Therefore you can see in the Event Log output that the time points can jump back. Except for larger additions this is a rare event.

The parameters of the time-step control algorithm are:

- initial time step a *t=0*,
- smallest allowed time step,
- largest allowed time step, and
- maximum allowed temperature change of a zone within a time step.

The initial time step as well as the largest allowed time step are defined in percent of the total duration of the process while the smallest allowed time step is given in seconds. This allows that these parameters normally need no change even if switching between processes with very short and very long duration.

Making the largest allowed time step bigger can reduce the number of steps and consequently the calculation time, but only if the time step is not limited by the maximum temperature change per time step. This means that both parameters need to be considered together.

Taking a too large smallest allowed time step can cause numerical difficulties, especially if large cold material additions are part of the process schedule.

The initial time step is usually of limited relevance for the overall calculation time, but should usually not be larger than the default value of 1.0%.

As different processes show very different temperature changes, it is probably most common to adapt the maximum temperature change per time step in order to have a good balance between accuracy of the results and calculation time. Usually it should be possible to change this parameter without adapting the other algorithm parameters.

The effects of the dynamic time step algorithm can be inspected by activating the data points in the plots.



To show the data points, in the **Results** window in Thermo-Calc, right-click in the plot area and choose **Properties**, then click **Show data points**.

About Pressure-Dependent Calculations

Defining the Process Simulation

It is possible to apply variable pressure during process metallurgical calculations, which is relevant in various processes such as Vacuum Oxygen Decarburization (VOD) or Ruhrstahl-Heraeus (RH).

The implementation includes all relevant features for a realistic modeling of the pressure-dependency:

- the set pressure at a time-step is valid for all bulk and reaction zones of the system
- the exhaust gas zone has always atmospheric pressure
- the added material (only relevant for gas) has initially always atmospheric pressure
- the material transferred to and from the zones (i.e. the added material and the exhaust gas from the zones) is undergoing an adiabatic expansion / compression because it is moved between different pressures

Generally there is no effect of pressure change on anything else than gas (due to physics and the implementation of the database).



PMET_07: Vacuum Oxygen Decarburization Kinetics

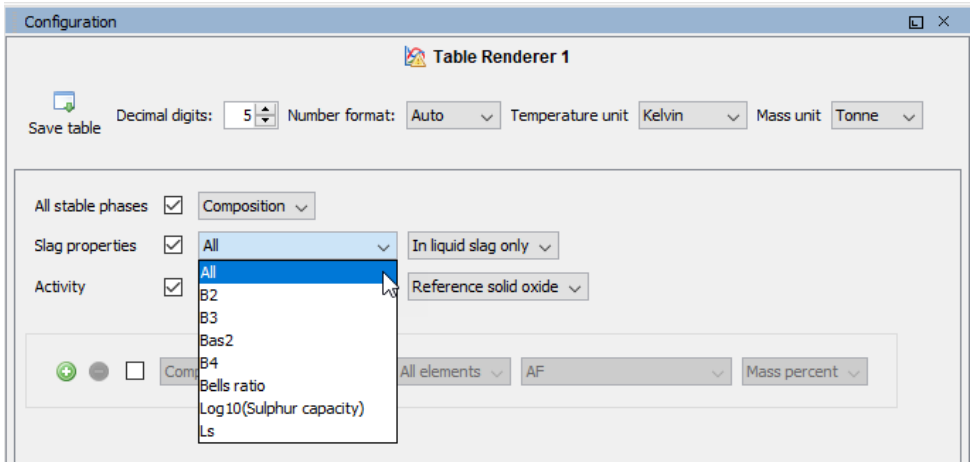
Process Metallurgy Slag Properties

The slag properties describe the capability of a slag to take up sulfur from the metal melt. The Process Metallurgy Module defines so-called phase groups. These contain all phases of a certain kind, for example all solid slag or all slag phases. The component composition of such a phase group is calculated by weighting the component composition of each phase with their fraction in the group.

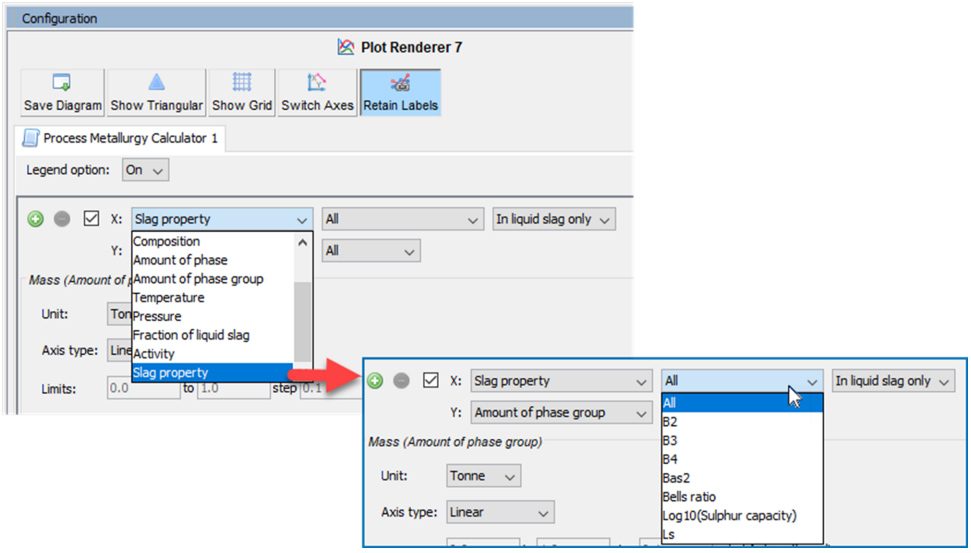
This allows to calculate slag properties for the phase groups, for example for the overall slag.

Various predefined slag properties such as different definitions of slag basicity, sulfur capacity and so forth are available for plotting or tabulating. On the **Process Metallurgy Calculator** when selecting axis variables on the **Plot Renderer** or choosing the properties to list with the **Table Renderer**, there is an option to include these slag properties.

The associated quantity selected from the next drop-down list has these options: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10(Sulphur capacity)**. Also choose **In liquid slag only**, **In solid slag only**, or **In all slag**. Depending on this setting, the composition averaged over liquid, solid, or all slag is applied as a basis for the slag property calculation.



Slag properties for a Table Renderer.



Slag properties for a Plot Renderer.

Equations and References

The equations and references for the slag properties are defined below. Composition can be given in mass (% or fraction).

The formulas are given in Thermo-Calc console-like syntax (B: mass, W: weight fraction, AC: activity). A slag property is available if all of its components are present in the phase group. Steel and slag are the actual phase groups chosen depending on the user request, i.e. the slag property can be calculated for the liquid slag only or for the overall slag (liquid and solid).

Basicity is defined as:

$$\mathrm{B2} = \frac{B(CaO)}{B(SiO_2)}$$

$$\mathrm{B3} = \frac{B(CaO)+B(MgO)}{B(SiO_2)}$$

$$\mathrm{B4} = \frac{B(CaO)+B(MgO)}{B(SiO_2)+B(Al_2O_3)}$$

$$\mathrm{Bas2} = \frac{B(CaO)+B(MgO)}{B(SiO_2)+B(Al_2O_3)+B(TiO_2)}$$

$$\mathrm{Bells\ ratio} = \frac{B(CaO)+0.7\cdot B(MgO)}{0.94\cdot B(SiO_2)+0.18\cdot B(Al_2O_3)}$$

Sulfur capacity is defined as:

$$\mathrm{Ls} = \frac{W_{(slag)}(S)}{W_{(steel)}(S)}$$

$$\mathrm{Log10}(C_s) = log10(W_{(slag)}(S) \cdot 100 \cdot (\frac{AC(O_2,GAS)}{AC(S_2,GAS)})^{(0.5)})$$

References

Basicity and MgO Saturation: For definitions of the basicity and MgO saturation properties B2, B3, B4 and Bells ratio see Keskitalo (2015). Also see the Slag Atlas (Verein Deutscher Eisenhuttenleute, 1995).

Sulfur Distribution and Capacity: For definitions of the sulfur distribution properties L_S see Andersson et al (1999). For the sulfur capacity, see Slag Atlas (Verein Deutscher Eisenhuttenleute, 1995).

Andersson, Margareta A. T., Par G. Jönsson, and Mselly M. Nzotta. 1999. “Application Ladle Slags of the Used Sulphide Capacity Concept on High-Basicity in Bearing-Steel Production.” ISIJ International 39 (11): 1140–49.

Keskitalo, Björn. 2015. “Model Studies on the Effects of Composition Differences of Direct Reduction Pellets and an Adaptive Addition of Slag Formers for the EAF Process.” Master's thesis, KTH Royal Institute of Technology, http://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-168296.

Verein Deutscher Eisenhuttenleute (VDEh), ed. 1995. Slag Atlas 2nd Edition. Dusseldorf, Germany: Verlag Stahleisen GmbH.

Adiabatic Calculations: Material Enthalpy

An adiabatic calculation requires the enthalpy of the input materials as an initial condition. The Process Metallurgy Module uses different approaches for the different material types metal, gas, and slag. Any mechanical mixture is only applied for 1 bar / 1013 hPa.

Metal

Frozen-in global equilibrium calculation at T=700 °C, taking the resulting enthalpy at the actual initial material temperature. This corresponds to a frozen-in microstructure. At initial material temperatures above 700 °C the equilibrium is instead calculated directly.

Gas

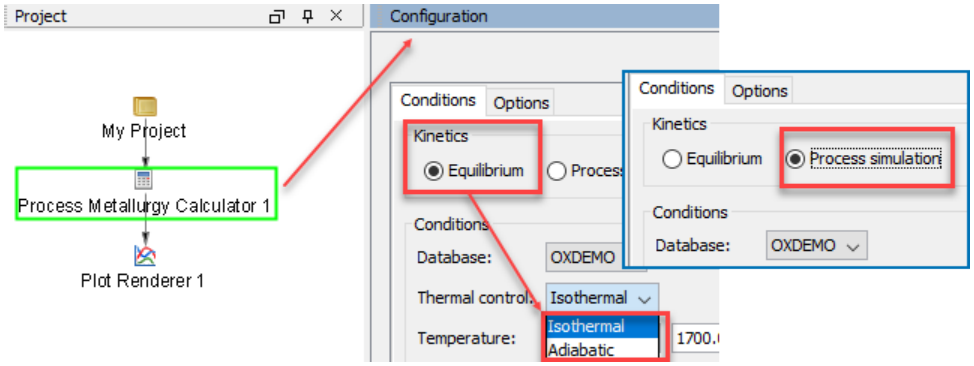
Mechanical mixture between the enthalpy of the gas components. This is no limitation, because all gas components in the databases are assumed to be ideal gas.

Slag

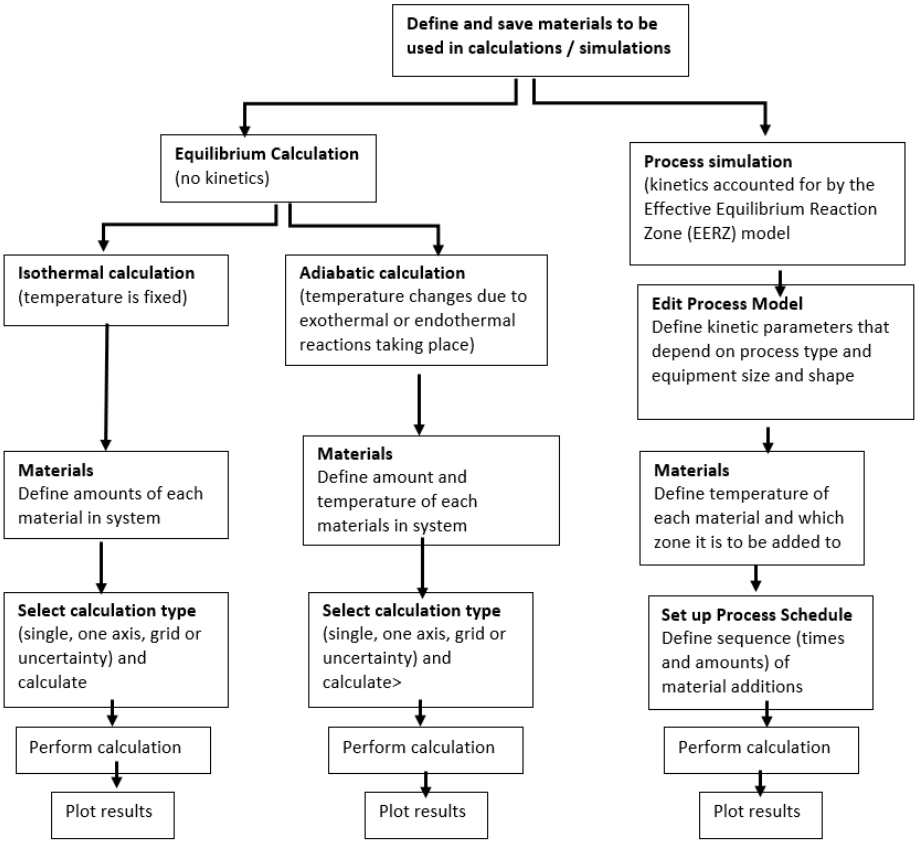
- Mechanical mixture: If the temperature is below T=1000 °C and every single material component (such as MgO, CaO, …) is fully solid at the requested material temperature, mechanical mixture is assumed. This means that the enthalpy of every component is calculated separately and summed up (weighted by mass fraction). This corresponds to the assumption that different separate components have been added to the slag (such as burnt lime and magnesite). If any component forms gas or liquid at the initial material temperature, this mode is not used. Note that mechanical mixture is also applied if pure elements are added to the slag material, i.e. it is not the same in respect to the material enthalpy to define CaO and Ca + O.
- Equilibrium: If no mechanical mixture of the material components is possible or if the temperature is above T=1000 °C. This corresponds to the assumption of a fully homogenized slag material.

Setting Up a Process Metallurgy Simulation

The following basic steps need to be carried out to set up calculations in the **Process Metallurgy Calculator**. There are three branches of simulation to choose from on the **Configuration** window when setting up the simulation an isothermal equilibrium calculation, an adiabatic equilibrium calculation, and a process simulation.



Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.



The three branches of simulations available for the Process Metallurgy Calculator (1) an isothermal equilibrium calculation, (2) an adiabatic equilibrium calculation, and (3) a process simulation.

Equilibrium Simulations

Two **Equilibrium** simulation types are available: **Isothermal** and **Adiabatic**. In general for the equilibrium simulation, the three most common material groups—*Steel*, *Slag*, and *Gas* are automatically included with the default composition input types that are relevant to each material group. You can add materials and save your material compositions directly from the Process Metallurgy Calculator and quickly access these for other simulations. For example, you might want to predefine compositions of steels, ferro-alloys, slags, and slag additions. The overall composition of the steel and slag is then obtained by adding amounts of these predefined materials.

Each group of materials is automatically added to the similar group where it is defined. You can manage these groups using the *Material Manager* (see Working with the Material Manager).

For adiabatic calculations, the selection of material type (steel, slag, gas) has an influence on the calculation. For isothermal calculations, the results are identical.

The reason the selection of materials for adiabatic calculations has an influence is because there are different strategies to calculate the enthalpy of the materials at the temperature at which these are added. Therefore, defining FeO as a *steel* containing 50at% Fe and 50at% O or as a *slag* with 50at% Fe and 50at% O or as *slag* with 100% FeO, all result in different enthalpies assigned to the component FeO, which in turn results in different equilibrium temperatures.

- Defining the Equilibrium Simulation
- Equilibrium Simulation: Conditions Tab
- Adiabatic Calculations: Material Enthalpy

Process Simulations

When you choose to do a **Process simulation** it includes the reaction kinetics. Using the EERZ (Effective Equilibrium Reaction Zone) model, you can first define your materials as you do with an **Equilibrium** simulation. You also need to define the **Process model** where you define the kinetic parameters of the simulation by setting up reaction zones, reaction rates, heat transfer coefficients, and so forth. You also need to define the **Process schedule** where the sequence and amounts of added materials are defined.

- Defining the Process Simulation
- Process Simulation: Conditions Tab

Calculation Types

The calculations available for an **Equilibrium** simulation, for both isothermic and adiabatic calculations, are *Single* equilibrium, *One axis*, *Grid*, and *Uncertainty*. After adding a **Plot Renderer** or **Table Renderer**, you can choose a variety of quantities, including slag properties such as Bells ratio and B2, to output results that provide useful visual representations of the steelmaking systems being analyzed.

- Process Metallurgy Calculator and Defining the Equilibrium Simulation



You can find several learning resources on the Process Metallurgy page of our website (or in Thermo-Calc, go to **Help → Thermo-Calc website**). You can also subscribe to the Thermo-Calc newsletter to be kept up-to-date about upcoming releases, training, examples, videos and much more.

Process Metallurgy Calculator

For information about licenses and availability, see About the Process Metallurgy Module.

Use a **Process Metallurgy Calculator** to set up calculations for steel and slag used in steelmaking. Define the composition of a steel (or other metal) and slag system using material groups: one each for steel, slag, and gas. You can save your material compositions directly from the calculator and quickly access and manage the materials and groups—it collects groups of saved materials according to type, thus making it easy to retrieve them.

You can add the calculator to **My Project** directly (right-click and select it from the **Create New Activity** menu) or use the Process Metallurgy Template.



Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.



You can find several learning resources on the Process Metallurgy page of our website (or in Thermo-Calc, go to **Help → Thermo-Calc website**). You can also subscribe to the Thermo-Calc newsletter to be kept up-to-date about upcoming releases, training, examples, videos and much more.

Kinetics - Equilibrium or Process Simulation

Once you have added a Process Metallurgy Calculator, the **Configuration** window is further branched based on the **Kinetics** option you choose, **Equilibrium**, where kinetics are not considered, or **Process simulation**, where kinetics are considered using the Effective Equilibrium Reaction Zone (EERZ) model.

All settings, no matter what kinetics branch, are defined on the **Configuration** window **Conditions** and **Options** tabs.

Conditions Tab

Equilibrium

- For information about the individual settings on this tab, see Equilibrium Simulation: Conditions Tab.

Set the conditions for your calculation that define the slag, metal, and gas. The topic, Defining the Equilibrium Simulation, has instructions that walk you through the steps that represent a simplified steelmaking process.

Process Simulation

- For information about the individual settings on this tab, see Process Simulation: Conditions Tab.

Set the conditions for your calculation that best describes the process you want to simulate. The topic, Defining the Process Simulation, has instructions that walk you through the steps. Also the description of the kinetics examples are useful to help you better understand the settings.

Options Tab

- For information about the individual settings, see Options Tab.

Use the **Material Manager** to create and delete groups of materials and delete materials you have saved directly from the Process Metallurgy Calculator. It is useful for frequently used materials. Also see Working with the Material Manager.

The settings in **Process Material Equilibrium and Grid** define certain numerical settings used by the Thermo-Calc calculation engine for equilibrium calculations such as whether tests for

global minimization should always be performed (this significantly slows down the calculations) or never be performed (this speeds up calculations but miscibility gaps might not be found), and so forth.

Calculations of oxide systems are numerically challenging, and they can often fail. The default values are chosen to give the best general performance and reliability and should only be changed by an expert user. Also, a large amount of logic is implemented in the Process Metallurgy Module to improve the convergence and calculation speed of equilibrium calculations. The timestep control is related to how finely the times defined in the **Process schedule** are resolved. See About Dynamic Time Stepping for more information.

Local versus Global Options Settings

The **Options** tab is where you can locally define specific Process Metallurgy Calculator settings. Settings can also be applied globally from the **Options** window.

To open the **Options** window: From the main menu select **Tools → Options → Graphical Mode** and click the **Activities** tab. Then click **Process Metallurgy**. See Global Settings: Process Metallurgy.

Plots and Tables

Right-click the node to add a Plot Renderer or Table Renderer to visualize your results. Although both nodes work the same as with the other calculators in Thermo-Calc, there are additional features and settings unique to the Process Metallurgy Module. Useful information is included throughout the documentation. You can also read more about the unique features in Working with the Process Metallurgy Module.

Defining the Equilibrium Simulation

After adding a **Process Metallurgy Calculator** to your project, you can choose to conduct an **Equilibrium** simulation, where you define the steel, slag, and gas groups of materials, or a **Process simulation**, where you set up a process using the EERZ (Effective Equilibrium Reaction Zone) model.

The following steps are for **Equilibrium** simulations. If you choose to do a **Process simulation**, see Defining the Process Simulation.

This is a general overview of the setup based on the PMET_01: Basic Oxygen Furnace (BOF) example, which walks you through the steps that represent a simplified steelmaking process.

1: Add the Calculator and Choose the Simulation Type

1. Add a **Process Metallurgy Calculator** node to **My Projects** node. If you used the **Process Metallurgy** template, click the node to display the **Configuration** settings window.
2. Under **Kinetics**, choose the simulation type, **Equilibrium** or **Process simulation**. For the following steps, choose **Equilibrium**.

2: Select a Database and Enter a Temperature

1. In the **Configuration** window, for the *Database* selection, the program automatically defaults to the highest available version of the TCOX database.

   The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

   It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

> All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

2. Set the **Thermal Control** as being **Isothermal** or **Adiabatic**.
3. Select a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**) and enter a numerical value in the field.
4. Select a **Pressure** unit (**Pascal**, **Atmospheres**, or **Bar**) and then enter a numerical value in the field.

3: Define the Conditions for the Steel, Slag and Gas Material Groups

Next define each material group—**Steel** (or any user-defined **Metal** group), **Slag**, and **Gas**.

- See Equilibrium Simulation: Conditions Tab for an overview of the layout of this section. There is also an overview of these material groups in Working with the Process Metallurgy Module.

1. Choose a **Material** to set up first, **Steel** (or any user-defined metal), **Slag**, or **Gas**.
2. Select an **Amount** from the list—**Tonne**, **Kilogram**, **Gram**, or **Pound**. Enter a numerical value in the field.
3. If this is the first time you are defining a material, or at any time when **User-defined** is selected, click **Show composition** to set the composition for the material (steel, slag, or gas or another user-defined metal).

> The composition for each material is hidden by default because the Module allows you to easily save materials and access these from the material menu. Once you save a collection of materials, you will rarely have to click **Show composition**. See Working with the Material Manager for details about saving and deleting materials.

4. To the right of the **Material** list (e.g. for the **Steel** group), choose the material composition you want to use for this simulation. Predefined **Example Steel** and **Example Slag** compositions are included with the installation.

- If you chose **Adiabatic** as the **Thermal Control**, also enter a **temperature** in the field for each material. This is the initial temperature before the material is added to the process.

5. From the first **Input type** list select **Mass percent**, **Mass fraction**, **Mole percent**, **Mole fraction**, or **Absolute amount**. For **Absolute amount**, you can directly enter values in the fields in the unit selected above for **Amount** (**Tonne**, **Kilogram**, **Gram**, or **Pound**).
6. For the next list, the default is based on which group you are defining. For the Steel (Metal) group it is **Element**, for Slag it is **Component**, and for Gas it is **Gas component**.
7. Choose **Major component** so that as you add other components, the major one is adjusted to be the rest of the composition. Choose **Normalize to total of 100%** so that the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100% If you select **Absolute amount**, **Normalize to total of 100%** is not available.
8. Based on which material group you are working with, add the **Element**, **Component**, or **Gas component**.



To add one or more material groups click the green add button. Click the red minus button to remove a material group. The new material inherits the default settings of that group.

9. After you have added and defined the element, component, or gas component it is recommended you save and name the material. This makes it easier to work with because the name of the material is automatically updated in the lists (and available as part of your library) instead of being named *User-defined* everywhere.

   The material is automatically saved in the relevant material group, so only steel materials are shown in the steel menu, only slag materials are shown in the slag menu, and only gas in the gas menu. You can also create additional material groups if there are groups you use regularly, such as scrap compositions, ferro-alloys or slag additions. See Working with the Material Manager for more details about creating and deleting material groups and deleting materials.

10. Continue adding and defining the material groups (e.g. Steel, Slag, and Gas). You could, for example, add another Steel group if you wanted to define a composition of a steel scrap to add to a basic oxygen furnace (BOF).

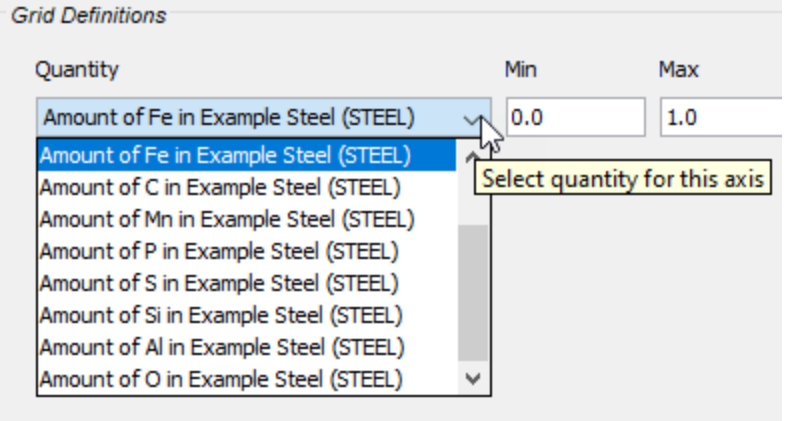
4: Select the Calculation Type and Associated Definitions

These settings are described more in Equilibrium Simulation: Conditions Tab.

1. Under *Calculation Type*, click to choose **Single** (no axes), **One axis**, **Grid**, or **Uncertainty**.

> For more complex calculations, it is good practice to start with a **Single** equilibrium calculation to make sure the calculation converges. Also see the settings described in Options Tab. These can be useful if your calculation fails.

2. Based on the calculation type, define either the *Grid Definitions* (for **One axis** or **Grid** calculations) or the *Sampling of Data from Gaussian Distributions* (for **Uncertainty** calculations). The **Quantity** displays all the stepping options set up with the material groups for **Steel**, **Slag**, and **Gas**. The example shows the steel group quantities.



> The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.

How these quantities relate to the material definition is described in Working with the Process Metallurgy Module.

5: Add and Define a Plot or Table and Run the Simulation

Once you have finished defining the Process Metallurgy Calculator, you also define the plot or table settings. To add a Plot Renderer or Table Renderer, right-click the calculator node and select an option from the **Create New Successor** menu.



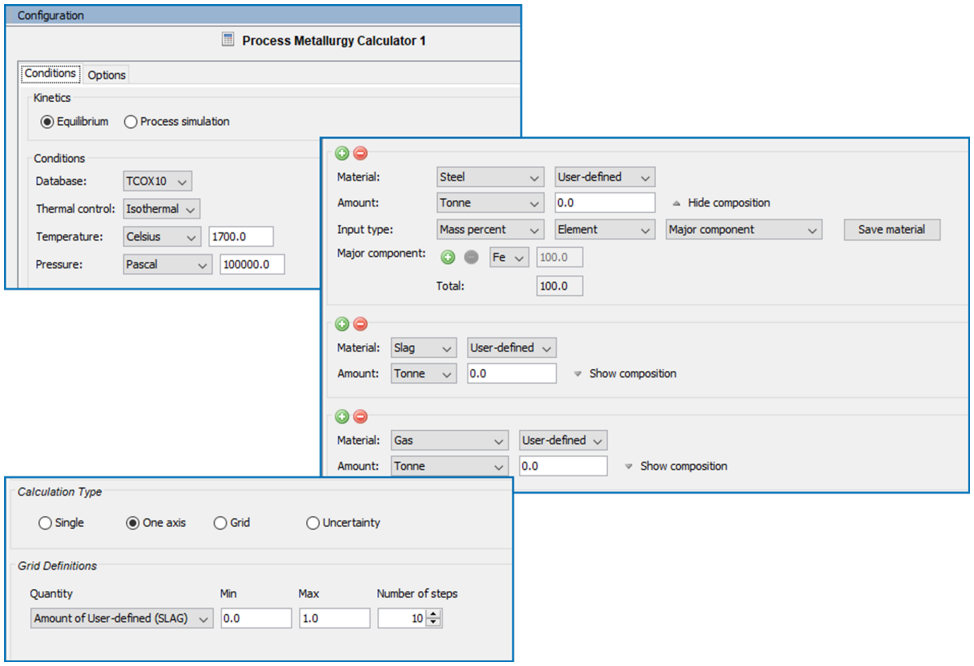
The settings are generally described for the individual nodes. See Plot Renderer and Table Renderer.

- Some useful information about the plots is also described in Working with the Process Metallurgy Module.

Equilibrium Simulation: Conditions Tab

The following outlines what you can set on the **Configuration** window **Conditions** tab when working with the **Process Metallurgy Calculator** and an **Equilibrium** simulation.

Also see Defining the Equilibrium Simulation for instructions that walk you through the steps that represent a simplified steelmaking process. A more complex process is described in Defining the Process Simulation.



An example of the different settings areas for a default Configuration window for a Process Metallurgy Calculator when an Equilibrium simulation type is selected. There are many settings available depending on the parameters.

Database

The most recent available version of TCS Metal Oxide Solutions Database (TCOX) is selected by default.

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

Thermal Control

Choose **Isothermal** or **Adiabatic**. When **Adiabatic** is selected, no global temperature is defined (as this changes during the process). Instead the initial temperature has to be defined separately for each material. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction. Certain types of processes run at almost constant temperatures. For such processes isothermal conditions are acceptable. But in most metallurgical processes the temperature will change sometimes dramatically in function of time due to heating or cooling of the system and due to exothermal or endothermal reactions taking place. For such processes adiabatic conditions are a better choice.

Temperature

Choose a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**) and then enter a numerical value in the field.

Pressure

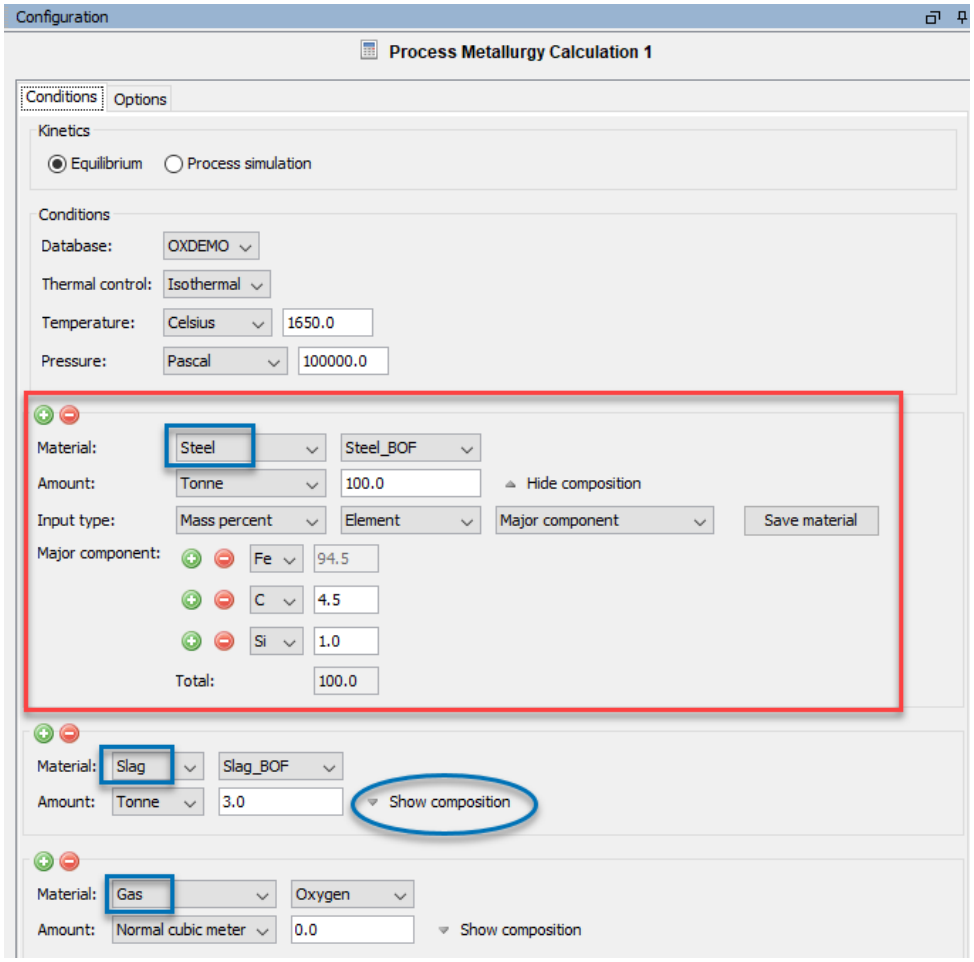
Choose a **Pressure**unit (**Pascal**, **Atmospheres**, or **Bar**) and then enter a numerical value in the field.

Material Groups (Steel, Slag and Gas)

- For more details about these fields, see Defining the Equilibrium Simulation. See also Working with the Material Manager.

There are three groups to define: **Steel** (or another user-defined **Metal** group), **Slag**, and **Gas**.

In the image below, the red-highlighted area is where the **Steel** material group is defined. The drop-down menu that displays *Steel_BOF* is a user-defined material. This can be defined and then saved to the material library.



The three material group areas on the Process Metallurgy Calculator where you can define components and save materials.

When you click **Show composition** next to any material group, additional fields display (e.g. **Input type**, **Major components**, and so forth) where you can further define each material group. You can add and remove materials using the Material Manager (available via the **Configuration** window → **Options** tab).



You can open the example project PMET_01: Basic Oxygen Furnace (BOF) from Thermo-Calc **(Help → Example Files → Process Metallurgy → PMET_01_ Basic_Oxygen_Furnace.tcu)**. Then click **Show composition** next to the **Slag** and **Gas** groups to see how the *Slag_BOF* and *Oxygen* materials are defined.

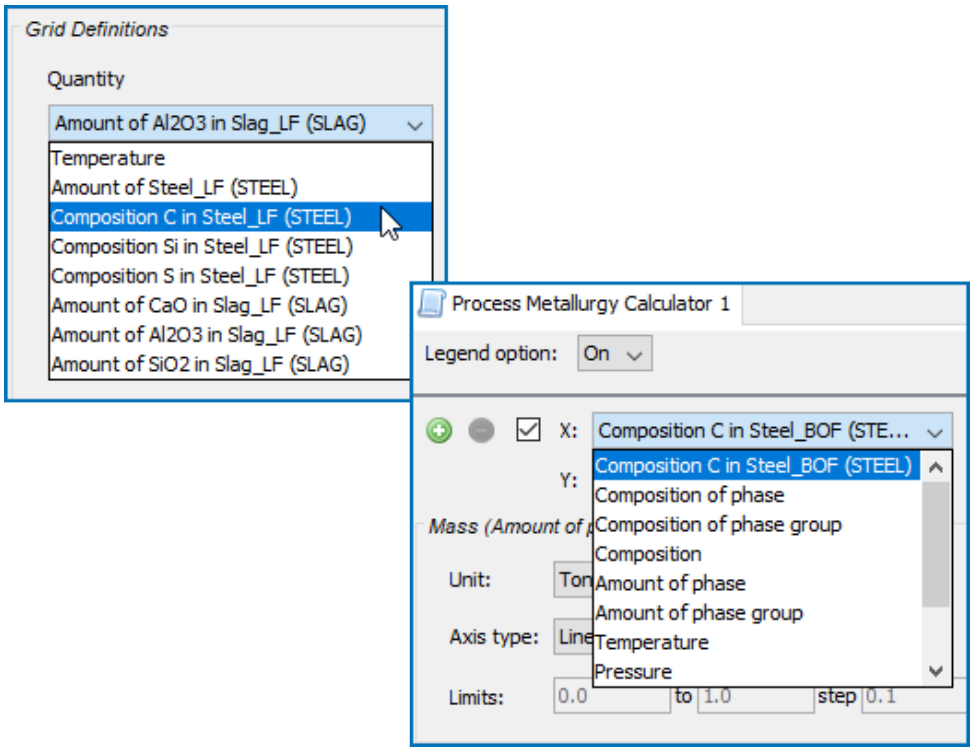
From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group. In this example, the *Steel_BOF* material was defined first and then named at the end. It is now automatically available wherever you select the Steel material or need to choose quantities to plot.



The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.



To add one or more material groups click the green add button. Click the red minus button to remove a material group. The new material inherits the default settings of that group.



After defining and saving a material composition, the named material is available for selection in a variety of places such as when choosing quantities on the calculator and defining axis variables on the Plot Renderer.

Calculation Type

Single (no axes), **One axis**, **Grid**, or **Uncertainty**.

The Calculation Types in Graphical Mode

- Select **Single** to calculate a single point. No additional settings are required. The results from this calculation can be displayed in the **Results** window using a **Table Renderer**.
- Select **One axis** to vary a quantity on the X-axis.
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.
- The **Uncertainty** calculation evaluates the equilibrium where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Grid Definitions (One axis or Grid)

The **Quantity** menu displays all the stepping options set up with the material groups for **Steel** (or any user-defined metal group), **Slag**, and **Gas**.

For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max**, and **Number of steps**.

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected equilibrium is evaluated.



For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour*, or *3D* diagram.

Heat Map, Contour, and 3D Plots

Sampling of Data from Gaussian Distributions (Uncertainty)

For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

- About the Uncertainty Calculations

Sampling Parameters (Uncertainty)

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

- About the Uncertainty Calculations

Defining the Process Simulation

Setting Up a Process Metallurgy Simulation

After adding a **Process Metallurgy Calculator** to your project, you can choose to conduct an **Equilibrium** simulation, where you define the steel, slag and gas groups of materials, or a **Process simulation**, where you set up a process using the EERZ (Effective Equilibrium Reaction Zone) model.

The following steps are for **Process simulation**. If you choose to do an **Equilibrium**, see Defining the Equilibrium Simulation.

1: Add the Calculator and Choose the Simulation Type

1. Add a **Process Metallurgy Calculator** node to **My Projects** node. If you used the **Process Metallurgy** template, click the node to display the **Configuration** settings window.

2. Under **Kinetics**, choose the simulation type, **Equilibrium** or **Process simulation**. For the following steps, choose **Process simulation**.

   Only adiabatic conditions are available for process simulations as this corresponds best to most practical processes.

2: Select a Database and Enter a Temperature

Process Simulation: Conditions Tab

1. In the **Configuration** window, for the *Database* selection, the program automatically defaults to the highest available version of the TCOX database.

   The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

2. Select a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**).
3. Select a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

3: Define the Process Model

Process Simulation: Process Model Settings

1. Enter a **Name** for the process and the total **Duration** of the process.
2. Choose a **Process model** from the list or click **Edit Process Model** to define a new model or edit an existing one.
3. In the **Process model** the following is defined:
    a. **Pressure**. This is can be either **Constant** throughout the process (enter a constant via the Edit Process Model) or be changed during the process (select **Table input** via the Edit Process Model) and then enter pressure in the **Process schedule** table.
    b. **Zones of the Effective Equilibrium Reaction Zone model**. Only two zones can be defined. The densities need to be given manually. They are used to calculate the volume of the reaction zones, which is in turn used for the calculation of the reaction kinetics. Choose to allow degassing or not.
    c. **Area of the Reaction zone and mass transfer coefficients**. The area is typically the area of the interface between the two zones. The mass transfer coefficients state how fast material is moved into the reaction zone. Large

values result in fast kinetics, small numbers in slower kinetics. These values strongly depend on the type of material (mass transfer in slags is slower than in liquid steel due to its higher viscosity) and type of process (the violent reactions in a basic oxygen furnace have higher mass transfer coefficients compared to the gentle stirring performed in a ladle furnace. These parameters are basically fitting parameters that need to be determined based on comparison with experimental data. Typical values can also be found in the literature. Choose to allow degassing or not.

d. **Transfer of phase group**. This defines how fast "foreign" phases are moved from one zone to the other. Foreign phases could be solid or liquid oxide inclusions in the liquid steel, or metallic droplets in the slag phase. A typical application is the simulation of the flotation of oxide inclusions out of the liquid steel into the slag phase during refining in a ladle furnace.

e. **The Heat entering or leaving the system and being transferred between the zones.** Constant cooling defines how much heat is lost from the system by radiation and convection. Separate values can be given to each zone if needed. Heat is used when the system is actively heated by an external heat source such as an electric arc or induction heater. Here only the heating efficiency is given, which is the percentage of for example electrical power that is transferred to the system as heat. The times and power are defined in the **Process schedule**. Different amounts of heat and material are added to the zones resulting in the zones having different temperatures. Heat transfer defines how heat flows from one zone to the other. A high value results in a quick equalization of temperature, a small value results in the zones keeping their different temperatures.

4: Define the Materials

- Process Simulation: Materials Tab

The materials can be defined, saved and retrieved in the same way as for an equilibrium simulation. For a process simulation, it must be defined to which zone the material is added. Typically, oxide materials are added to the slag zone and metallic materials are added to the steel zone. Gas or other injected materials (such as carbon or lime powder) are typically added to the reaction zone. But this choice depends on the process to be simulated and must be carefully chosen. By defining the same material twice or even three times, it can be split, so that part of the material is added to one zone and part of it to another zone.

5: Define the Process Schedule

- Working with the Process Schedule

Process Simulation: Process Schedule Tab

On the **Process schedule** tab, the sequence and amounts of additions during the duration of the process are defined. All the materials defined in the **Materials** tab automatically are included in the table. If a heat addition is defined in the Process Model this is also included in the table. If the units **Tonne**, **Kilogram**, or **Pound** are selected, then the additions are defined as one-time additions at a certain time. If a rate is chosen as unit of the addition (such as **Kilogram per minute** or **Kilogram per second**, for gas also **Normal cubic meter per minute** or per second can be given) then the rate of addition is entered into the table. The additions are visualized in a plot for clarity.

6: Run the Simulation and Add and Define a Plot or Table

When the simulation is set up, click **Perform Tree** to run it. Plots and tables can be added in the same way as for equilibrium calculations.

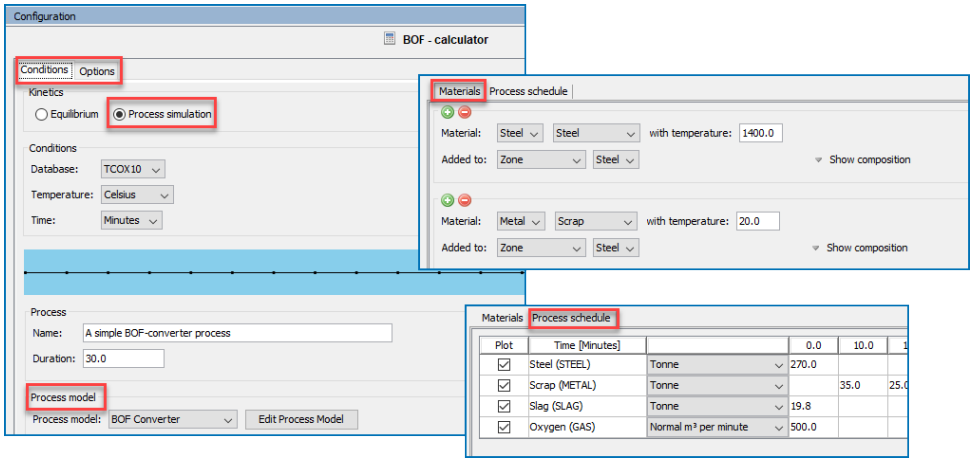
Process Simulation: Conditions Tab

See Defining the Equilibrium Simulation for instructions that walk you through the steps that represent a simplified steelmaking process. A more complex process is described in Defining the Process Simulation and where the settings in the following topics are described.

Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.

The following outlines what you can set on the **Configuration** window **Conditions** tab when working with the **Process Metallurgy Calculator**.

Below is based on selecting a **Process simulation** under **Kinetics**. The settings to complete are for the **Process Model**, the **Materials**, and the **Process Schedule**.



An example of the different sections on the Configuration window for a Process Metallurgy Calculator when a Process simulation type is selected. This screen shot is from the example PMET_04. There are many settings available depending on the parameters.

Database

The most recent available version of TCS Metal Oxide Solutions Database (TCOX) is selected by default.

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

Temperature

Select a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**).

Time

Select a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

Process Simulation: Process Model Settings

The following outlines what you can set on the **Configuration** window under Process and when you click **Edit Process Model**. The overall steps to set this up are described in Defining the Process Simulation.

Process

Under *Process*, enter a **Name** and **Duration**.

For more complex processes, you could, for example, enter the process reference as its *Name* as is done for the EERZ example **PMET_06_Ladle_ Furnace_Kinetics.tcu**.

Process Model

Choose a *Process model*. Click **Edit Process Model** to enter details as below.

You can create your own **Process model** and name them so these are available to choose from the list in the future. This is done using the **Edit Process Model** window.

Edit Process Model

To open the **Edit Process Model** window, click **Edit Process Model** to access the following settings.

Pressure

For **Pressure**, this is can be either **Constant** throughout the process or be changed during the process (using **Table input** here and then entering values in the Process Schedule). Choose:

- **Constant** to choose a unit (**Pascal**, **Atmospheres**, or **Bar**) and then enter a numerical value in the field.

  Only constant pressure throughout the process can be used. Also, the pressure only influences reactions involving the gas phase.

- **Table input** to add or use the values entered in the **Process Schedule** table.

Zones

In this section define the material zone(s), which are added to a **Zone** or **Reaction zone** on the **Materials** tab.

Enter a **Name** and **density** (in kg/m^3) for the zones.

For example, enter `Steel` and `Slag`, which in the next section are available to define for **Zone 1** or **Zone 2** in the Reaction zone.

Select the **Allow degassing** check box to be able to simulate vacuum degassing, for example.

Click the **Add** button to define additional items and the **Remove** button to delete items.

Reactions

In this section you are defining either a **Reaction zone** and/or **Transfer of phase group**.

Select the **Allow degassing** check box to be able to simulate vacuum degassing, for example.

Click the **Add** button to define additional items and the **Remove** button to delete items.

Reaction Zone

If you choose **Reaction zone** from the list then enter an *area* (in m^2).

Next choose from each **Zone 1** and **Zone 2** list the Zone as defined above, for example **Steel** or **Slag**.

For **mass transfer coefficient** choose:

- **Constant** to enter a numeric value in the field in m/s for each.
- **Table input** to add or use the values entered in the **Process Schedule** table.

Reaction zone area and mass transfer coefficient defines the kinetics of the reaction between the two zones. A large area and fast mass transfer results in fast kinetics.

Transfer of Phase Group

If you choose to define a **Transfer of phase group**, then choose the state as **Liquid metal**, **Solid metal**, **All metal**, **Solid oxides**, **Liquid oxides**, **All oxides**, or **Gas**.

Then choose the two zones (e.g. Steel or Slag) to define **from zone** and **to zone** and enter a value of the **%/min**.

This parameter defines how fast “foreign” phases are transferred from one zone to another. A typical example is the flotation of oxide inclusions in liquid steel up into the slag phase.

Heat

Choose the type of heat to apply to the process: **Constant cooling**, **Heat transfer**, and/or **Heat**.

Click the **Add** button to define additional items and the **Remove** button to delete items.

Constant Cooling

If you choose **Constant cooling**, enter a **Name**, choose either **Zone** or **Reaction Zone** and enter a numerical value in the field in MW (megawatts).

If you choose **Zone**, you can further choose either Zone defined above (e.g. **Steel** or **Slag**). If you choose **Reaction Zone**, then heat is lost from the EERZ, the size of which is calculated at each timestep depending on the kinetic parameters defined in **Reaction Zone**.

This parameter defines how much heat is lost from a zone (or the reaction zone) by radiation or convection and results in an overall cooling of the system.

Heat Transfer

If you choose **Heat transfer**, select two zones between where heat should flow and enter a **heat transfer coefficient** in Wm^2/K.

As different amounts of material and also different amounts of heat can be added to the different zones, these temperature are different. As the two zones are in contact heat flows from the hotter zone to the cooler zone thus equalizing the temperature. The amount of heat flowing from one zone to the other is defined by the **Heat transfer**. A high heat transfer coefficient leads to fast temperature equalization, a small heat transfer coefficient results in the zones keeping different temperatures.

Heat

If you choose **Heat**, enter a *Name*, then select **Zone** or **Reaction zone**, choose a Zone (e.g. **Steel** or **Slag**) and enter a percentage of **MW efficiency** in the field.

Select **Heat** if the system is actively heated by an external heat source such as an electric arc or induction coil. Here only the efficiency is defined, which is the percentage of power (for example electrical power) that is transformed into heat that enters the system and heats it up. The profile of power versus time is defined in the **Process Schedule**.

Click **Save** when the Process Model is defined and enter a **Process model name**. Each time you save a process model it adds it to the list on the main **Configuration** window, which you can use in future set ups.

Process Simulation: Materials Tab

The following outlines what you can set on the **Configuration** window **Materials** tab. The overall steps to set this up are described in Defining the Process Simulation.

This section is similar to how you define the materials for the Equilibrium branch. Some information is explained in more detail for Equilibrium Simulation: Conditions Tab and not repeated here.

Material

Materials are grouped into **Steel** (or another user-defined **Metal** group), **Slag** (or another user-defined non-metallic group), and **Gas**.

Some of what you choose from lists in this section depend on what you have entered as the **Process Model** above. For example, the **Zone** or **Reaction zone** options are based on those entries (e.g **Steel** or **Slag**).

To add one or more material groups click the green add button. Click the red minus button to remove a material group. The new material inherits the default settings of that group.

After choosing the Material for the section being defined, also enter a value of the *temperature* in the field. Choose what **Zone** or **Reaction zone** it is to be **Added to**.

The times and amounts of additions are defined in the **Process schedule**.

Show Composition

When you click **Show composition** next to any material group, additional fields display where you can further define each material group.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group.

From the first **Input type** list select **Mass percent**, **Mass fraction**, **Mole percent**, **Mole fraction**, or **Absolute amount**. For **Absolute amount**, you can directly enter values in the fields in the unit selected above for **Amount** (**Tonne**, **Kilogram**, **Gram**, or **Pound**).

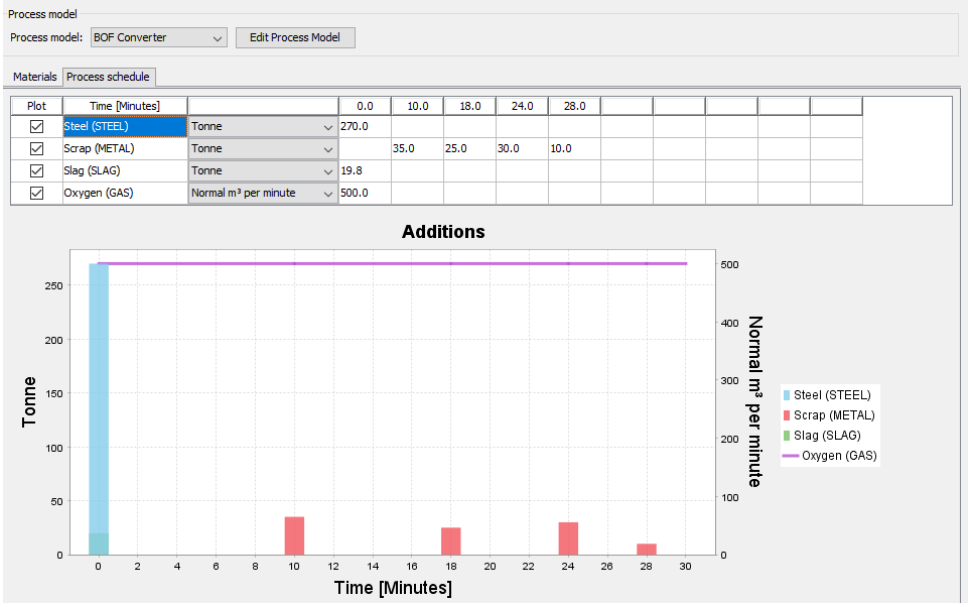
For the next list, the default is based on which group you are defining. For the Steel (Metal) group it is **Element**, for Slag it is **Component**, and for Gas it is **Gas component**.

Choose **Major component** so that as you add other components, the major one is adjusted to be the rest of the composition. Choose **Normalize to total of 100%** so that the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100% If you select **Absolute amount**, **Normalize to total of 100%** is not available.

Process Simulation: Process Schedule Tab

The following outlines what you can set on the **Configuration** window **Process Schedule** tab. The overall steps to set this up are described in Defining the Process Simulation. Also see Working with the Process Schedule.

On the **Process schedule** tab, the sequence and amounts of additions during the duration of the process are defined. All the materials defined in the **Materials** tab automatically are included in the table. If a heat addition is defined in the *Process Model* this is also included in the table.



Plot

Select the **Plot** check box to include or exclude the components in the process schedule plot area, for example, to help you examine the changes in the plot window, after defining the Steel, Scrap, Slag, or Gas rows, see what happens when you remove one or more items from the plot.

Unit

Enter a value and choose a unit **Tonne**, **Kilogram**, **Pound**, **Kilogram per second**, or **Kilogram per minute**. For **Gas** you can also choose **Normal m3 per minute** as the unit.

If a unit **Tonne**, **Kilogram**, or **Pound** is selected, then the additions are defined as one-time additions at a certain time. If a rate is chosen as unit of the addition (such as Kilogram per minute or second, for gas Normal cubic meter per minute or second) then the rate of addition is entered into the table and it stays constant until a different value is entered.

Options Tab

These settings are for the **Process Metallurgy Calculator** and are located on the **Configuration** window → **Options** tab. Only unique settings are described below.

> You can change some of these settings locally for a specific Process Metallurgy Calculator or globally in the **Options** settings. To open the Options window: From the main menu select **Tools → Options**. Click the **Graphical Mode** tab then click **Process Metallurgy**.

- Equilibrium Simulation: Conditions Tab

Material Manager

- See Working with the Material Manager for details.

Use the **Material group** and **Material** lists to create and delete material groups, as well as delete material compositions that are saved from the Process Metallurgy Calculator. It is useful for frequently used materials.

- **Material group**: To create or delete a group, choose it from this list, e.g. **Steel**, **Slag**, or **Gas**. The *Steel* group is simply a generic **Metal** group. You can create other user-defined metal groups and then these are listed. Click **Create group** or **Delete group** as required to manage the list.
- **Material**: To delete a material, choose the group type then select the material composition to delete. For example, select the **Slag** material group, then choose the **Example Slag** material and click **Delete material** to remove it from all lists.

Process Material Equilibrium and Grid

Minimization Strategy

Under *Process Material Equilibrium and Grid*, the *Minimization strategy* setting is used to ensure that the most stable minimum under the specified conditions is computed. The default uses the **Global test preferred** option for **Equilibrium** simulations and the **Local minimization preferred** option for **Process simulations**.

With either the *Global* or *Local preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred** the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.



For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

Max no of iterations

Under *Process Material Equilibrium and Grid*, the default for the **Max no. of iterations** is that the program tries 2000 iterations before it gives up.

Required accuracy

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Smallest fraction

Under *Process Material Equilibrium and Grid*, the default **Smallest fraction** is `1.0E-16`. If this value fails, the program tries other values. This is the value assigned to constituents that are unstable.



The default value is for all phases except for the IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) where the default value is always as 1E-30.

Max grid points (in Global minimization)

Under *Process Material Equilibrium and Grid*, from the **Max grid points** list choose:

- **Coarse** for 2000 grid points, the default,
- **Medium** for 20,000 grid points,
- **Fine** for 200,000 grid points, or
- **Custom** to set your own number of grid points.

Approximate driving force for metastable phases

Under *Process Material Equilibrium and Grid*, the **Approximate driving force for metastable phases** check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus these driving forces may be only approximate.

Force positive definite phase Hessian

Under *Process Material Equilibrium and Grid*, the **Force positive definite phase Hessian** check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

Control step size

Under *Process Material Equilibrium and Grid*, the **Control step size** check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

Timestep Control



This section is used with the **Process simulation** calculations. Read About Dynamic Time Stepping to better understand these settings.

Timestep

Under *Timestep control*, enter numerical values in the fields for the **Timestep**:

- **Initial %**
- **Smallest allowed** in seconds (s)
- **Max % of duration**

Max temperature change per time step

Under *Timestep control*, in the field enter the **Max temperature change per time step** in Kelvin (K).

Scheduler and Event Log Windows

In this section:

Using the Scheduler 355

Event Log Window 357

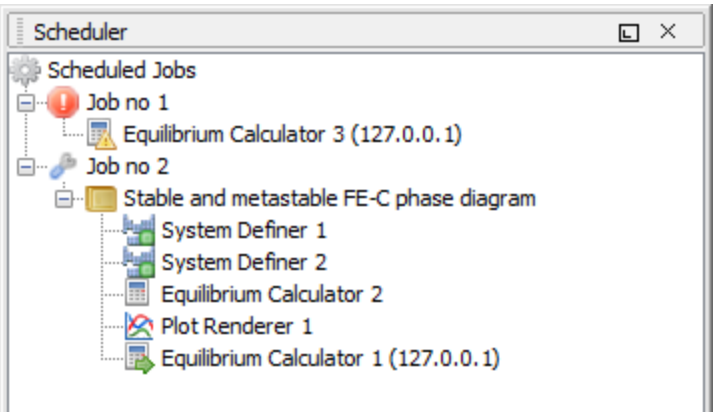
Using the Scheduler

The **Scheduler** window has activity information about current or scheduled jobs. A *job* is any activity you have selected to be performed. The Scheduler also indicates if there is an error during a job and when a job has stopped. If you have set an activity, tree or project to be performed at a later time then this is also listed.

About the Scheduler Jobs

- Whenever you trigger the performance of a whole project, tree or individual activity, all the activities to be performed are shown under a job heading.
- When all the activities belonging to a job are completed the job and its activities disappear from the Scheduler window.
- If there is an error during the performance of an activity, icons for that job and activity remain in the Scheduler window until removed.

Node or Window Status Markers



Managing the Schedule

In the Scheduler window, you can cancel scheduled jobs, remove errors and show information about errors.

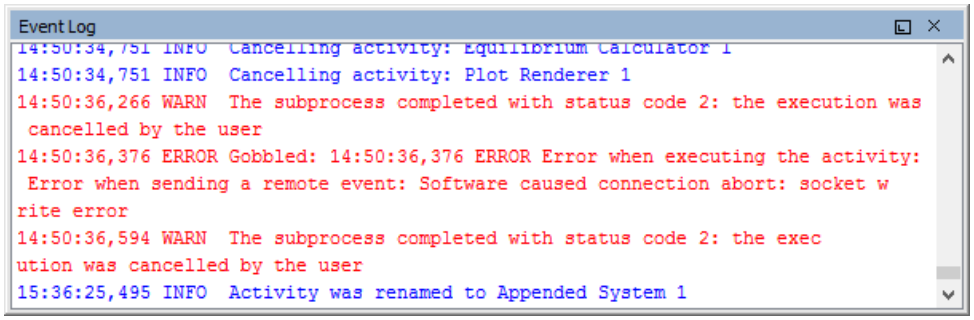
- To cancel all jobs: Right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Cancel All Jobs**
- To remove (clear) all failed activities and jobs: Right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Clear All Errors**

- To cancel a specific job: Right-click the job label (for example, **Job no 1**) and select **Cancel Job**
- To remove (clear) a specific failed job: Right-click the job label (for example, **Job no 1**) and select **Cancel Job**
- To open a window with error details: Right-click the label for the failed job (for example, **Job no 1**), and select **Show Error Log**

Event Log Window

The **Event Log** window is closed by default. Information about what Thermo-Calc is processing or doing is in blue text and error or warning messages are in red text.

Global Settings



- To open the Event Log window: Click the **Event Log** window once to expand it or select it from the **Window → Event Log** menu. Double-clicking the window maximizes it
- To specify the level of detail in the Event Log: From the main menu select **Tools →Options**. In the **General** tab set the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed)

Working with Plots and Tables

In this section:

Performing Projects, Trees and Activities 359
Saving and Printing the Output (Graphical Mode) 360
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Plot Renderer: Convert a Plot to a Table and Export the Data 371
Merging Plots into One Diagram 373
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Performing Projects, Trees and Activities

You can trigger the performance of an activity (also called a *job*) and all the activities below it in the same tree in either the **Project** or **Configuration** window. In the Project window you can also perform a single activity without performing its successors or perform the whole project (all the activity trees).

In the **Configuration** window, click **Perform Tree** to perform the currently selected activity and all the activities below it. If there are no activities below the selected activity, then the button says **Perform** instead.



All activities that must be completed as prerequisites are automatically performed first. For example, if you Perform Tree for a Plot Renderer, then the predecessors, Equilibrium Calculator and System Definer, are automatically performed before the Plot Renderer.

In the Project window, you can do any of the following:

- Perform an activity: Right-click the activity and select **Perform Now**, or **Perform Later** and schedule a time to perform the activity
- Perform an activity and all activities below it in the tree: Right-click any node in the tree and select **Perform Tree Now**. Or select **Perform Tree Later** and schedule a time for all activities in the tree to be performed
- Perform a project: Right-click **My Project** and select **Perform Now** or **Perform Later** and schedule a time to perform all project activities in the tree



If there is an error during the performance of an activity, icons display status markers, which are described in Node or Window Status Markers.

Saving and Printing the Output (Graphical Mode)

Global Settings: Graphical and Console Mode Plotting

Output can refer to results in the form of tabulated data in a table or a diagram.

The terms *diagram* and *plot* are interchangeable. The commands in Console Mode generally use the term diagram and in Graphical Mode it is also called a plot (e.g. the Plot Renderer).

In Graphical Mode the output is displayed in the **Results** window. The output can be in the form of a table or a diagram (plot). In both cases you can save from the **Configuration** or **Results** windows. You can print the table or diagram from the **Results** window.

Saving Diagrams

You can save the output in a variety of file formats. For JPG and PNG images you can also adjust the image quality.

In Console Mode, the diagram is output to the **Console Results** window after using the PLOT_DIAGRAM command.

In Graphical Mode, the diagram is output to the **Results** window after performing a tree that includes a Plot Renderer.

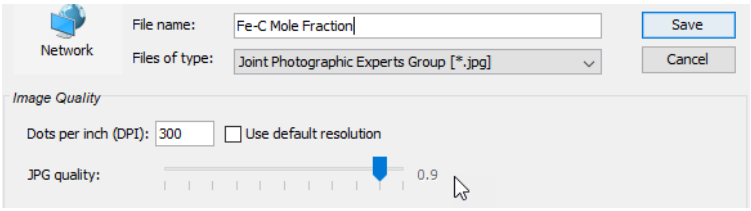
1. In the **Results** window, right-click the diagram and select **Save as**.

   In the Graphical Mode **Configuration** window you can also click the **Save Diagram** (or **Save table**) buttons to open the **Save** window.

2. In the **Save** window:
   a. Navigate to where you want to save the diagram.
   b. Enter a **File name**.
   c. From the **Files of type** list choose **png** (the default), **jpg**, **ps**, **pdf**, **gif**, **svg**, or **emf**.

d. For PNG and JPG files only, under the **Image Quality** section, choose to improve the resolution of the image. For JPG files you can also adjust the file size.

- To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** check box. Then enter a numerical value in the **Dots per inch (DPI)** field.
- For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.



e. When you are ready, click **Save**.

Saving (Exporting) Tables

You can save the table output in different file formats from the Table Renderer and Plot Renderer **Configuration** and **Results** windows.

In Graphical Mode, a table is output to the **Results** window after performing a tree that includes a Table Renderer. It is also output using the **Table View** button located on the Plot Renderer **Configuration** window.

1. Generate a table. Then depending on which window you are in:
   - In the **Results** window, right-click the table and select **Save as**, or
   - In the **Configuration** window click the **Save table** button.
2. In the **Save As** window:
   a. Navigate to where you want to save the table.
   b. Enter a **File Name**.
   c. From the **Files of Type** list choose **Text [*.txt]**(the default), **Hyper Text Markup [*.html]**, or **Excel [*.xls]**.
   d. When you are ready, click **Save**.

Printing Output

In the **Results** window, right-click the table or diagram and choose **Print**. Select additional settings as required on the **Print** window.

Zooming In and Out

In the **Results** window (where the plots are):

- Use the mouse scroll wheel to zoom in and out.
- Click and drag the mouse from left to right to highlight an area of the plot to zoom into a specific point. Use the scroll wheel to continue zooming in or out.

Resetting a Plot to the Default View

- For 2D plots, click and drag the mouse from right to left.
- For 2D and 3D plots, click **Perform Tree** to regenerate the plot in the **Results** window.

Rotating 3D Plots

In the **Project** window (where the activity nodes are):

- Right-click and select **Zoom In** or **Zoom Out**.
- To go back to the default zoom, select **Reset Zoom**.

Plotting Options

The Plot Renderer is a dynamic activity node with options such as being able to:

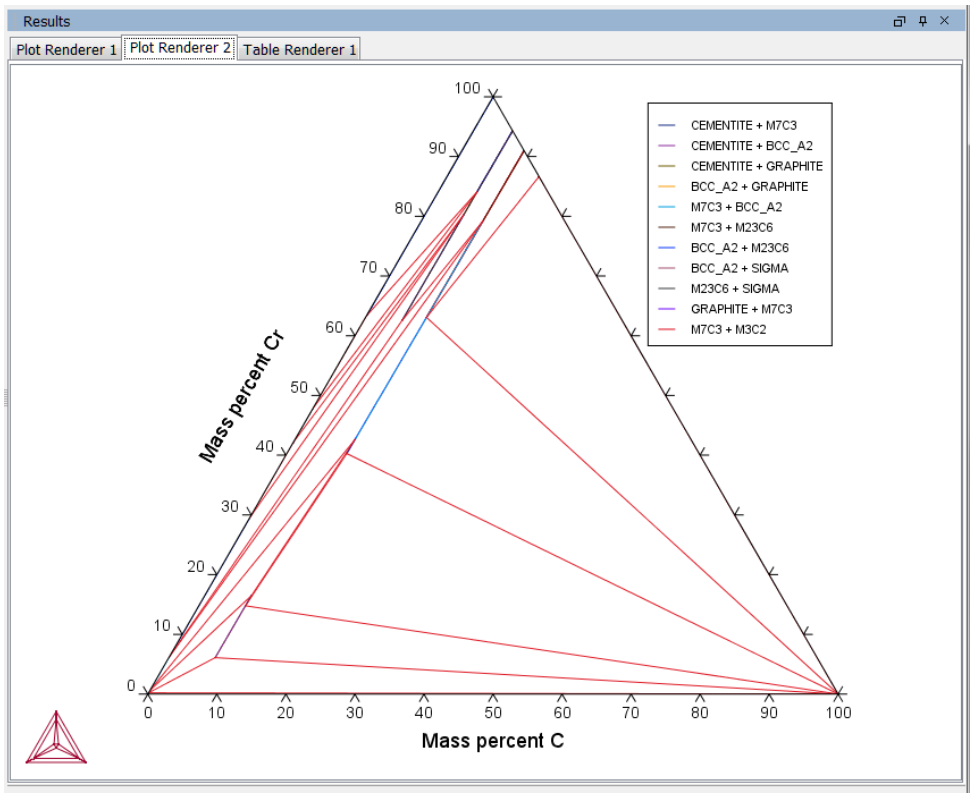
- add more than one Plot Renderer to its predecessor node (i.e. one of the calculator activities),
- add axes to the plots,
- merge results in one plot, and
- choose from a variety of plotting modes (grouped, flexible, cross plot, statistical, CCT, or TTT).

Additional settings are also described in Configuration Settings.

Plots Can Have More Than One Predecessor

A Plot Renderer can have several predecessors (if you want to plot several calculations in the same diagram), in which case there are several tabs in the Configuration window, one for each predecessor.

Plotting Several Calculations in One Diagram

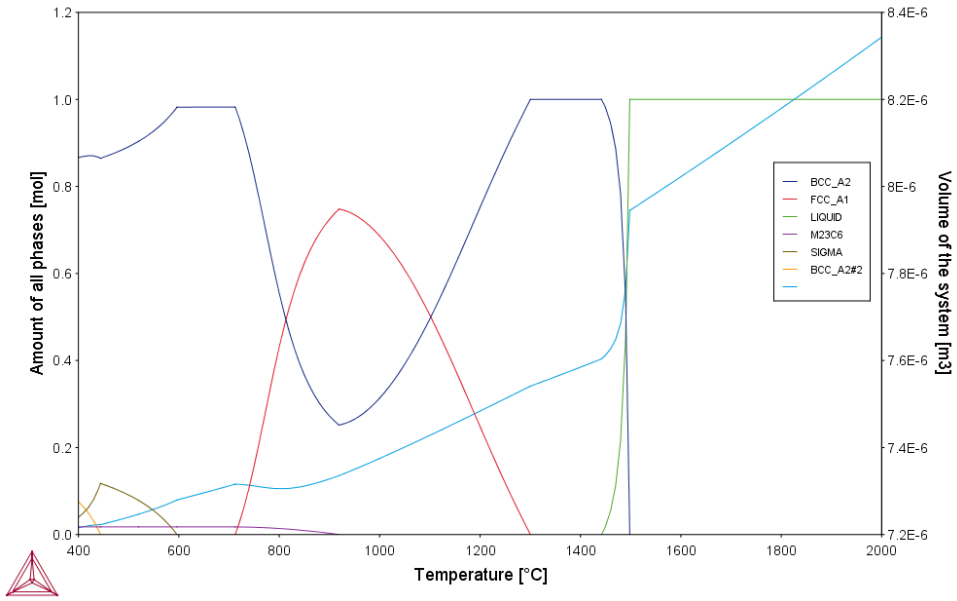


Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Results window as different tabs. The figure is from Graphical Mode example T_04.

Add Axes to Plots

You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time as in the figure.

- Adding Axes to a Diagram



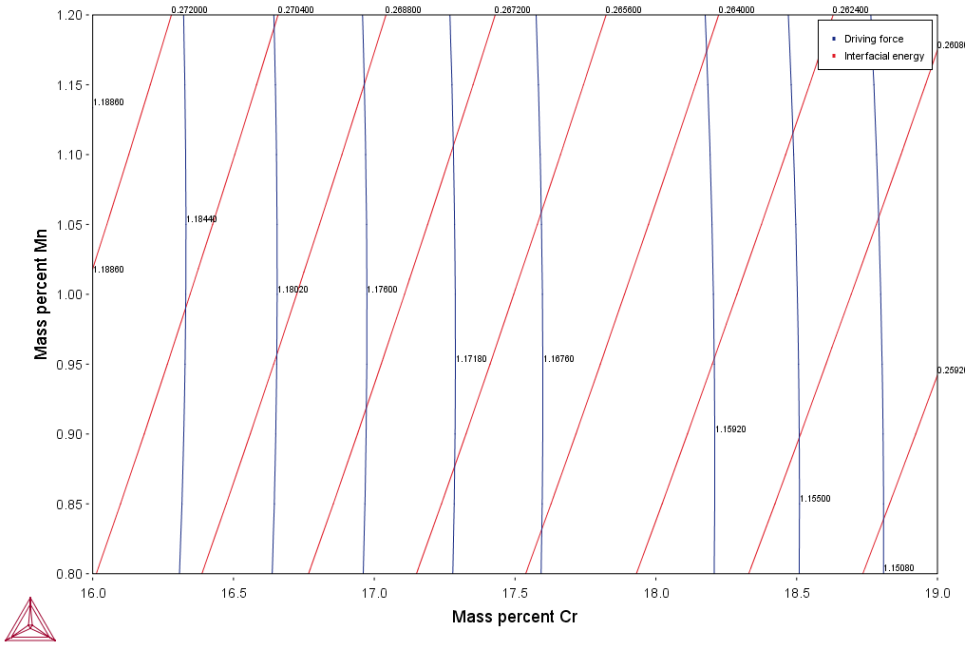
Two variables plotted on the Y-axis.

Merge Results in One Plot

You can merge (or overlay) calculated results for several variables into one plot. This is similar to adding an axis, but instead of displaying different variables along the X- and/or Y-axes, the same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).

As in the figure (from example PM_G_03 in Graphical Mode Examples), the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

- Merging Plots into One Diagram



A contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.

Choose a Plot Mode

Plotting Modes and Working with Batch Calculations

- Use **Flexible mode** to individually add and configure axes quantities and change the units or other associated settings one at a time.
- Use **Grouped mode** to add and configure groups of axis quantities at the same time and of the same type. For example, change units or settings in groups with similar settings like temperature units or axis types.
- Use **Statistical mode** to select **Frequency** or **Normal probability** as the *Axis variable* and then the *Axis type* is set to **Histogram** or **Probability**, respectively.
- Use **Cross plot mode** to plot the experimental data from a Batch calculation with the calculated result, e.g. you might be looking at liquidus temperature and now can plot both to compare the experimental data against the Thermo-Calc calculated results.

You choose the experimental data value (which is read from the data file) as an X- or Y- Axis variable and then the calculated result as the other X- or Y- Axis variable.

Two other modes are available with a Steel Model Library license and when using the **Property Model Calculator**.

- Use **TTT mode** to make a TTT diagram from a One-axis calculation with temperature. The x- and y-axes are time and temperature, respectively. Time quantities (such as pearlite-start, bainite-start) are plotted as functions of temperature. Temperature quantities (such as Ms, M50) are independent of time and plotted as horizontal lines.

- Use **CCT mode** to make a CCT diagram from a One-axis calculation with Log10 (cooling rate [K/s]) from the CCT Diagram Property Model. The x- and y-axes are time and temperature, respectively. Result quantities defined as time-temperature pairs are identified and plotted. Cooling curves are also automatically added in the plot.

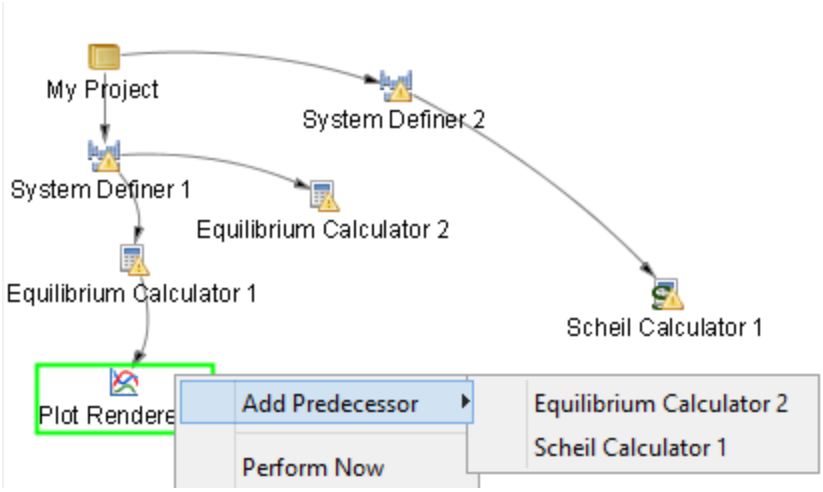
Plot Settings: TTT Mode and Plot Settings: CCT Mode

Plotting Several Calculations in One Diagram

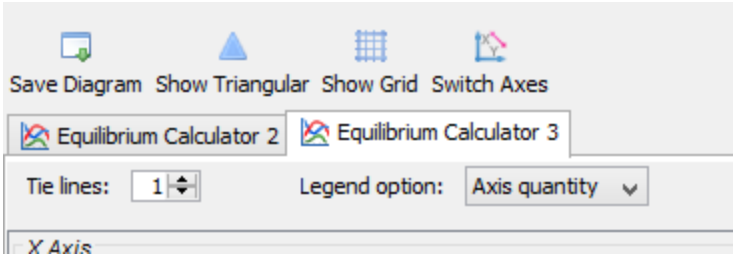
To plot several calculations in one diagram, you must have, in addition to the Plot Renderer's original predecessor, at least one available Plot Renderer predecessor in your project, for example, the additional predecessor can be an Equilibrium Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator or Experimental File Reader.

1. In the Project window click the **Plot Renderer** node.

2. In the **Configuration** window click **Add Predecessor**. Or right-click the **Plot Renderer** and choose **Add Predecessor**.

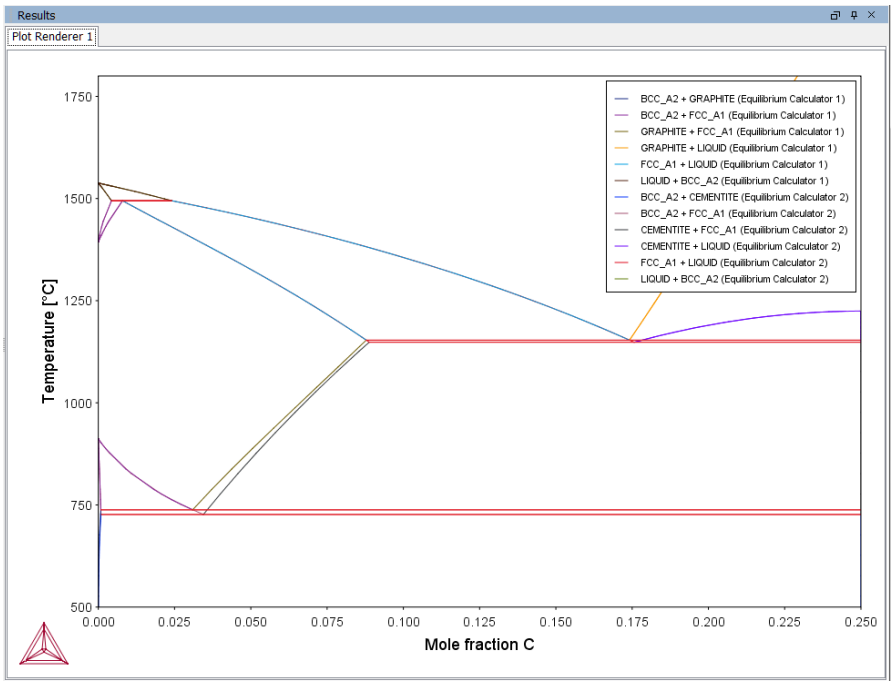


3. Select a predecessor. When added, the extra predecessor is linked to the Plot Renderer. On the Plot Renderer's Configuration window, the predecessors are shown as two tabs:



4. Configure how you want each calculation plotted on the tabs in the **Configuration** window, then click to **Perform** the Plot Renderer activity.

The calculations are plotted in the same diagram in a tab in the **Results** window. If any of the axis variables of the plots differ, then the label and scale of all calculations are shown parallel to each other. The following shows two calculations where different axes variables are plotted.



Plot Renderer: Convert a Plot to a Table and Export the Data

For all calculation types and calculators, the associated Plot Renderer has a Table View button you can use to convert a plot to table data. Once the plot data is converted, you can toggle between displaying the Plot or Table in the Results window as well as save the table and export to file.

For the Table Renderer only single equilibrium and property diagram (stepping) calculations are available.

Converting a Plot to a Table on the Plot Renderer

1. Set up the Plot Renderer for your particular calculation and click **Perform** to display the plot in the **Results** window.
2. On the Plot Renderer **Configuration** window, click the **Table View** button (toggled ON).
3. Choose the **Decimal digits** and **Number format** (**Auto**, **Decimal**, or **Scientific**) to display in the table.
4. Click **Perform**. This converts the plot data to display table data in the **Results** window.

Switching Between a Plot and a Table in the Results Window

Once the plot data is converted, you can toggle between displaying the Plot or Table in the Results window

- To display the Table: On the Plot Renderer **Configuration** window, click the **Table View** button to toggle it ON and then click **Perform** to generate the table.
- To display the Plot: On the Plot Renderer **Configuration** window, click the **Table View** button to toggle it OFF and then click **Perform** to generate the plot.

Saving the Table (Exporting the Data)

Once the plot data is converted to a table, you can save/export this to file.

1. Convert the plot to a table (the **Table View** button is toggled ON).
2. Click **Save table** to export the table data.
3. In the **Save As** window navigate to where you want to save the table.
4. Enter a **File Name**.
5. From the **Files of Type** list choose **Text [*.txt]**(the default), **Hyper Text Markup [*.html]**, or **Excel [*.xls]**.
6. Click **Save**.

Saving and Printing the Output (Graphical Mode) for more options.

Merging Plots into One Diagram

You can merge (or overlay) calculated results for several variables into one diagram. The same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).

You cannot overlay heat map or frequency plots.

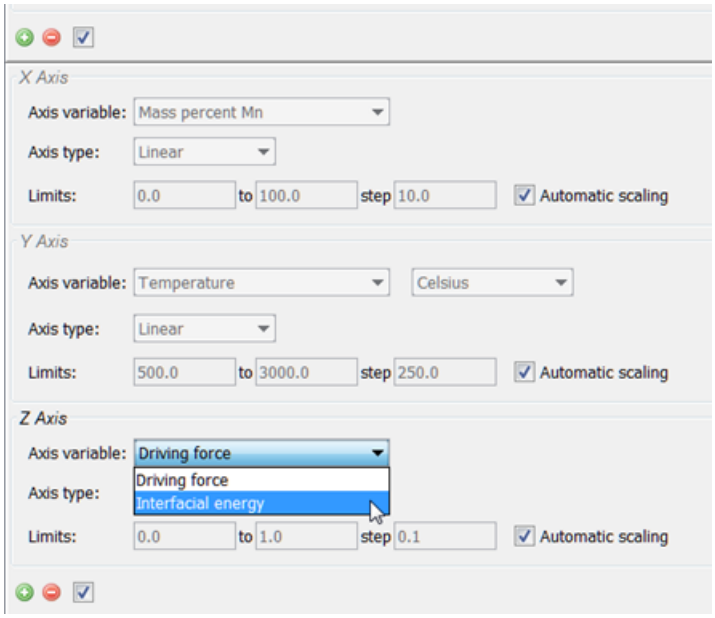
The following uses example PM_G_03: Driving Force and Interfacial Energy to describe the steps to overlay two plots: the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

1. In the **Project** window right-click the calculator node (e.g. Property Model Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.

Example

In this example the Property Model Calculator is set to a *Grid* calculation type.

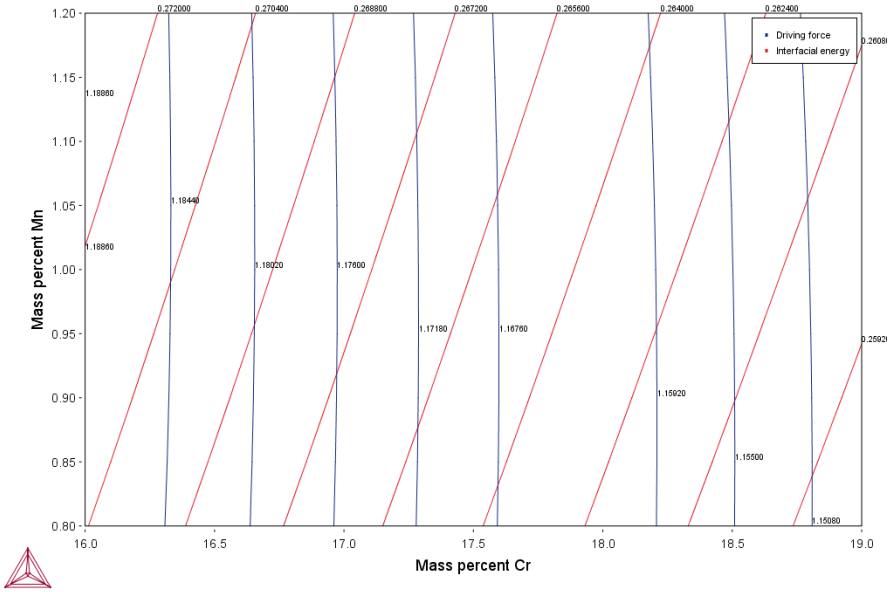
Choose **On** for the **Legend option** and **Contour** as the **Plot type**.



4. Click the **Add an axis** button. A new axes settings section is added underneath.

5. From the *Z Axis* section choose the **Axis variable**. In this example, **Interfacial energy**.
6. Click **Perform** to plot both on the same diagram.

   In this case, a contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.

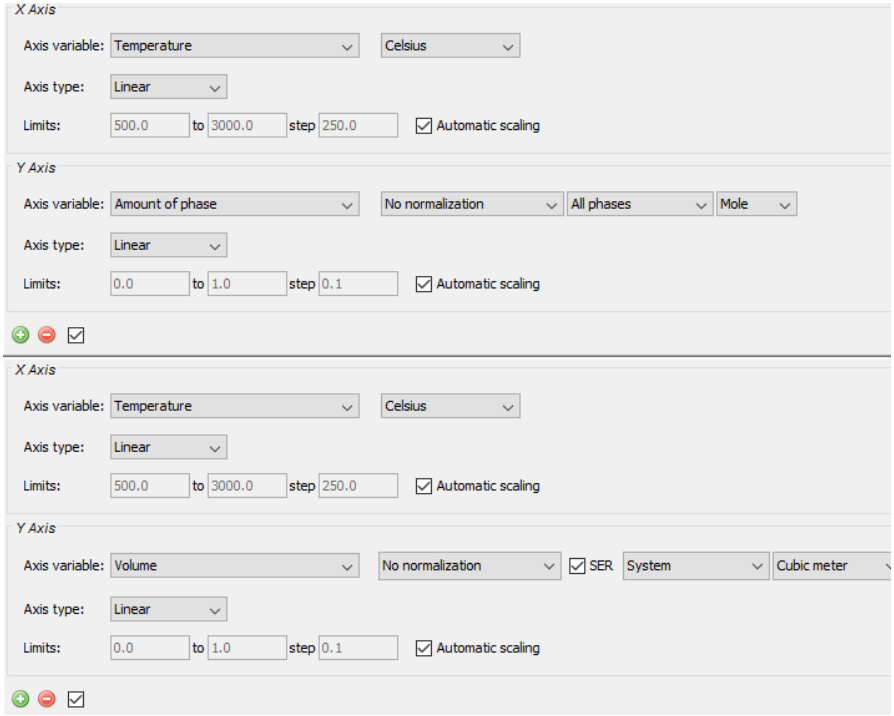


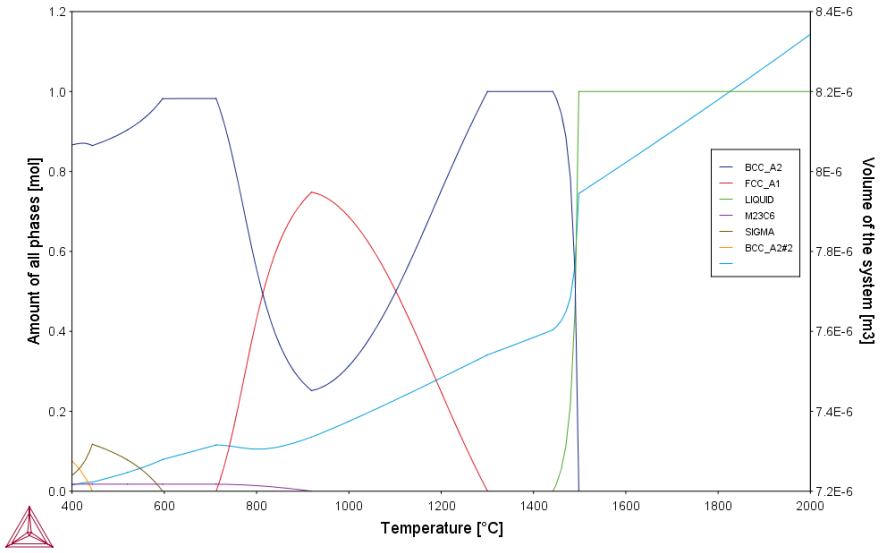
Adding Axes to a Diagram

You can add additional *X*- and/or *Y*-axes to a plot to compare two or more variables at the same time.

1. In the **Project** window right-click the calculator node (e.g. an Equilibrium Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.
4. Click the **Add an axis** button. A new settings section is added underneath.
5. From the *X Axis* and/or *Y Axis* sections define another **Axis variable** and choose an **Axis type**.
6. Click **Perform** to plot both variables on the selected axis, in this example, the Y-axis.

   In this example **Amount of phase** and **Volume** are selected as the Y-axis variables and **Temperature** as the X-axis variable. The plot is an example of the output.




Amount of all phases [mol]
Volume of the system [m3]
Temperature [°C]
BCC_A2
FCC_A1
LIQUID
M23C6
SIGMA
BCC_A2#2
1.2
1.0
0.8
0.6
0.4
0.2
0.0
8.4E-6
8.2E-6
8E-6
7.8E-6
7.6E-6
7.4E-6
7.2E-6
400
600
800
1000
1200
1400
1600
1800
2000

Plotting Modes

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of plotting modes (grouped, flexible, cross plot, statistical, CCT, or TTT).

Additional settings are also available as described in Configuration Settings.

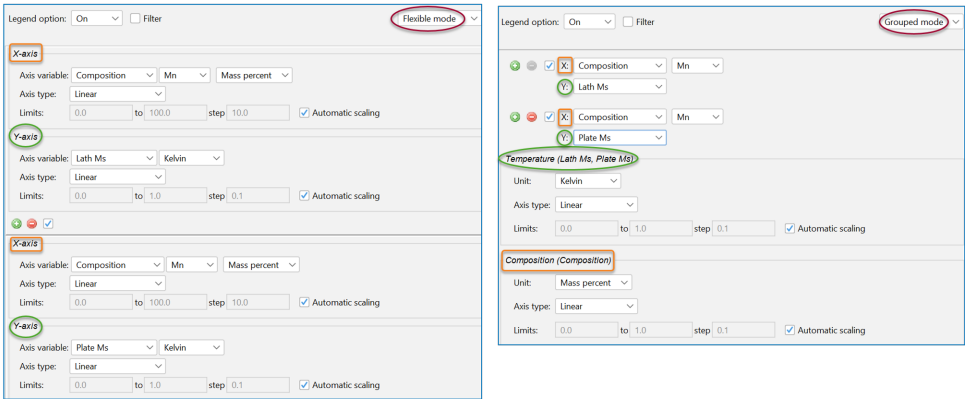
Flexible Mode and Grouped Mode

Both are available with the **Equilibrium Calculator** and **Property Model Calculator** > **One axis** *Calculation Type*. Flexible mode is also available with Property Model Calculator **Min/Max** calculations.

- Use **Flexible mode** to individually add and configure axes quantities and change the units or other associated settings one at a time.

- Use **Grouped mode** to add and configure groups of axis quantities at the same time and of the same type. For example, change units or settings in groups with similar settings like temperature units or axis types.

This example uses Property Model example *PM_G_06_Yield_Strength_HEA.tcu*. If you have a license for the Steel Model Library, you can also see an example of switching between Flexible and Group mode in the **Steels** example *PM_Fe_02_Fe-Mn_Martensite_Morphologies.tcu*.



Comparing Flexible mode (left) to Grouped mode (right) on a Plot Renderer as a successor to a Property Model Calculator. The advantage of the Grouped mode is that you can, for example, configure or edit settings in one place, making it easier to manage and work with the plot quantities.

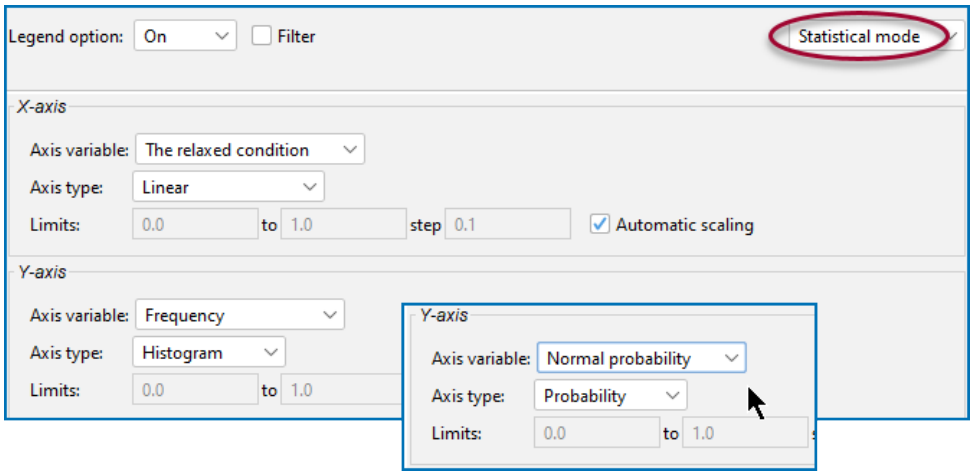
STATISTICAL MODE

Available with:

- **Property Model Calculator** > **Batch** or **Uncertainty** *Calculation Type*.
- **Process Metallurgy Calculator** > **Uncertainty** *Calculation Type*.

Use **Statistical mode** to select **Frequency** or **Normal probability** as the *Axis variable* and then the *Axis type* is set to **Histogram** or **Probability**, respectively.

This example uses Property Model example *PM_G_01_Phase_Transition.tcu*.



The two combination options, Frequency>Histogram or Normal probability> Probability, selected with the Statistical mode on a Plot Renderer as a successor to a Property Model Calculator.

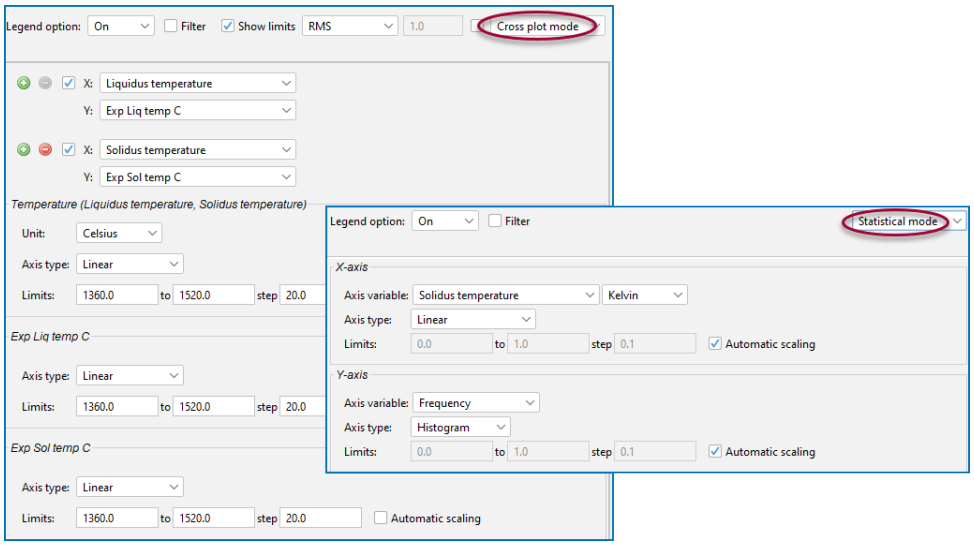
CROSS PLOT MODE

Available with **Property Model Calculator** > **Batch** *Calculation Type*.

Use **Cross plot mode** to plot the experimental data from a Batch calculation with the calculated result, e.g. you might be looking at liquidus temperature and now can plot both to compare the experimental data against the Thermo-Calc calculated results. You choose the experimental data value (which is read from the data file) as an X- or Y- Axis variable and then the calculated result as the other X- or Y- Axis variable.

Working with Batch Calculations

This example uses Property Model example *PM_G_12_Solidus_Liquidus_Batch_Calculation.tcu*.



For a Batch calculation, and when the data file contains experimental (Exp) data, you can use the Cross plot mode on a Plot Renderer to compare it to the simulated results. You can also switch to using Statistical mode.

TTT Mode and CCT Mode

Available with a Steel Model Library license and when using the **Property Model Calculator** and a **One axis** *Calculation Type*.

- Use **TTT mode** to make a TTT diagram from a One-axis calculation with temperature. The x- and y-axes are time and temperature, respectively. Time quantities (such as pearlite-start, bainite-start) are plotted as functions of temperature. Temperature quantities (such as Ms, M50) are independent of time and plotted as horizontal lines.

- Use **CCT mode** to make a CCT diagram from a One-axis calculation with Log10 (cooling rate [K/s]) from the CCT Diagram Property Model. The x- and y-axes are time and temperature, respectively. Result quantities defined as time-temperature pairs are identified and plotted. Cooling curves are also automatically added in the plot.

For examples of these settings windows, see Plot Settings: CCT Mode and Plot Settings: TTT Mode

Heat Map, Contour, and 3D Plots

Grid Calculations

Using the Equilibrium, Property Model, or Process Metallurgy Calculators, you can choose to plot a *Heat map*, *Contour*, or *3D* diagram.

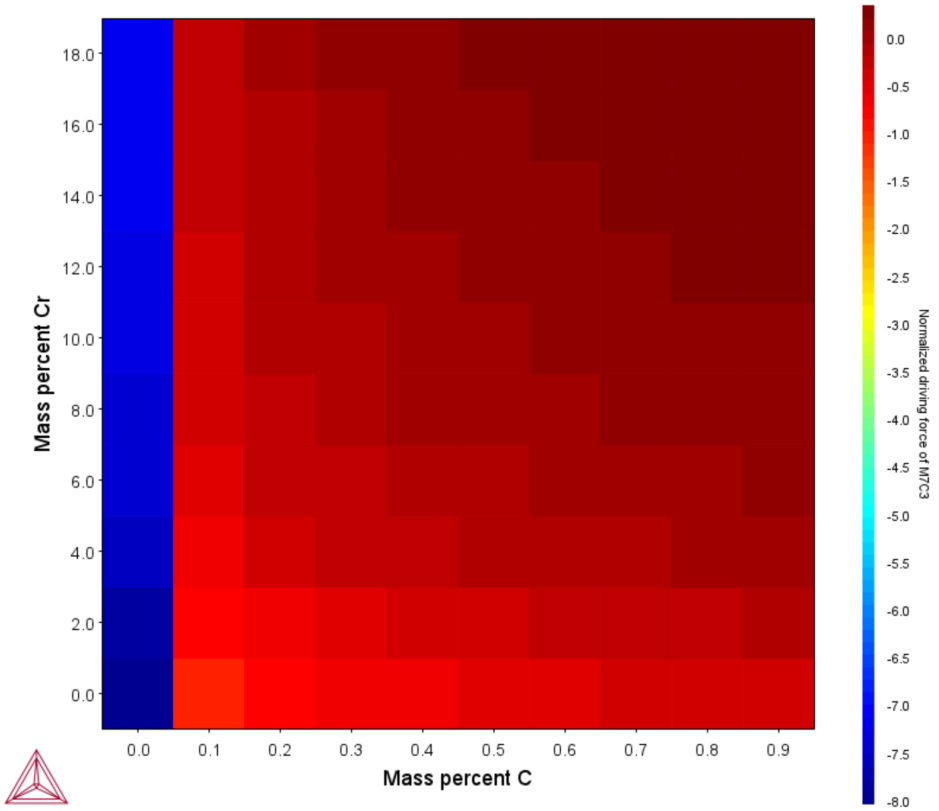
- Equilibrium Calculator, Property Model Calculator, and Process Metallurgy Calculator

Heat Map

Each Z-axis variable value in the grid is represented by a color-coded area, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.

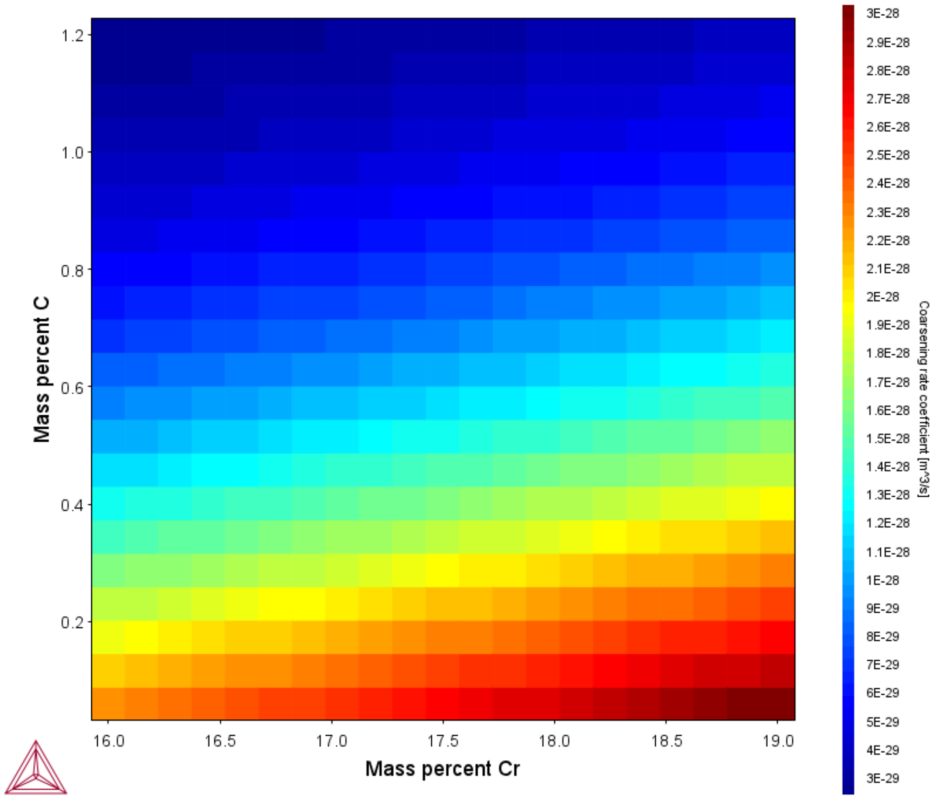
Using an Equilibrium Calculator

Equilibrium Calculator: T_09: Carbide Driving Force Heat Map



Using a Property Model Calculator

Property Model Calculator: PM_G_02: Coarsening and Interfacial Energy

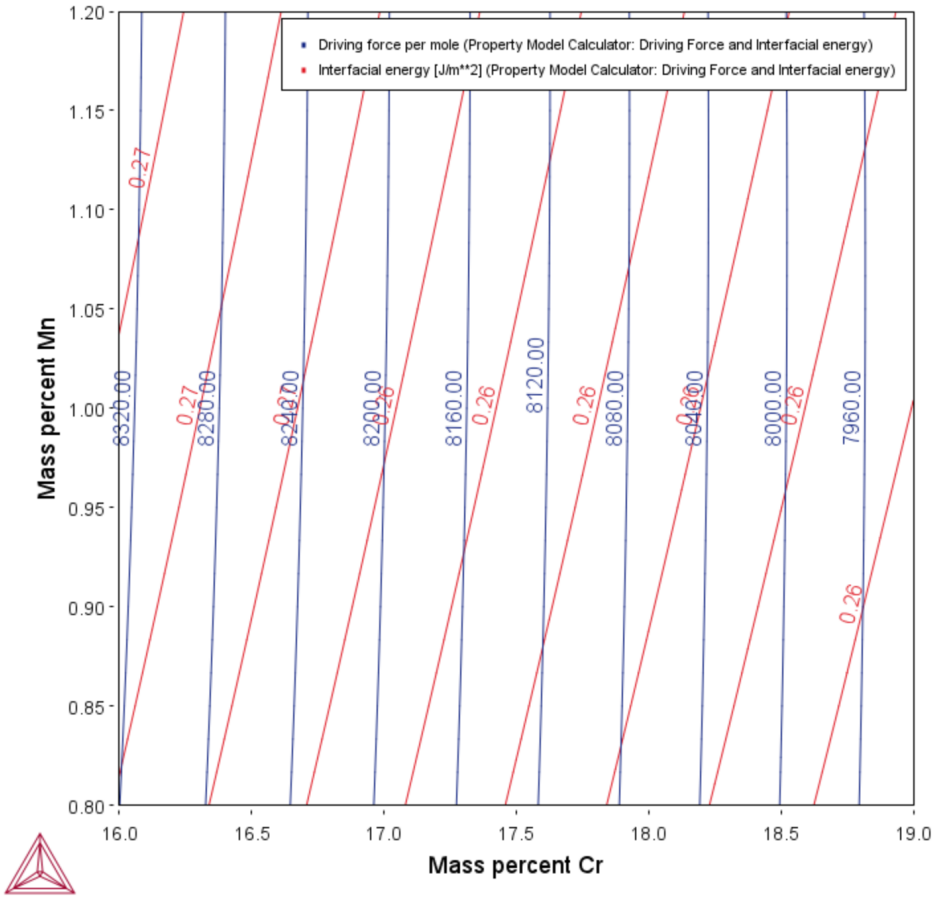


Contour

Using a Property Model Calculator

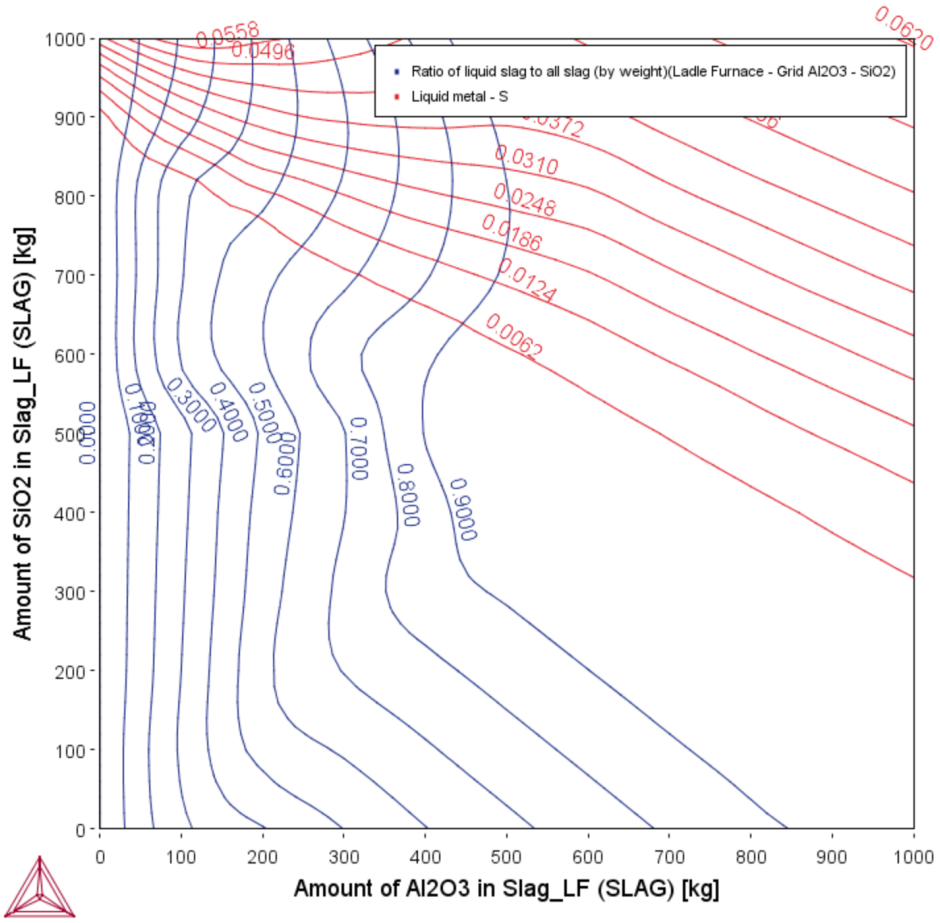
Property Model Calculator: PM_G_03: Driving Force and Interfacial Energy

Z-axis variable values are traced with curves in the same way that height values are traced with curves on a topographical map. The colors used originate from the different data series.



Using a Process Metallurgy Calculator

Process Metallurgy Calculator: PMET_02: Desulphurization in a Ladle Furnace (LF)

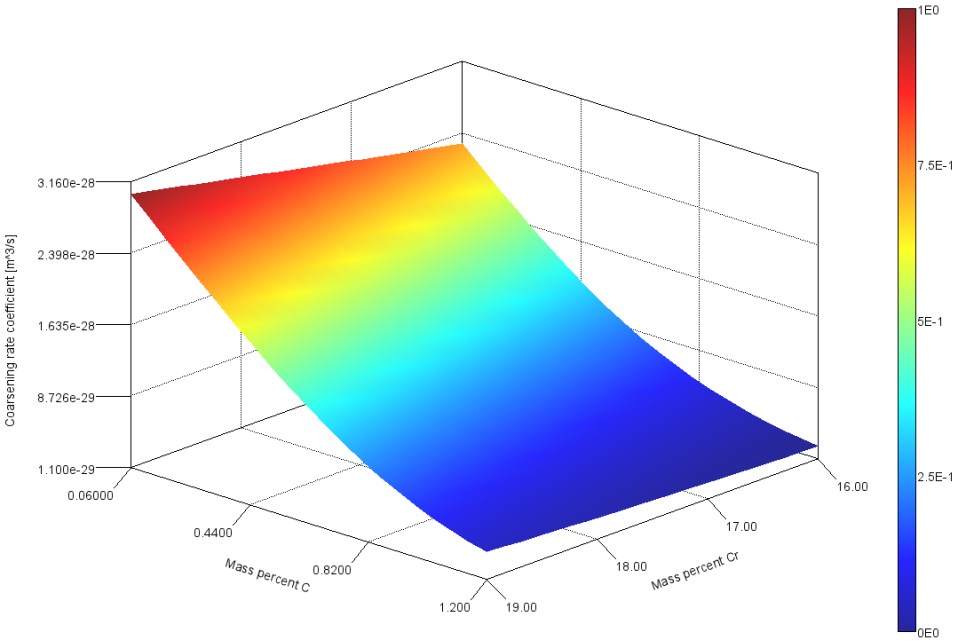


3D

When in the Thermo-Calc help (press F1), go to Rotating 3D Plots to watch a short video showing you how to rotate this plot in the Results window.

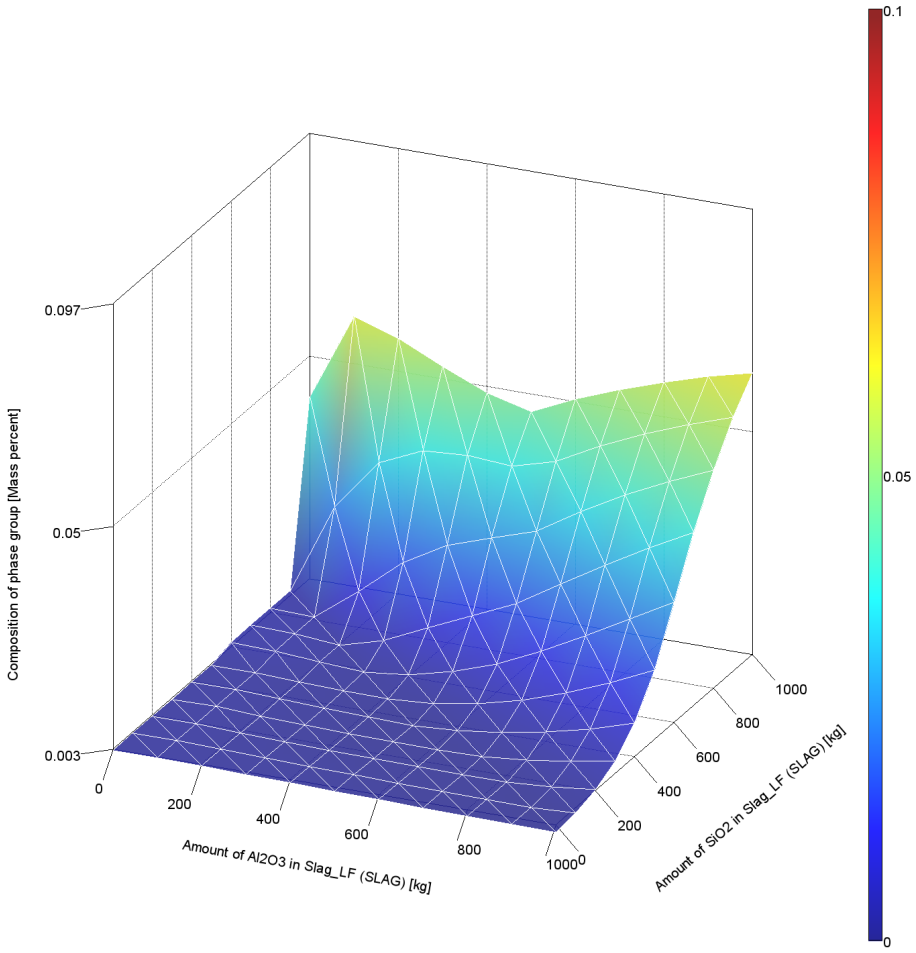
Using a Property Model Calculator

Property Model Calculator: PM_G_02: Coarsening and Interfacial Energy



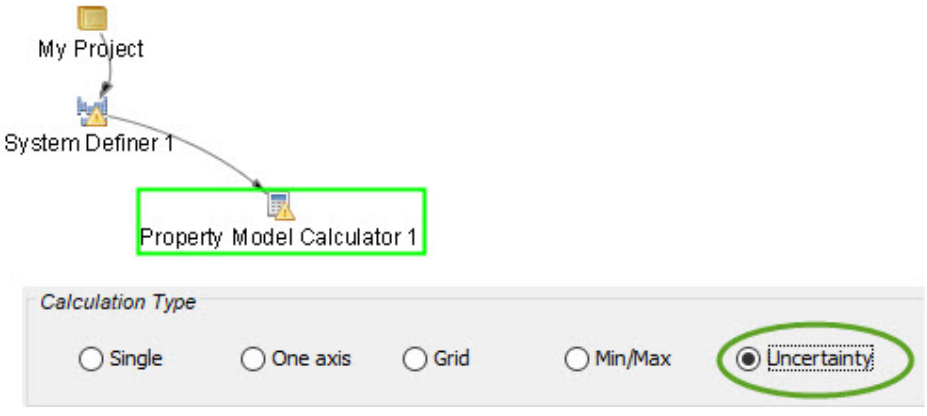
Using a Process Metallurgy Calculator

Process Metallurgy Calculator: PMET_02: Desulphurization in a Ladle Furnace (LF)



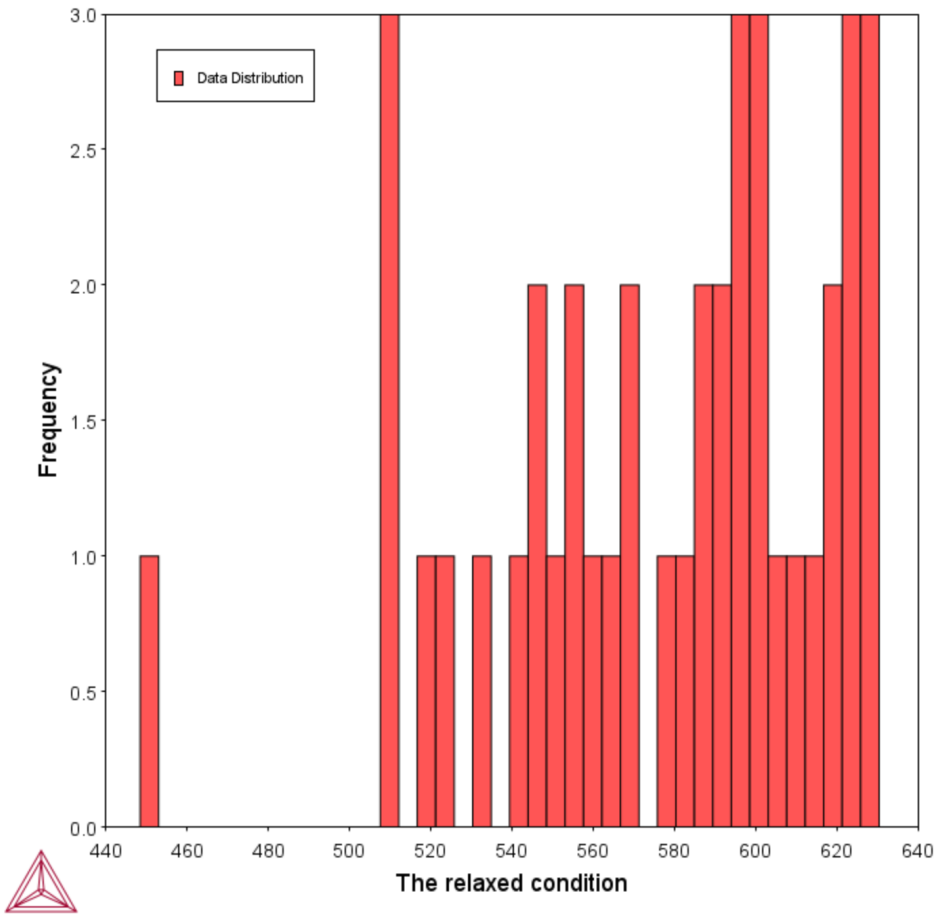
Uncertainty Calculations

Using a **Property Model Calculator** or **Process Metallurgy Calculator** (Uncertainty calculation) you can choose to create either a *histogram* or *probability* plot.

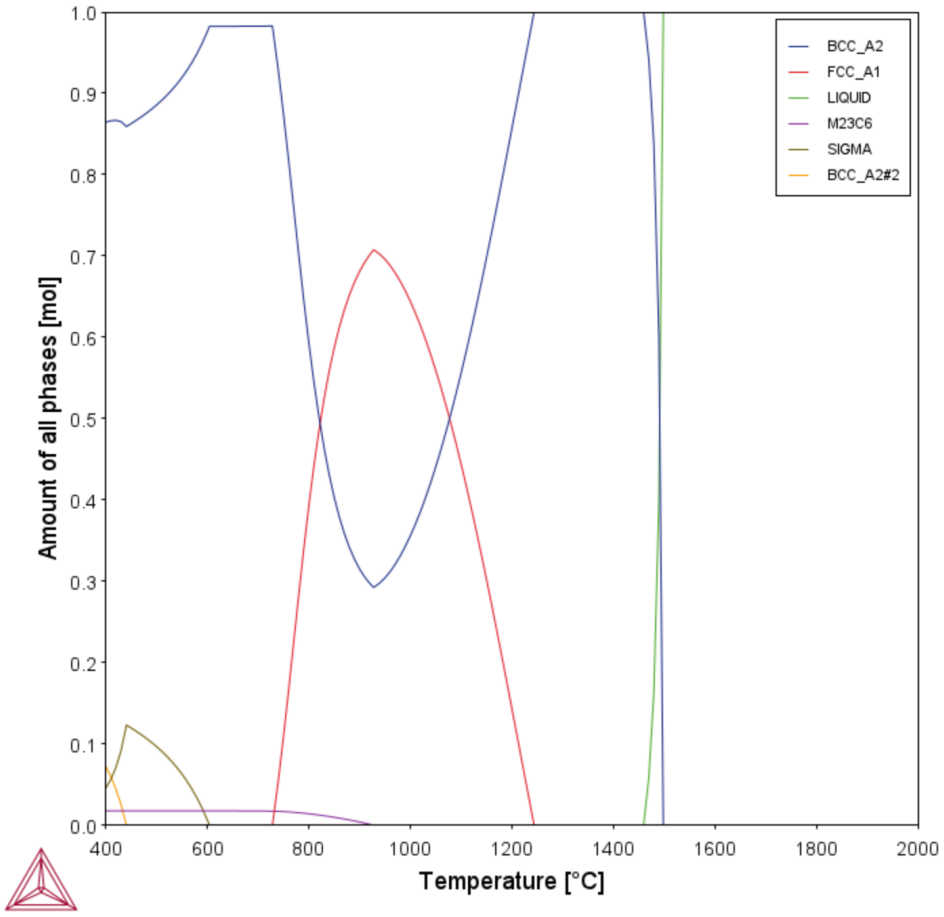


The following use the Property Model Calculator example: PM_G_01: Phase Transition

Histogram



Probability



About the Uncertainty Calculations

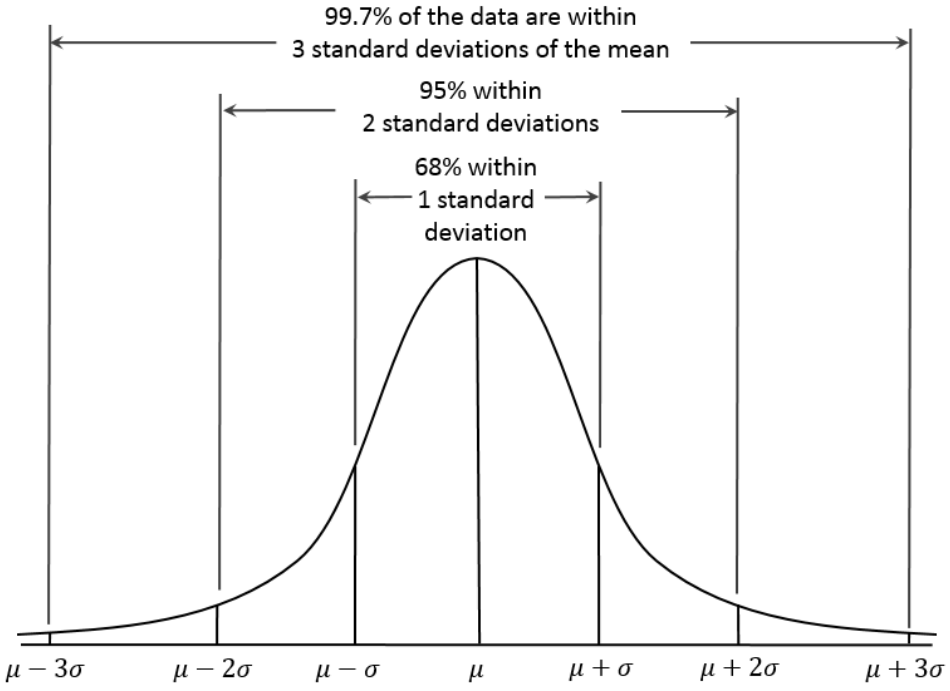
The **Uncertainty** calculation in Thermo-Calc uses the values (the mean) entered for quantities under the *Condition Definitions* section as the starting point to estimate, within a certain probability, the true variation of the quantity. Uncertainty calculations are available with the Property Model Calculator and the Process Metallurgy Calculator.

An example of a Gaussian distribution is shown next. The example uses the Phase Transition Property Model Settings and an **Uncertainty** *Calculation Type* to describe how the sampling of data is performed. The example PM_G_01: Phase Transition predicts the transition temperature to the unwanted brittle Sigma phase and shows how the temperature is influenced by changes to a steel alloy's composition.

Gaussian Distribution, the 3-Sigma Rule

- The *mean* is at the peak of the curve (labeled μ).
- The *standard deviation* (σ) is a plus and minus range, ±1σ, ±2σ or ±3σ, of the variance from the mean.

Image by Dan Kernler: https://en.wikipedia.org/wiki/Normal_distribution#/media/File:Empirical_Rule.PNG.

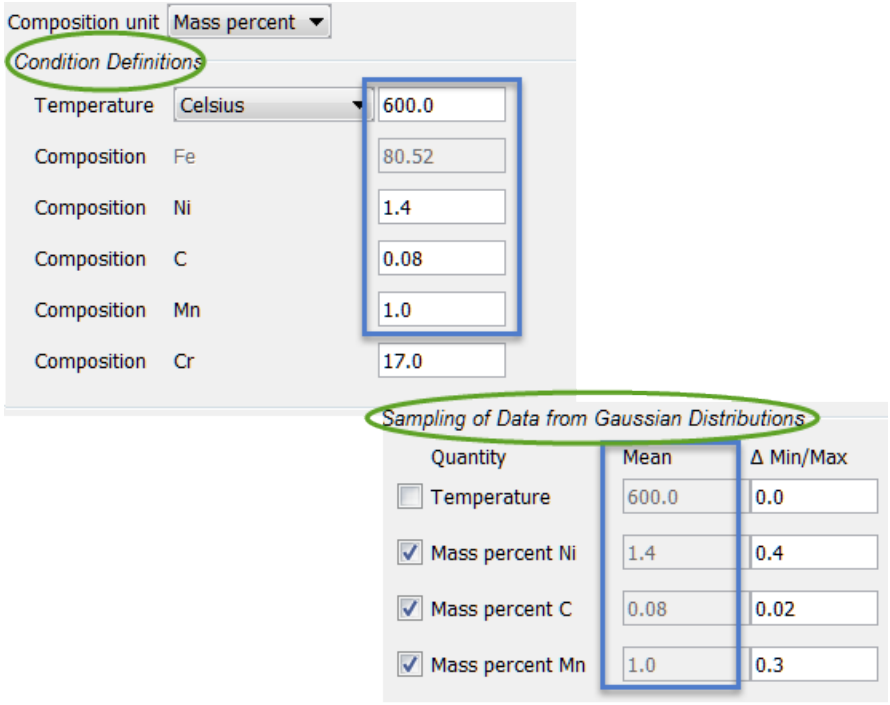


As long as the number of events (the sample size) is very large, then the Gaussian distribution function can be used to describe physical events. A Gaussian distribution is assumed to describe how each quantity varies in an uncertainty calculation, as shown next.

Condition Definitions and Sampling Settings

In Thermo-Calc, the mean of the quantity's distribution is defined in the *Condition Definitions* section. The **Mean** is then used in the *Sampling of Data from Gaussian Distributions* section as the starting point for how much you want to deviate from this value.

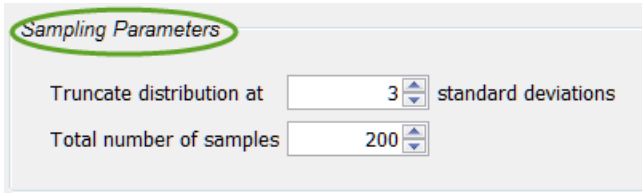
The mean defined under *Condition Definitions* is used during the sampling.



The values entered in the Δ **Min/Max** fields are the resulting width of the distribution corresponding to the 95% confidence interval (approximately μ ± 2σ) shown in *Gaussian distribution, the 3-sigma rule*.This confidence interval means that approximately 95% of the sampled values fall within these limits, as shown next.

Sampling Parameter Settings

The default value for truncating the distribution is set at **3 standard deviations** in the *Sampling Parameters* section. This is also where you set the **Total number of samples**. The default is 200. In order to maintain a Gaussian distribution for the varied quantities, this number should not be too low.

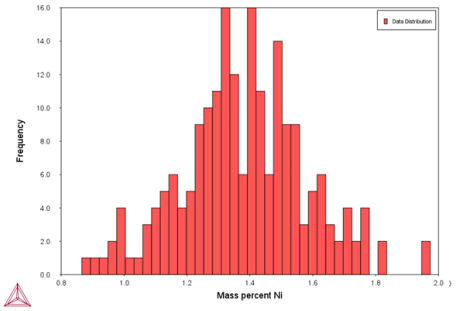


You can experiment by varying the conditions and the number of samples to see the distribution results smooth out as is to be expected based on the Central Limit Theorem, as shown in the histogram plot. You can also plot the results as a normal probability.

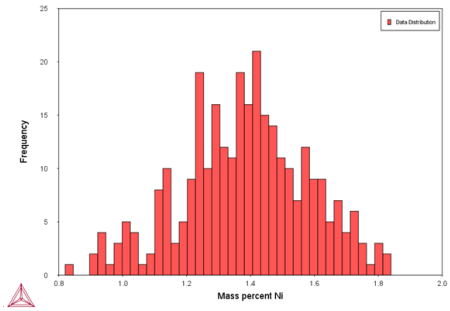
Histogram Plot

This series of histogram plots shows the uncertainty calculations sampling data from Gaussian distributions. On the **Plot Renderer** the variable is set to measure the **Composition** of **Ni**. It compares the Ni composition where the total sample size is increased. In the example, the initial sample size uses the default, 200, and then the sample size is increased to 300, 400, 600, 800, and 1000, showing how the plot follows the Gauss distribution.

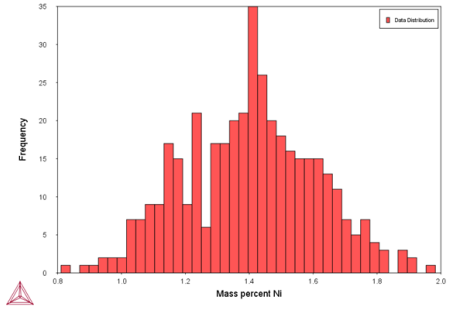
Total samples = 200



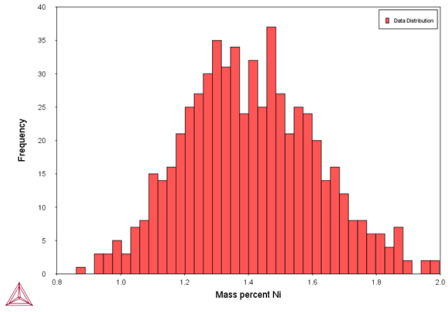
Total samples = 300



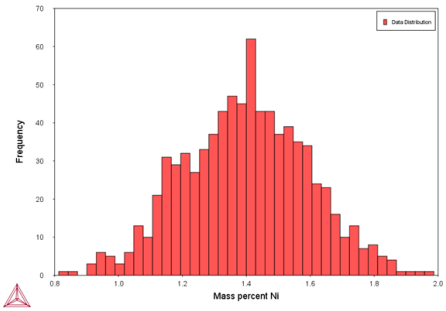
Total samples = 400



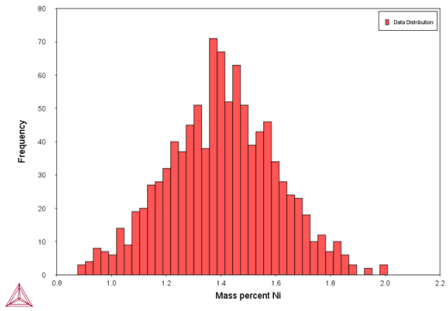
Total samples = 600



Total samples = 800

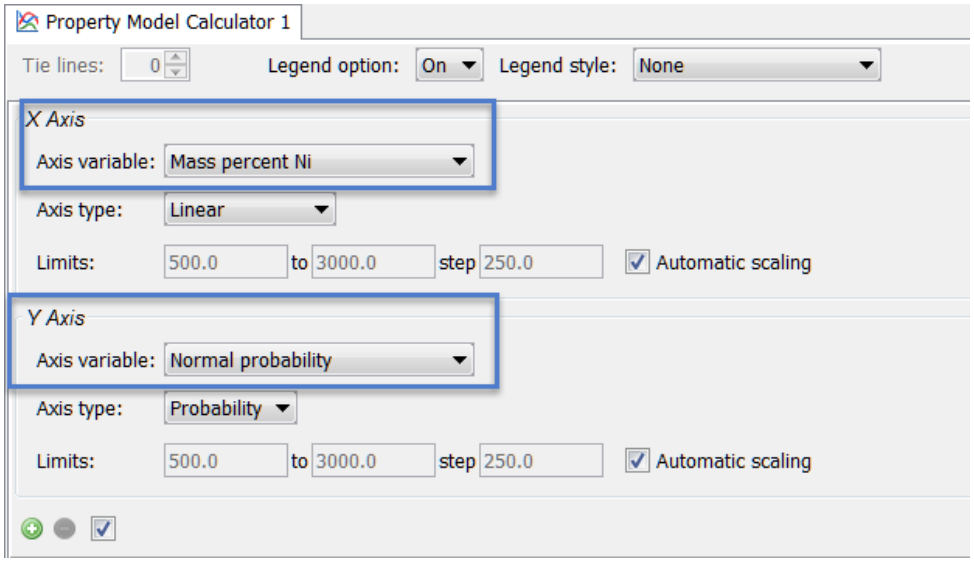


Total samples = 1000

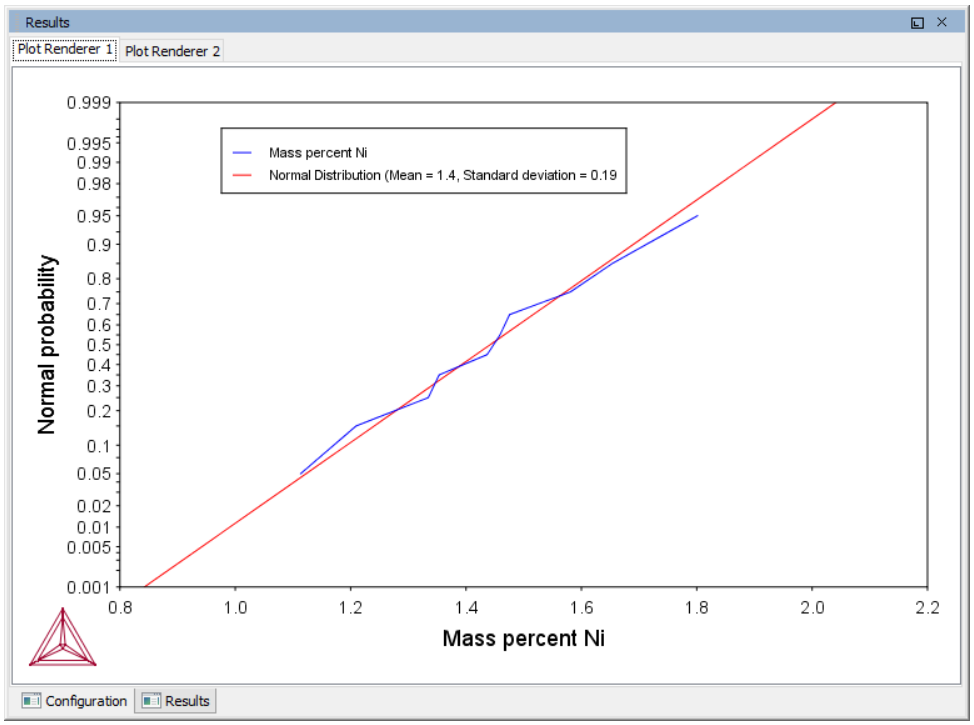


Normal Probability Plot

You can also plot the results as a Normal probability. Continuing with this example, for the Property Model Calculator the *X Axis* variable is plotted as **Mass percent Ni** and the *Y Axis* variable is plotted as the **Normal probability**.



This is a normal probability plot example of the uncertainty calculations sampling data from Gaussian distributions. It compares the Ni composition where the total sample size is 200. The sampled data (blue line) closely follows the ideal normal distribution (red line). Deviations are naturally larger at the tails (≈1%Ni and ≈2%Ni) since the number of samples are fewer there compared to the center of the distribution.


Results
Plot Renderer 1
Plot Renderer 2
Mass percent Ni
Normal Distribution (Mean = 1.4, Standard deviation = 0.19
Normal probability
0.999
0.995
0.99
0.98
0.95
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.05
0.02
0.01
0.005
0.001
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
Mass percent Ni
Configuration
Results

Rotating 3D Plots

- Heat Map, Contour, and 3D Plots
- The Calculation Types in Graphical Mode

When you use a *Grid* calculation type you can plot the diagram in 3D.

In the **Results** window after you create the 3D plot:

- Rotate the diagram automatically. Double-click in the **Results** window and the diagram rotates clockwise. Left-click once to stop the automatic rotation.
- Rotate the diagram manually. Left-click and hold the mouse and move it around the **Results** window.
- Scroll the mouse wheel/use your fingers on a trackpad to zoom on the Z-axis values.
- Right-click and move the mouse to shift the surface up or down without zooming.
- To reset the plot to its default view click **Perform Tree** to regenerate the plot.

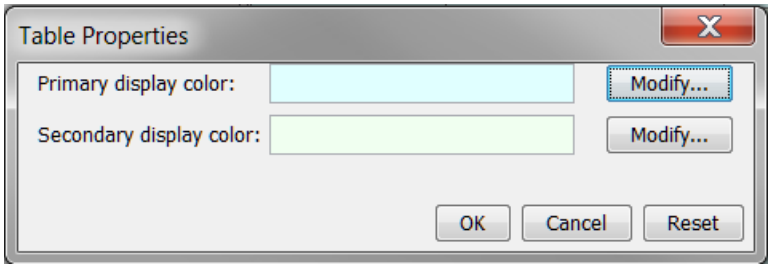
Plot and Table Formatting

In this section:

Setting Background Colours 396
Changing the Plot Properties 397
Plot Labels 398
Plot Labels: Entering a Mixture of Plain Text and Equations 399
Plot Labels: Rotation Angle and Show Anchor 400
Moving Plot Labels 401
About Legend Styles 402
Legend and Label Styles 403

Setting Background Colours

To change the background colours of the table, in the **Results** window right-click a Table Renderer tab, and select **Properties**. Modify as required.



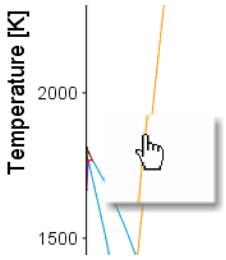
The defaults for these settings can be changed globally. To open the Options window: From the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

Changing the Plot Properties

For global changes to the default settings plots see Global Settings: Graphical and Console Mode Plotting. The settings are the same but applied to all new plots.

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included).

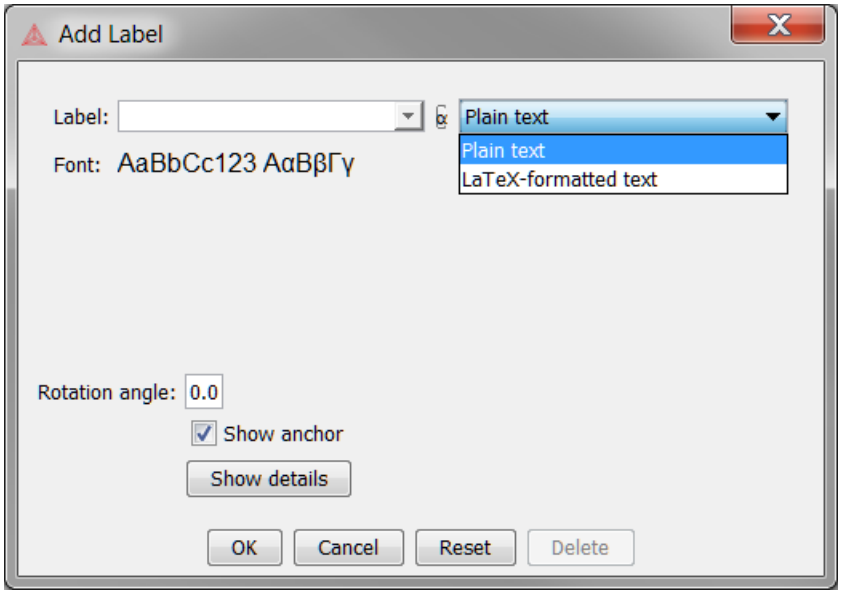
In the **Results** window, hover the mouse over a plot line. When it is over a line that can clicked the crosshair cursor turns into a pointing finger.



To prevent unintended edits, hold down <Ctrl> while moving the cursor around the plot to only display it as a crosshair.

Plot Labels

To add a label text at a certain point in a plot, right-click the point, and select **Add Label**. For phase diagrams, the program suggests a label that you can keep or edit. The suggested label specifies the names of the stable phases at the coordinate where you clicked. For all other plot types, you enter your own text, which can either be Plain text or LaTeX formatted text.



You can enter the label as **Plain text** or in **LaTeX-formatted text**. For **LaTeX-formatted text** enter or edit the text as required. For example, underscores (_) are added before the numbers to make subscripts in the label.

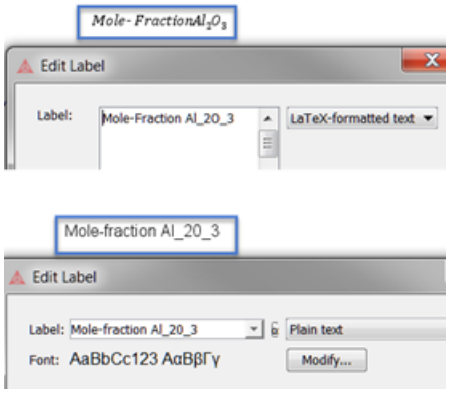
For a list of supported LaTeX commands, see: http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html.

By default when using LaTeX, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.

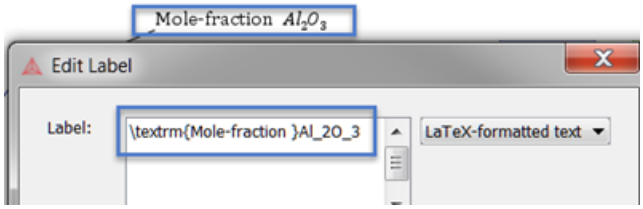
Plot Labels: Entering a Mixture of Plain Text and Equations

When you enter text using LaTaX formatted text it displays by default on the plot in italics and treats the text as an equation.

As in the following example, the top label does not display correctly because the label is a mixture of text (Mole-Fraction) and an equation (Al_2O_3). In the bottom image, when the same information is added as Plain text to the plot it now does not include the subscripts.



To add a mixture of plain text and equation text, you can exit math mode using the string `\textrm` followed by the text to display enclosed in curly brackets. For example `\textrm {Mole-fraction }Al_2O_3` results in the label as shown:



In this example, you need to add a space at the end of fraction in order to separate the text from the equation part of the label.

When working in Console Mode, you can also use the above windows on the Console Results window to add and edit labels. In addition, you can use the command.

Plot Labels: Rotation Angle and Show Anchor

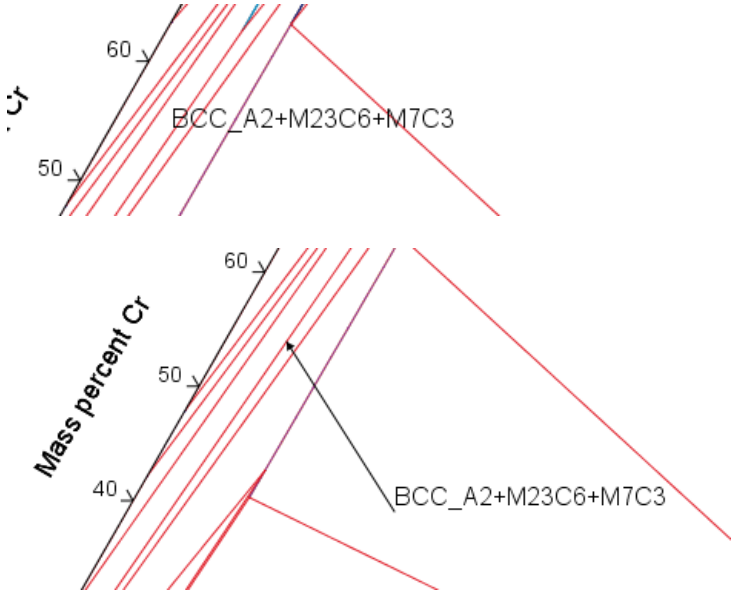
By default the **Show anchor** check box is selected, which includes an arrow from the label point to the coordinates.

If you do not want the label oriented horizontally in the Plot Renderer tab, then specify the number of degrees of rotation in the **Rotation angle** field.

Click **OK** to add the label to the plot. You can also move a label by clicking and dragging it. The default anchor arrow is added to indicate the point that belongs to the label.

Moving Plot Labels

Drag and drop labels anywhere on the plot. The anchor arrow points to the point of origin.



Close up of a plot label before being moved (top) and after being moved (bottom). The arrow in the lower image points to the label's original location on the plot.

About Legend Styles

There are a variety of legend styles you can use to display detail about the phases. The same legend styles are available for both Graphical Mode and Console Mode plots.



For Console Mode, use the command CHANGE_LEGEND.

In Graphical Mode the label styles are defined when using the Plot Renderer. You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for *Legend option*.

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

If constituent description is included in the legend, then for each equilibria along a line in the diagram, the largest constituent fractions are summed until they are equal or greater than 0.6. This is done separately for each sublattice. If the equilibria along the line gets different sets of constituents these are all appended to the list for that sublattice.

The ordering description is only printed for partitioned phases (phases that have a disordered contribution) that begins with at least two identical sublattices (sublattices where the set of constituents are identical). `DISORD` (disordered) is shown if site fractions are identical between identical constituents on all identical sub lattices (with an error margin) otherwise `ORD` (ordered) is shown in the legend.

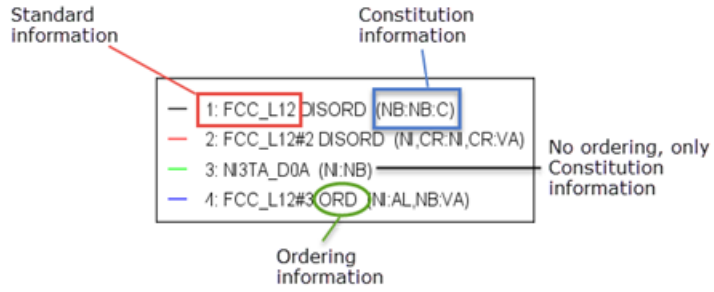
If ordering between equilibria in a line are different, then `ORD + DISORD` is shown in the legend.

Legend and Label Styles

Legend Styles

To show the differences between labels, the following uses the same example file that creates Figure 6 in TCNI database extended information document (found on the Thermo-Calc website).

When **All** is selected for this specific example the label includes the following:



Specifically:

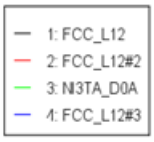
- There are two disordered FCC phases (matrix and carbide), one ordered FCC (gamma prime), plus a phase NI3TA_D0A (called Delta in Ni-alloys).
- ORDERING shows the different FCC phases.
- CONSTITUTION shows that FCC_L12#1 is NbC, FCC_L12#2 is matrix with Ni and Cr as major constituent, FCC_L12#3 is Ni3Al with Nb addition and NI3TA_D0A is Nb-rich (eg. Ni3Nb).

Label Styles

These examples are for each label style choice - **None**, **All**, **Constitution** or **Ordering**. The instructions are for when you are setting the options using the Plot Renderer. In Console Mode, you choose the options (`ALL`, `NONE`, `CONSTITUTION`, or `ORDERING`) after the command CHANGE_LEGEND.

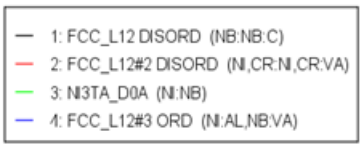
None

When **None** is selected the legend includes the standard information about the phases.



All

When you select **All** the **Constitution description** and the **Ordering description** (when there is ordering) are included.



Constitution description

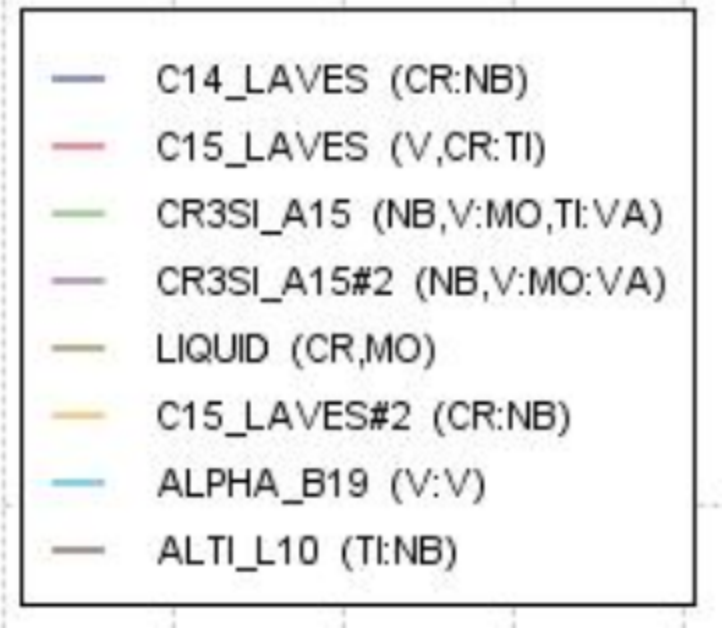
When you select **Constitution description**, this is added to the standard description.



Here is an example with a brief explanation of what you might see when choosing this option.



Only major constituents are listed.

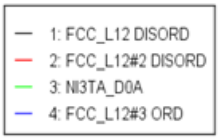


First there is the phase name then (NB, V : MO, Ti : VA) meaning the first sub-lattice contains mostly NB and V. The second sub-lattice contains mostly Mo and TI, the third sub-lattice contains mostly VA= Vacancy= No atom/molecule at all.

Mostly" means Thermo-Calc sums the largest site fractions in a sub-lattice until it reaches 0.6. E.g. If sorted values are FE=0.5, AL=0.15, CR=0.15, NI=0.09 + smaller values then you will get "(Fe,AL,CR)" because FE+AL > 0.6 and then CR because it has same size as AL.

Ordering description

When you select **Ordering description** and when there is ordering, this is added to the standard description.



Graphical Mode Examples

About the Examples

This guide includes descriptions of the following examples.

Category	Example number
Thermo-Calc Graphical Mode Examples Collection includes binary and ternary system examples, Scheil, the Equilibrium Calculator, plus more	T_01 to T_12
Thermo-Calc General Property Model Examples Collection: General Models Library	General Models: PM_G_01 to PM_G_12
Steel Model Library Examples Collection	Steel Models: PM_Fe_01 to PM_Fe_08
Process Metallurgy Module Examples Collection	PMET_01 to PMET_08
Diffusion Module (DICTRA) Graphical Mode Examples	D_01, D_02, D_03 (the Quick Start Guide Examples) D_04 to D_08
Precipitation Module (TC-PRISMA) Graphical Mode Examples	P_01 to P_13

Thermo-Calc Graphical Mode Examples Collection

In this section:

T_01: Calculating a Single-Point Equilibrium 408
T_02: Stepping in Temperature in the Fe-C System 410
T_03: Fe-C Phase Diagrams 412
T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K 414
T_05: Stable and the Metastable Fe-C Phase Diagrams 417
T_06: Serially Coupled Equilibrium Calculators 419
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T_08: Scheil and Equilibrium Solidification 427
T_09: Carbide Driving Force Heat Map 430
T_10: Scheil Solidification with Back Diffusion 431
T_11: Surface Tension in Cu-Zr 433
T_12: Viscosity in Cr-Ni 435
T_13: Scheil Solidification with Solute Trapping 437

T_01: Calculating a Single-Point Equilibrium

This example shows the result from a single-point equilibrium calculation in the Fe-C system. It demonstrates the use of the Equilibrium Calculator and generates a Table Renderer in the **Results** window. The number of equilibrium conditions is C+2 where C is the number of components, meaning that four conditions are needed in this example:

- **Temperature** is 1000 K
- **Pressure** is 100000 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%



This example is included as a tutorial on our website and our YouTube channel.

Project File Information

- Folder: Thermo-Calc
- File name: *T_01_Single-point_equilibrium.tcu*

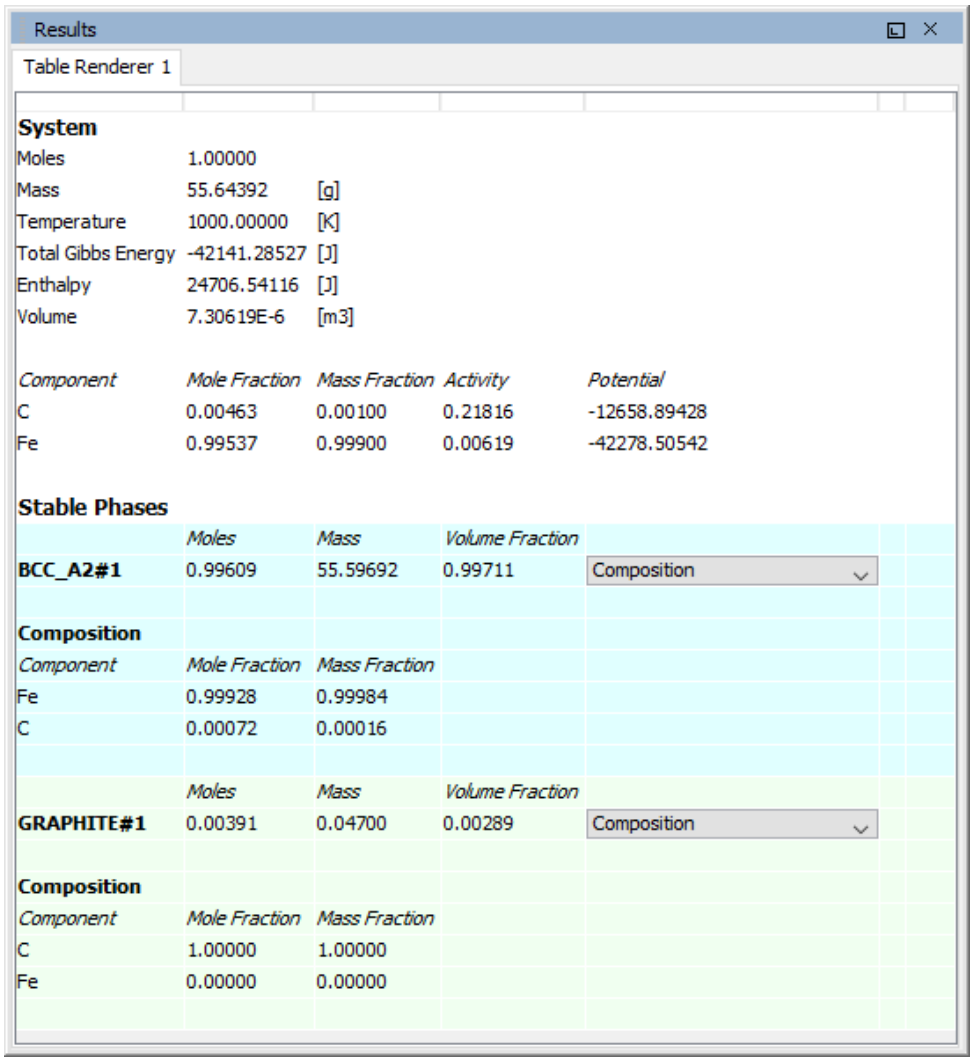


Figure 15: The displayed results of the calculation show that the BCC_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

T_02: Stepping in Temperature in the Fe-C System

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the temperature is varied between 500 and 2000 K. It demonstrates the use of the Equilibrium Calculator. To allow temperature to vary, the corresponding **Axis Definition** check box is selected.

This example is included in the tutorial on our website and YouTube channel.

Project File Information

- Folder: Thermo-Calc
- File name: *T_02_Step_in_temperature_in_Fe-C.tcu*

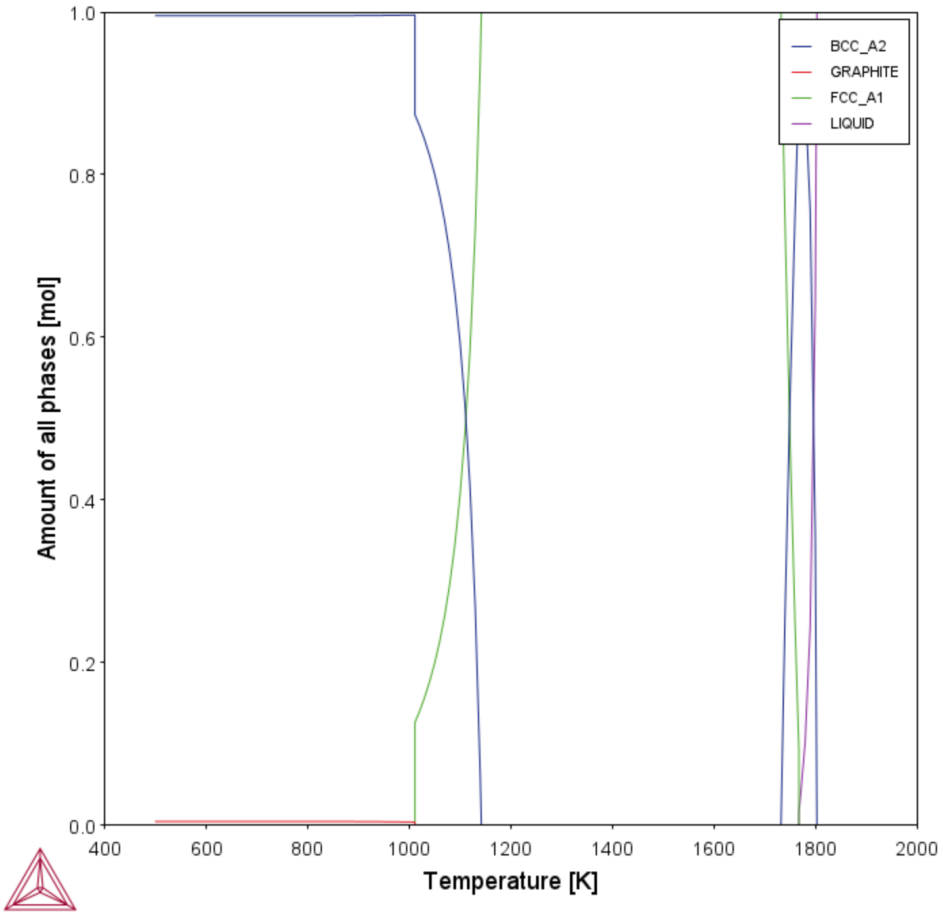
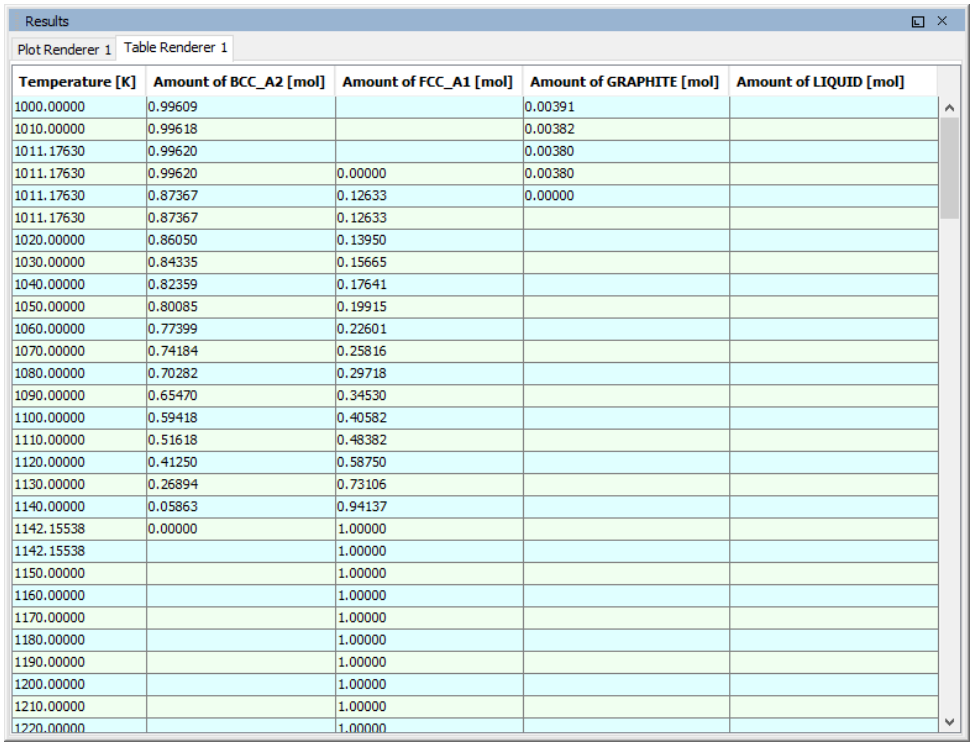


Figure 16: In this example, results are displayed graphically using a Plot Renderer activity.

If you want, you can use a Table Renderer to generate text results instead, as shown in this example after adding a Table Renderer to the Equilibrium Calculator and clicking **Perform**.


Results

Plot Renderer 1 | Table Renderer 1

Temperature [K]	Amount of BCC_A2 [mol]	Amount of FCC_A1 [mol]	Amount of GRAPHITE [mol]	Amount of LIQUID [mol]
1000.00000	0.99609		0.00391	
1010.00000	0.99618		0.00382	
1011.17630	0.99620		0.00380	
1011.17630	0.99620	0.00000	0.00380	
1011.17630	0.87367	0.12633	0.00000	
1011.17630	0.87367	0.12633		
1020.00000	0.86050	0.13950		
1030.00000	0.84335	0.15665		
1040.00000	0.82359	0.17641		
1050.00000	0.80085	0.19915		
1060.00000	0.77399	0.22601		
1070.00000	0.74184	0.25816		
1080.00000	0.70282	0.29718		
1090.00000	0.65470	0.34530		
1100.00000	0.59418	0.40582		
1110.00000	0.51618	0.48382		
1120.00000	0.41250	0.58750		
1130.00000	0.26894	0.73106		
1140.00000	0.05863	0.94137		
1142.15538	0.00000	1.00000		
1142.15538		1.00000		
1150.00000		1.00000		
1160.00000		1.00000		
1170.00000		1.00000		
1180.00000		1.00000		
1190.00000		1.00000		
1200.00000		1.00000		
1210.00000		1.00000		
1220.00000		1.00000		

T_03: Fe-C Phase Diagrams

This example shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using the Binary Calculator activity and then using a System Definer and Equilibrium Calculator.

In both cases, a Plot Renderer is used to display results. The purpose of the Binary Calculator is to simplify common calculations for binary systems. In the Equilibrium Calculator two axes are defined: *Mass percent C* and *Temperature*. An axis variable must also be an equilibrium condition.

This example is included as a tutorial on our website and our YouTube channel.

Project File Information

- Folder: Thermo-Calc
- File name: *T_03_Fe-C_phase_diagram.tcu*

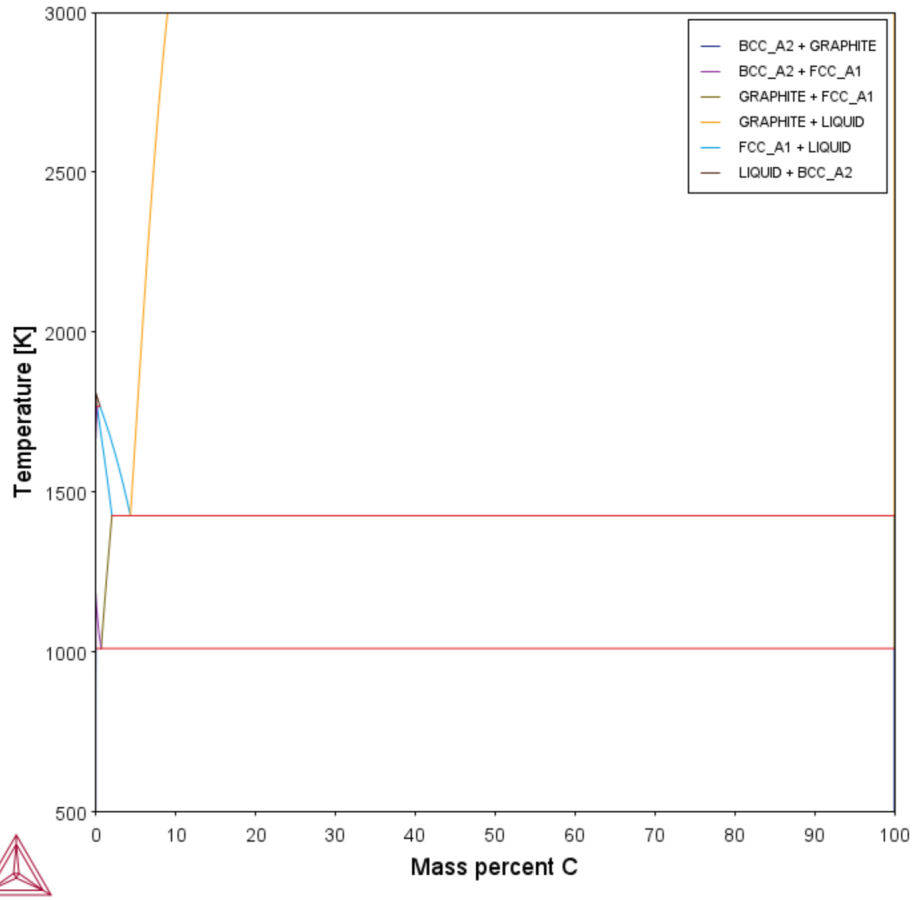


Figure 17: The plot result of the System Definer and Equilibrium Calculator.

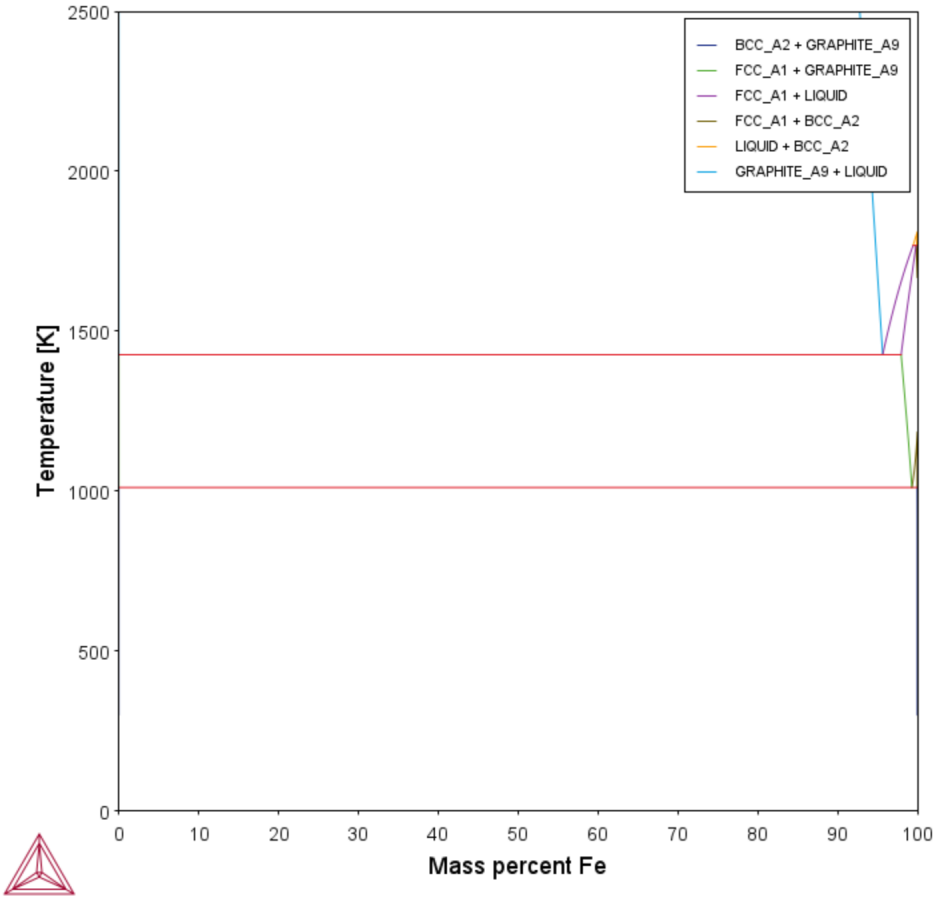


Figure 18: The plot result of the Binary Calculator simulation.

T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to example T_03: Fe-C Phase Diagrams, the same diagram is calculated using a Ternary Calculator and then using a System Definer and Equilibrium Calculator. Two Plot Renderer activities are added to create two plots.

This example is included as a tutorial on our website and our YouTube channel.

Project File Information

- Folder: Thermo-Calc
- File name: *T_04_Fe-Cr-C_ternary_phase_diagram.tcu*

Try practicing with two features on the Plot Renderer Configuration window. To toggle between a triangular and a rectangular diagram, click the **Show Triangular** button then click **Perform** to see what happens. To toggle the X and Y axis variables, click the **Switch Axes** button and then click **Perform**.

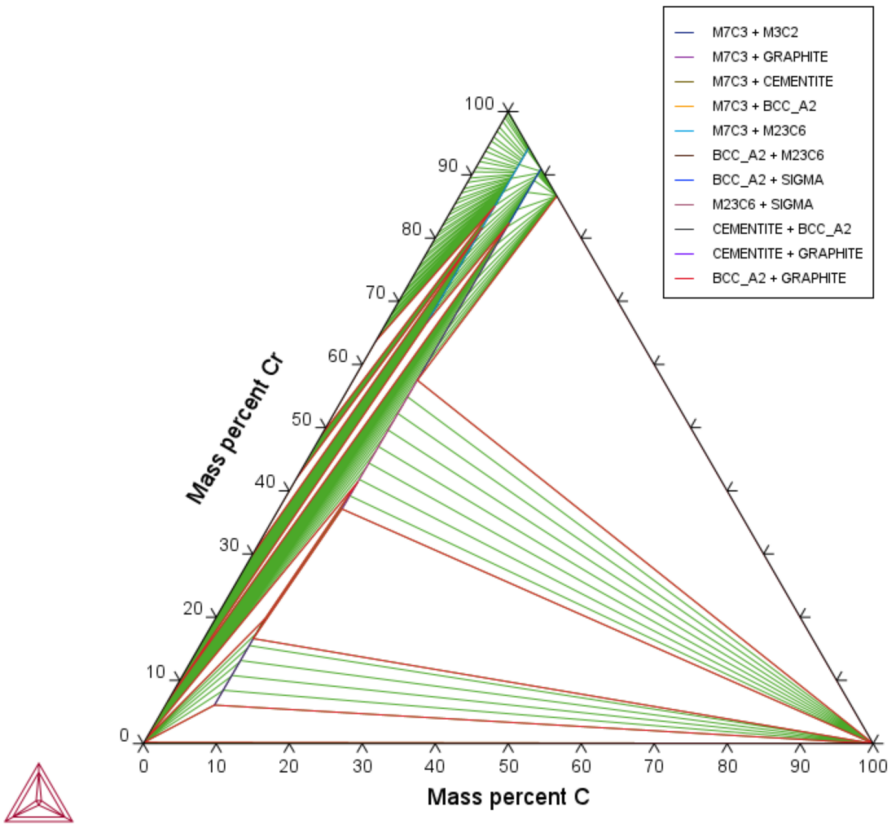


Figure 19: Ternary Calculator

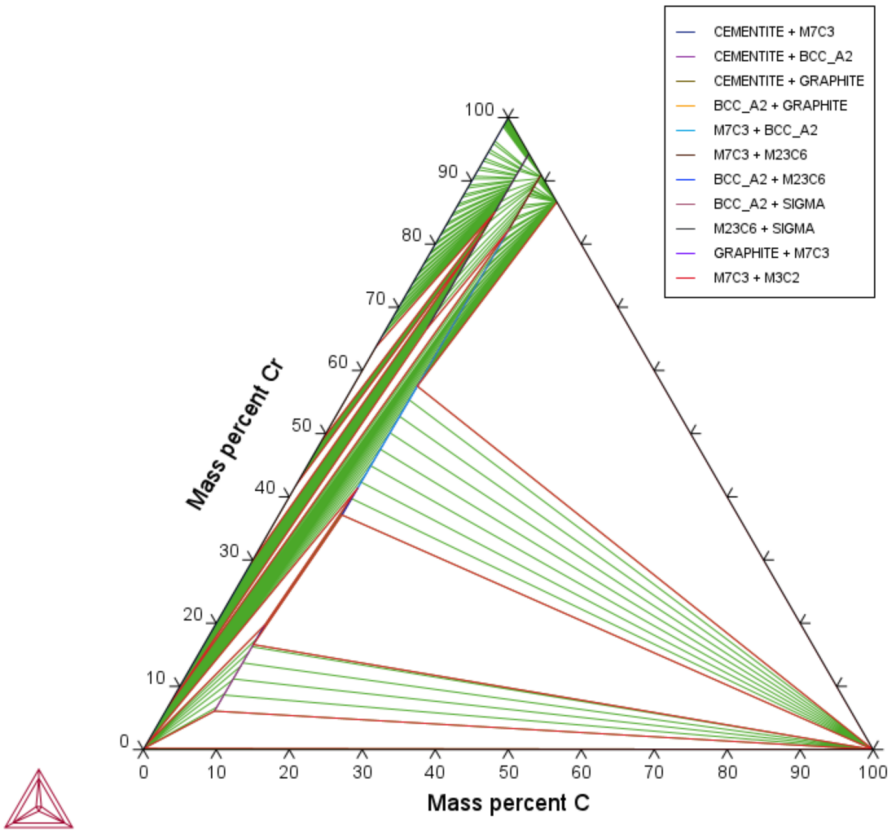
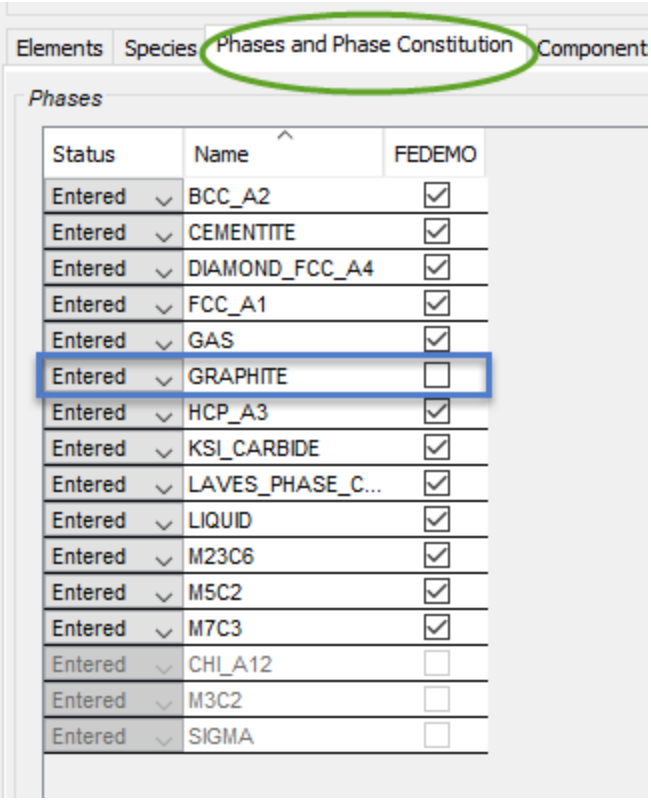


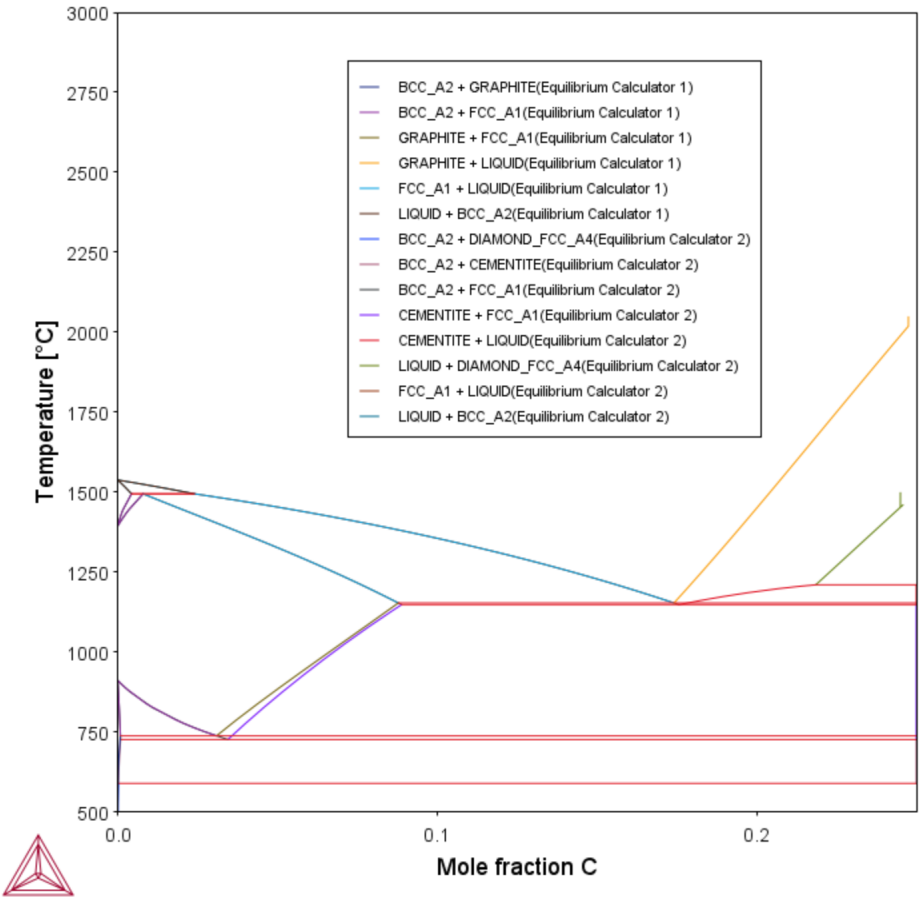
Figure 20: Equilibrium Calculator

T_05: Stable and the Metastable Fe-C Phase Diagrams

This example shows how to overlay results from two calculations in the same plot using the Equilibrium Calculator.

1. The Plot Renderer activity is first created as a successor to Equilibrium Calculator 1.
2. Then right-click the Plot Renderer node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. In **Equilibrium Calculator 1** the stable phase diagram is calculated and in **Equilibrium Calculator 2** the metastable phase.
3. The metastable diagram is obtained by deselecting the graphite phase on System Definer2 → **Phases and phase constitution** tab.





Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_05_Fe-C_stable_and_metastable_phase_diagram.tcu*

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.

T_06: Serially Coupled Equilibrium Calculators

Sometimes there are multiple solutions for a given set of equilibrium conditions. In other cases the equilibrium calculation does not converge. You can then aid the final calculation by, in effect, telling the software where it should start the search for the equilibrium.

This example shows how to serially couple two Equilibrium Calculator nodes together for more complex equilibrium conditions. For each calculation, the output is to a Table Renderer.

Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_06_Serial_equilibrium_calculators.tcu*



Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.

Table Renderer Results

Equilibrium Calculator 1

In the first example, the objective is to calculate the equilibrium at 850° C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.

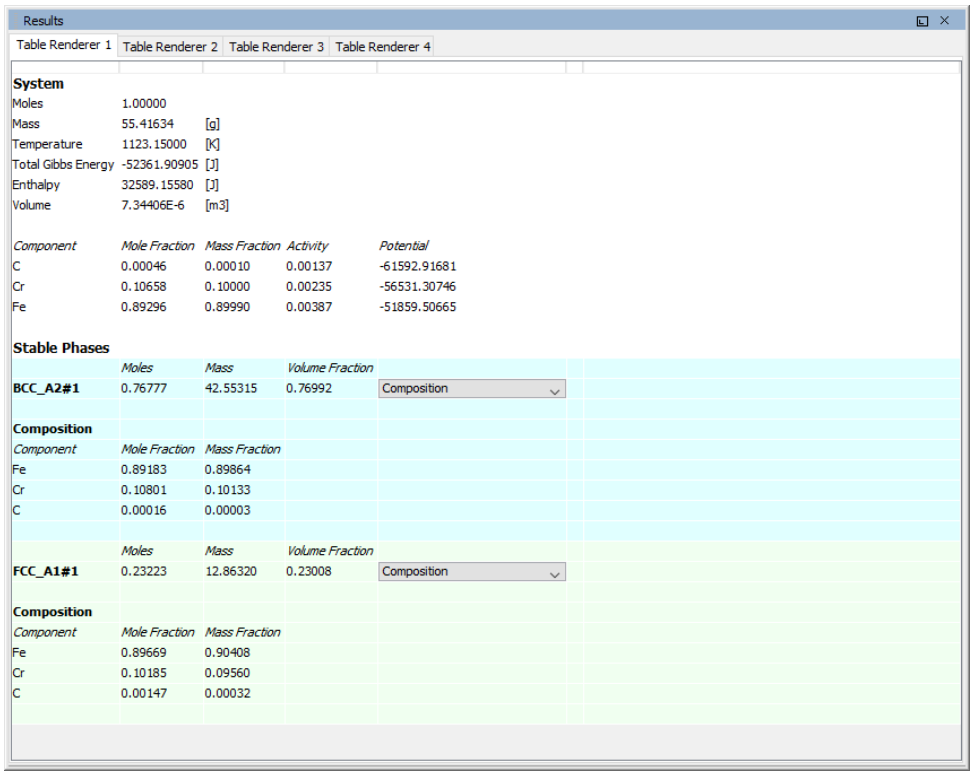

Results

Table Renderer 1 | Table Renderer 2 | Table Renderer 3 | Table Renderer 4

System

Moles	1.00000	
Mass	55.41634	[g]
Temperature	1123.15000	[K]
Total Gibbs Energy	-52361.90905	[J]
Enthalpy	32589.15580	[J]
Volume	7.34406E-6	[m3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
C	0.00046	0.00010	0.00137	-61592.91681
Cr	0.10658	0.10000	0.00235	-56531.30746
Fe	0.89296	0.89990	0.00387	-51859.50665

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.76777	42.55315	0.76992	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.89183	0.89864
Cr	0.10801	0.10133
C	0.00016	0.00003

	Moles	*Mass*	*Volume Fraction*	
FCC_A1#1	0.23223	12.86320	0.23008	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.89669	0.90408
Cr	0.10185	0.09560
C	0.00147	0.00032

Equilibrium Calculator 2

In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.

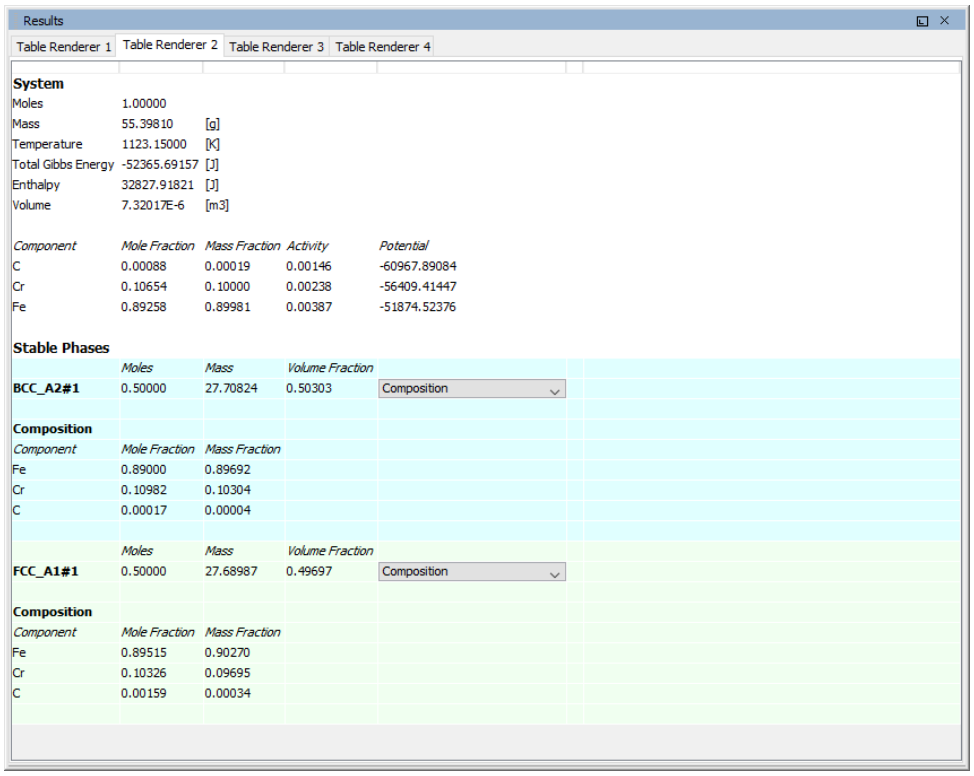

Results

Table Renderer 1 | Table Renderer 2 | Table Renderer 3 | Table Renderer 4

System

Moles	1.00000	
Mass	55.39810	[g]
Temperature	1123.15000	[K]
Total Gibbs Energy	-52365.69157	[J]
Enthalpy	32827.91821	[J]
Volume	7.32017E-6	[m3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
C	0.00088	0.00019	0.00146	-60967.89084
Cr	0.10654	0.10000	0.00238	-56409.41447
Fe	0.89258	0.89981	0.00387	-51874.52376

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.50000	27.70824	0.50303	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.89000	0.89692
Cr	0.10982	0.10304
C	0.00017	0.00004

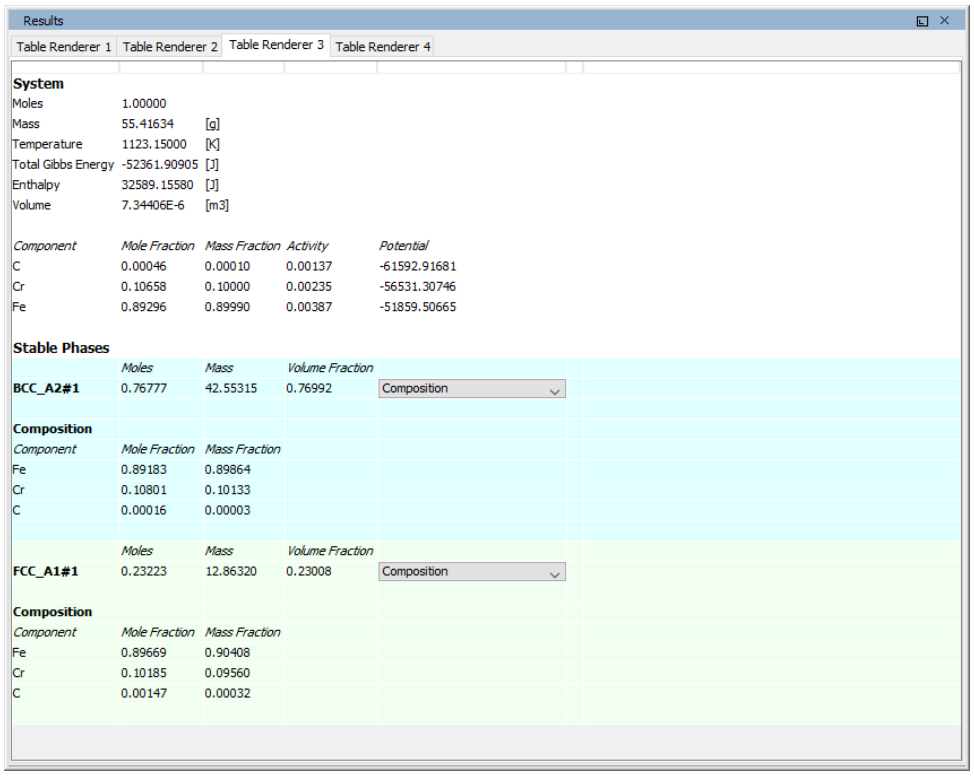
	Moles	*Mass*	*Volume Fraction*	
FCC_A1#1	0.50000	27.68987	0.49697	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.89515	0.90270
Cr	0.10326	0.09695
C	0.00159	0.00034

Equilibrium Calculator 3

In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.



Equilibrium Calculator 4

In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.

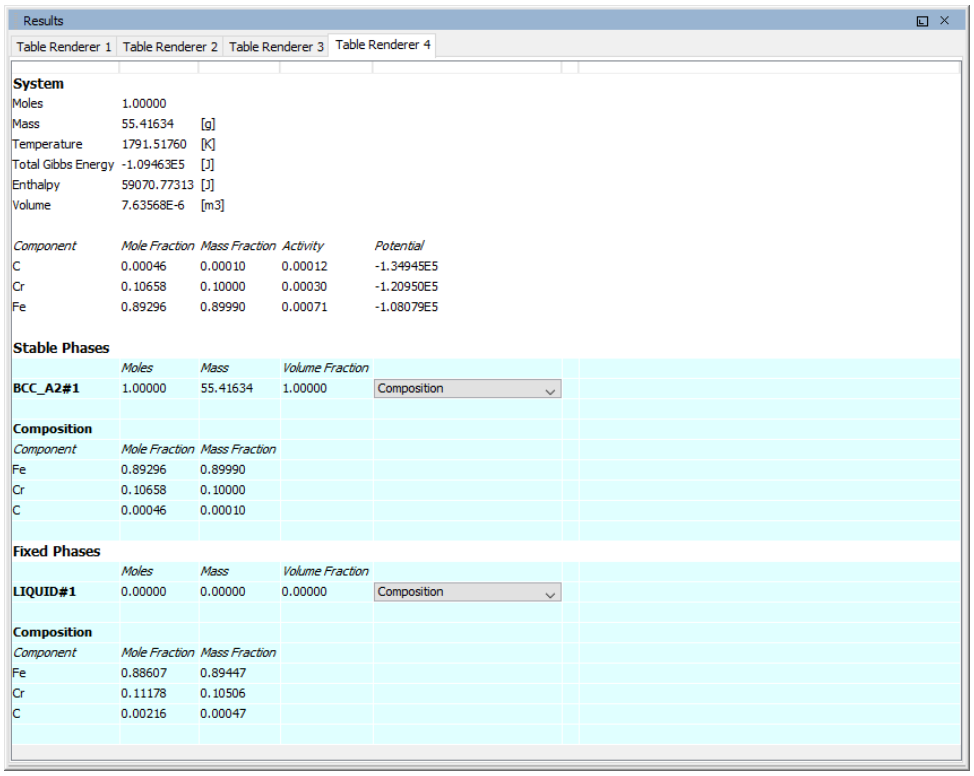

Results

Table Renderer 1 | Table Renderer 2 | Table Renderer 3 | Table Renderer 4

System

Moles	1.00000	
Mass	55.41634	[g]
Temperature	1791.51760	[K]
Total Gibbs Energy	-1.09463E5	[J]
Enthalpy	59070.77313	[J]
Volume	7.63568E-6	[m3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
C	0.00046	0.00010	0.00012	-1.34945E5
Cr	0.10658	0.10000	0.00030	-1.20950E5
Fe	0.89296	0.89990	0.00071	-1.08079E5

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	1.00000	55.41634	1.00000	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.89296	0.89990
Cr	0.10658	0.10000
C	0.00046	0.00010

Fixed Phases

	Moles	*Mass*	*Volume Fraction*	
LIQUID#1	0.00000	0.00000	0.00000	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.88607	0.89447
Cr	0.11178	0.10506
C	0.00216	0.00047

T_07: User-Defined Functions

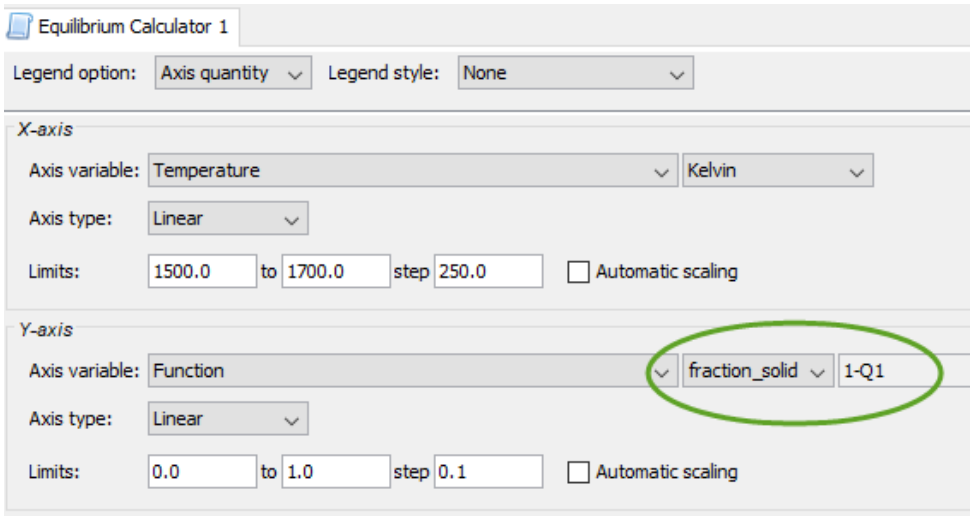
This example shows how to implement user-defined functions.

A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the Equilibrium Calculator under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted against temperature in two Plot Renderer activities. Functions can be entered in terms of *QuantitiesQ1*, *Q2*, *Q3* and so forth, or by using the Thermo-Calc syntax.

Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_07_User_defined_functions.tcu*

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.



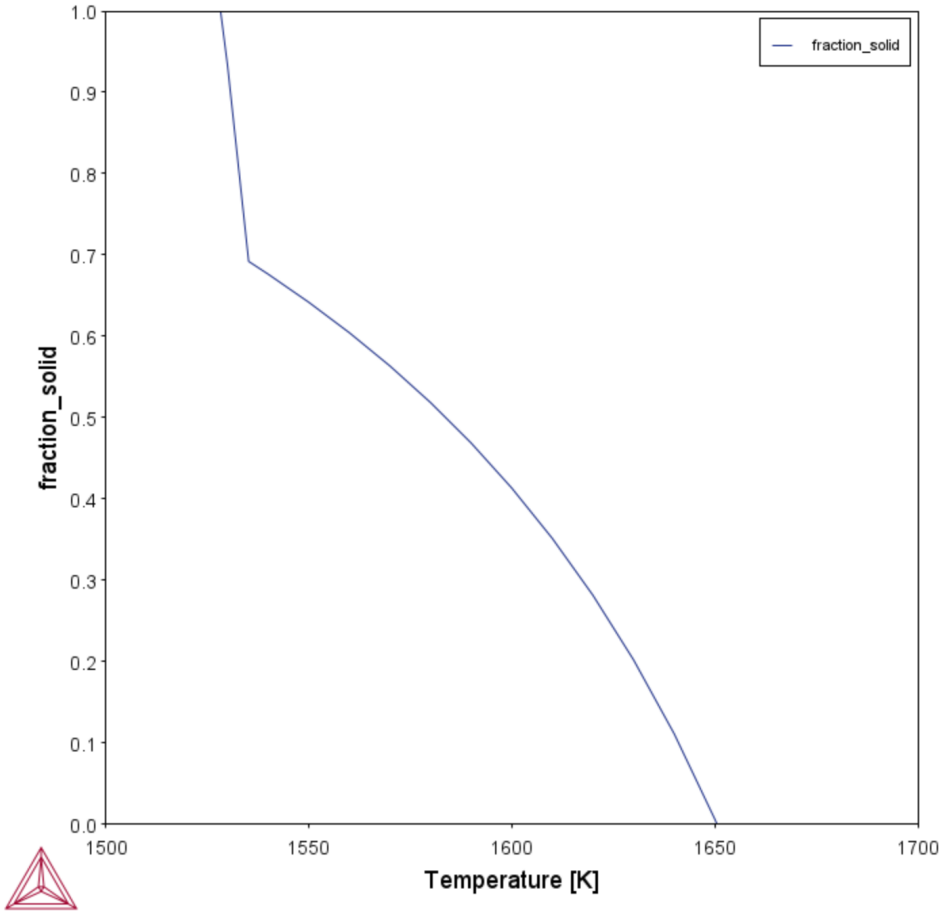


Figure 21: The result of the fraction_solid function.

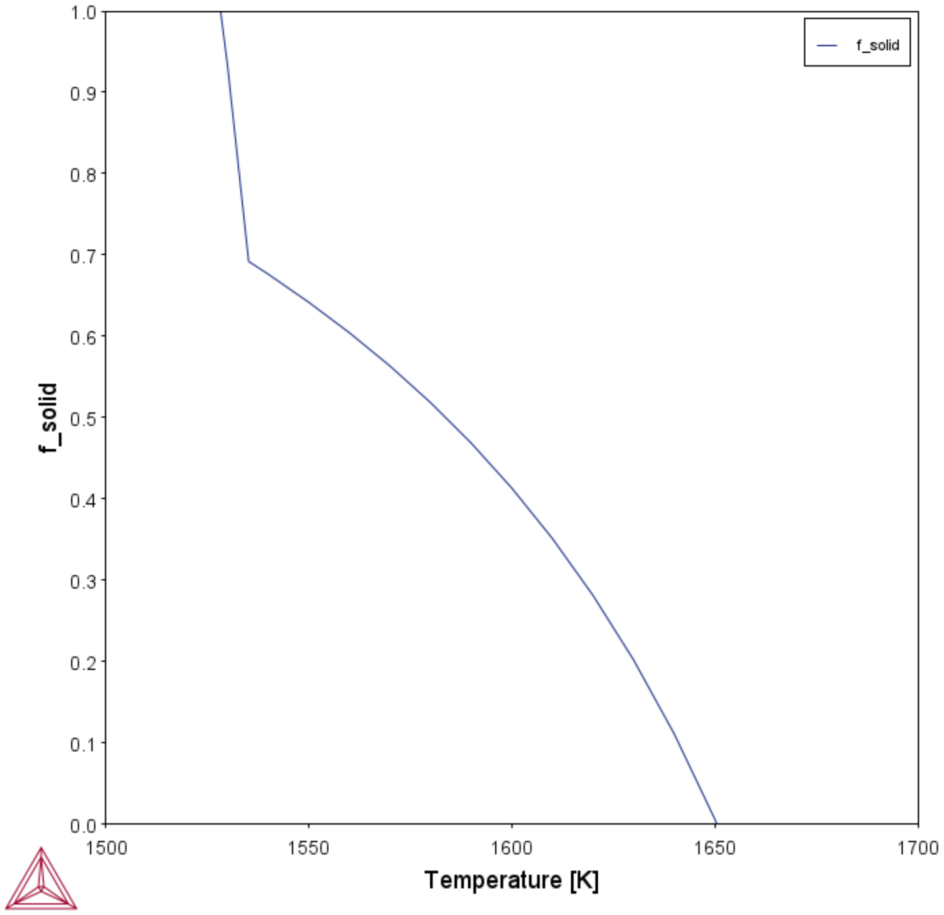


Figure 22: The result of the f_solid function.

T_08: Scheil and Equilibrium Solidification

This example shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions, i.e. zero diffusion in the solidified material and infinitely fast diffusion in the liquid. The example uses the Scheil Calculator and adds a Plot and Table Renderer.

Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_08_Scheil_and_equilibrium_solidification.tcu*.

For video tutorial examples using Scheil, see our website and YouTube channel.

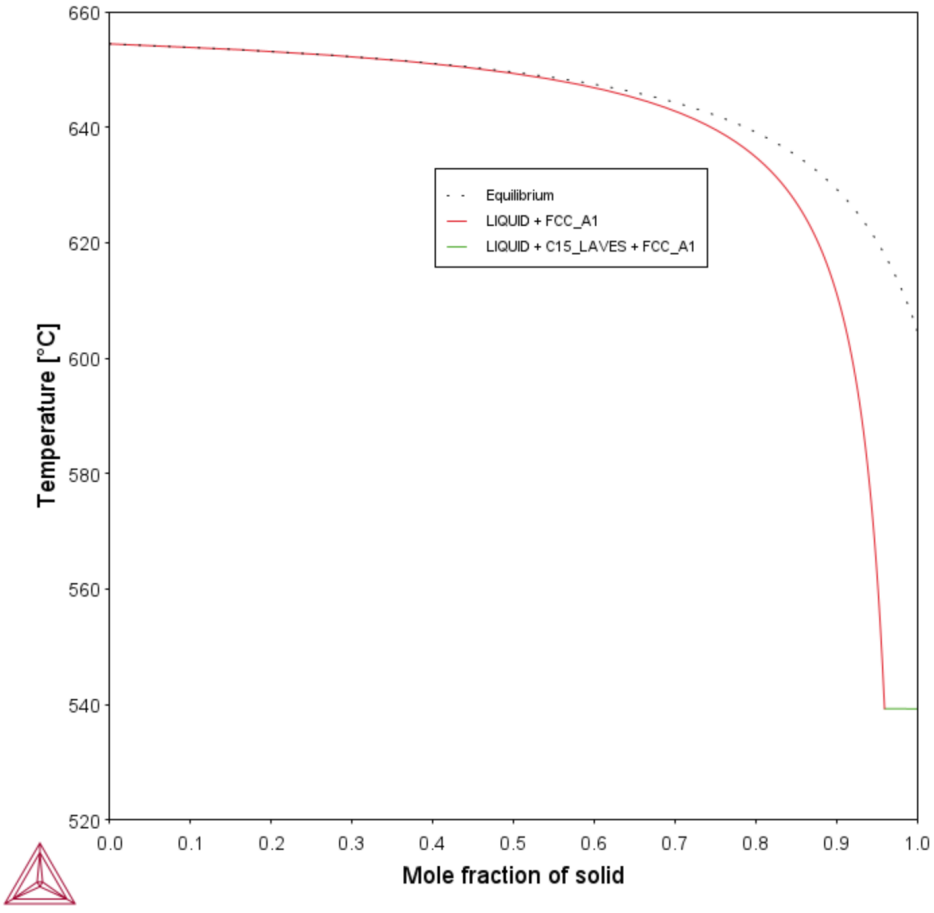


Figure 23: The plot compares the mole fraction of a solid vs temperature.

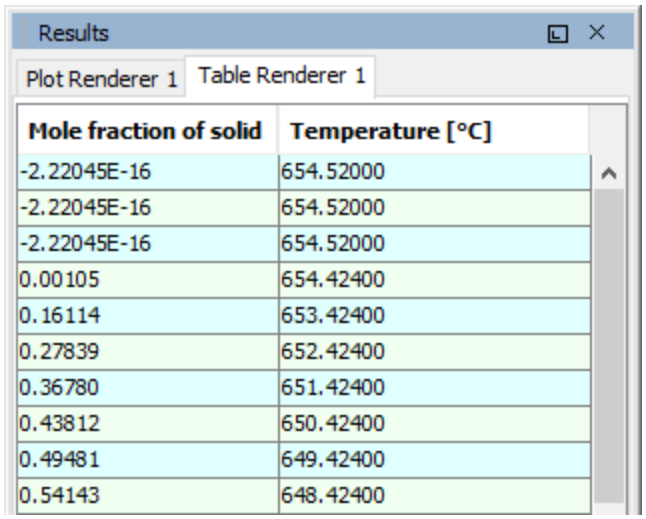


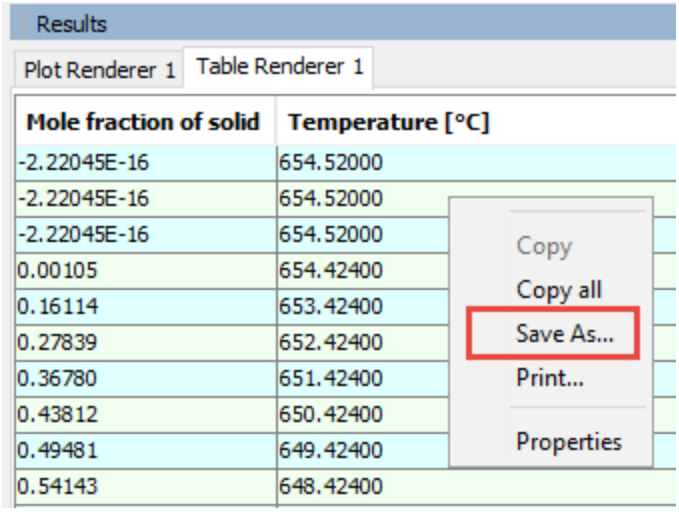
Figure 24: The table provides the data, which you can also export.

To Save the Table (via Table Renderer)

There are two ways to save the table from the Table Renderer **Results** or **Configuration** windows.

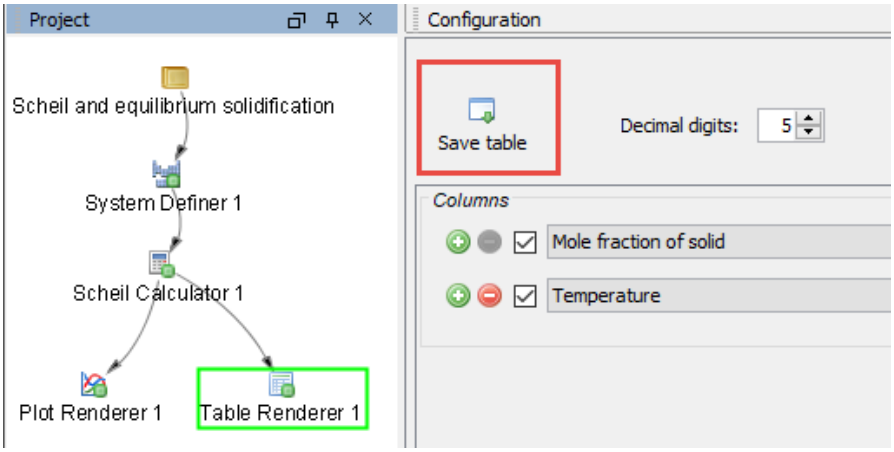
Method 1

In the **Results** window, right click the table and select **Save As...**



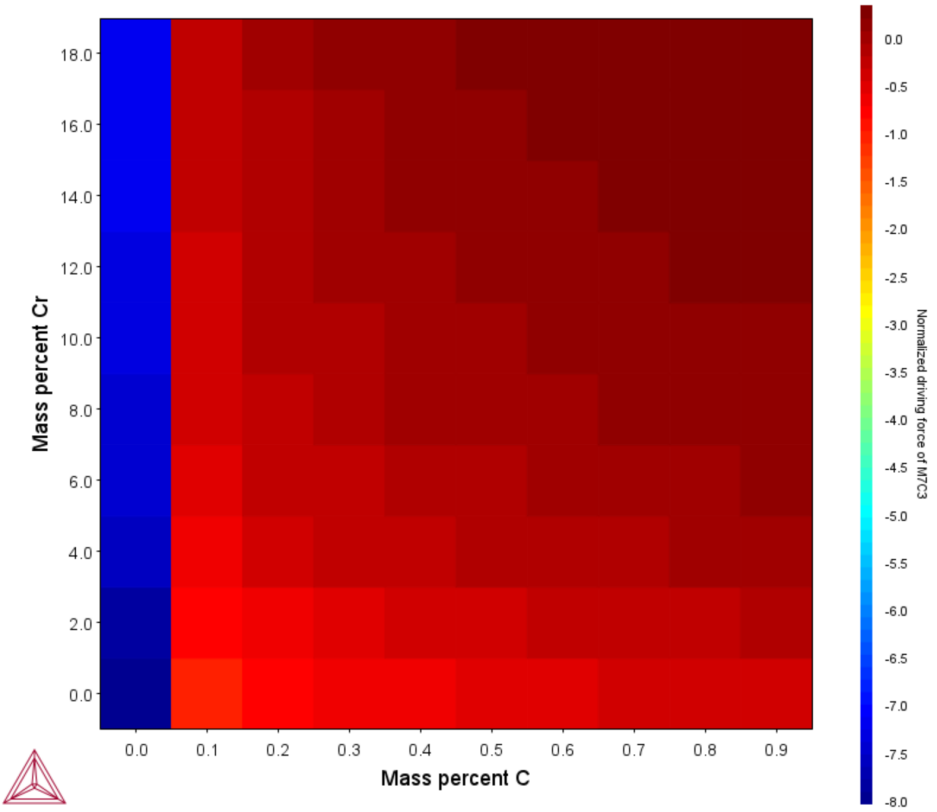
Method 2

1. In the **Project** window, click the **Table Renderer**.
2. In the **Configuration** window, click **Save table**.



T_09: Carbide Driving Force Heat Map

This is an example of using *Grid* calculations to plot the driving force for a carbide as a function of two composition variables. With the *Grid* calculation type, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A Plot Renderer connected to a grid calculation plots the *z*-axis property for each equilibrium as a function of the two calculation axes. The final plot can be either a heat map or a contour plot.



Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_09_Heat_map_of_carbide_driving_force.tcu*

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.

T_10: Scheil Solidification with Back Diffusion

See Scheil Calculator for an overview of the different Scheil simulation models available.

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

This is an example of a Scheil solidification simulation of a Al-2.1Cu-1Si alloy including back diffusion in the primary phase.

The example uses two of the Scheil Calculator activity nodes with different cooling rates, 10 K/s and 0.005 K/s. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve as shown in the plot result. Both a thermodynamic ALDEMO (aluminum demo) and mobility MALDEMO (Al-alloys mobility) database are used for this calculation.

Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_10_Scheil_with_back_diffusion.tcu*.

For video tutorial examples using Scheil, see our website and YouTube channel.

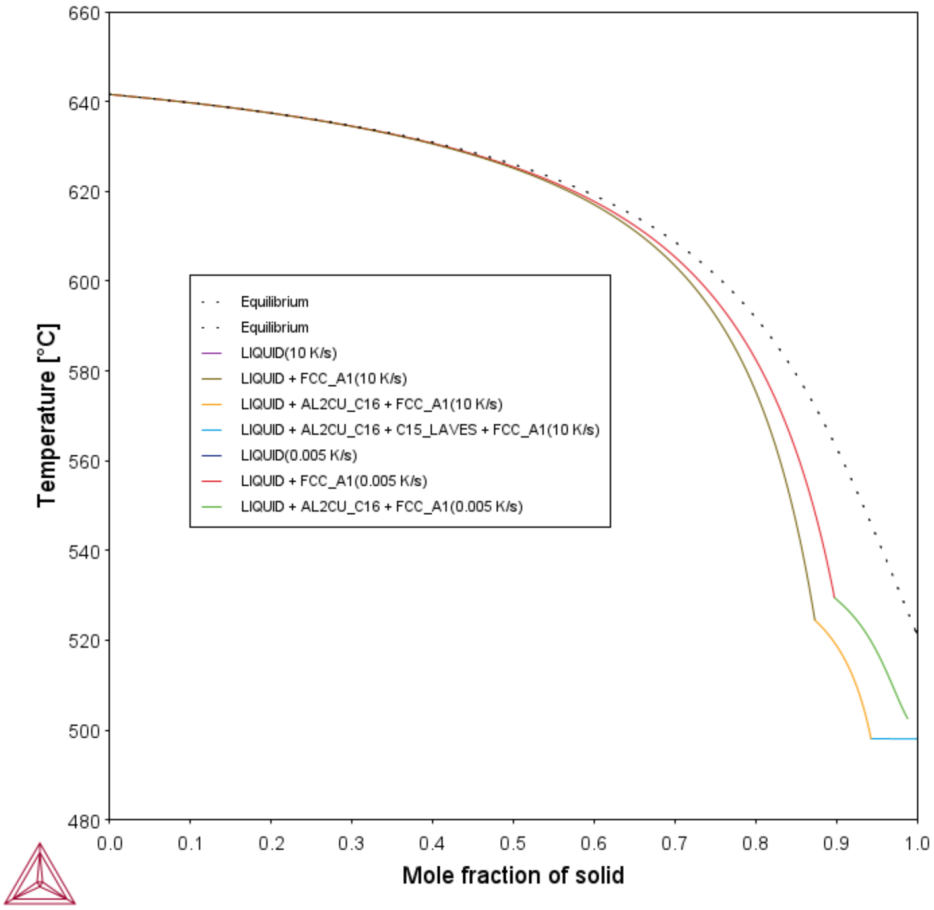


Figure 25: Scheil solidification. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve .

T_11: Surface Tension in Cu-Zr

This is an example of including surface tension in the calculations. This property, and others, are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

Using the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL), the surface tension of liquid metallic is plotted at 1373 K for Cu-Zr and compared to experimental data from Krasovskyy (2005).

Not all databases have this property although it is being added to databases as these are updated over time. Currently it is available with the latest versions of TCNI and TCAL.

Reference

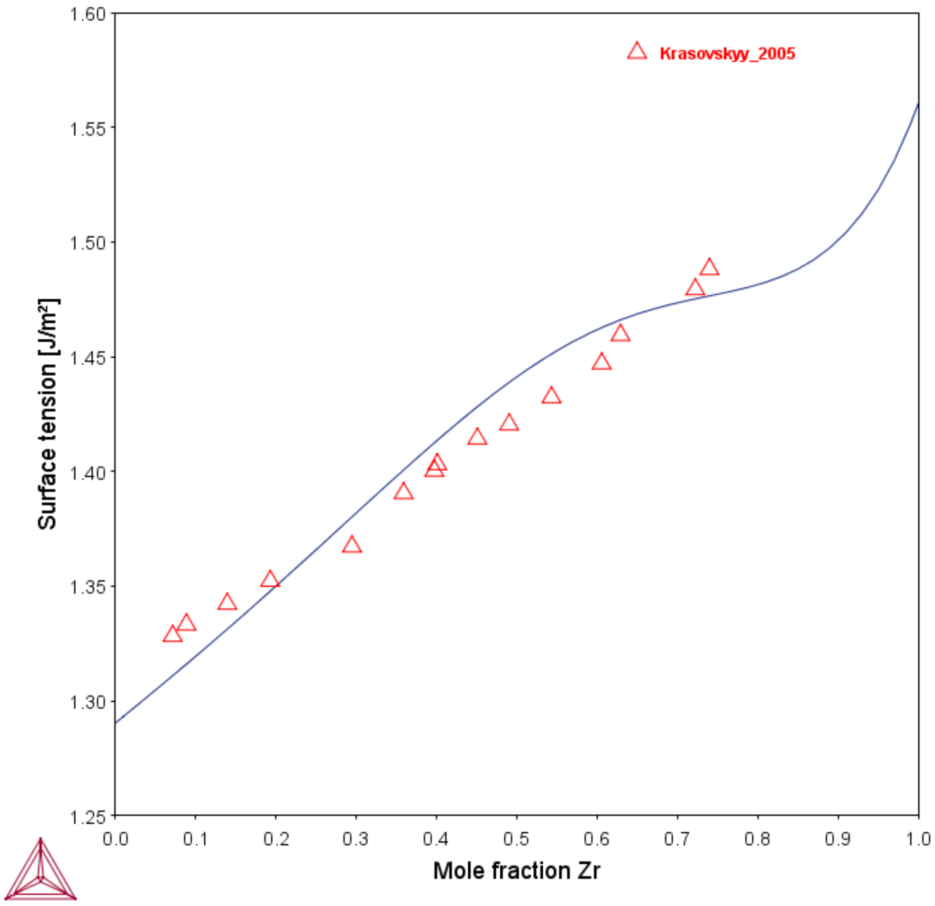
[2005, Krasovskyy] V. P. Krasovskyy, Y. V. Naidich, N. A. Krasovskaya, "Surface tension and density of copper–Zirconium alloys in contact with fluoride refractories," J. Mater. Sci. 40, 2367–2369 (2005).

You can learn more about the surface tension model by searching the help (press F1 when in Thermo-Calc).

The same example is also provided in Console Mode as `tcex56`.

Project File Information

- Folder: Thermo-Calc
- File name: *T_11_Surface_tension_in_Cu-Zr.tcu*.



T_12: Viscosity in Cr-Ni

This is an example of including viscosity in the calculations. This property, and others, are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

Using the FEDEMO database, which is the free demonstration version of the TCS Steel and Fe-alloys Database (TCFE), the viscosity of metallic liquids is plotted at 1873 K for Cu-Ni and compared to experimental data from Sato (2005).

Not all databases have this property although it is being added to databases as these are updated over time. Currently it is available with the latest versions of TCFE, TCHEA, TCNI and TCAL.

Reference

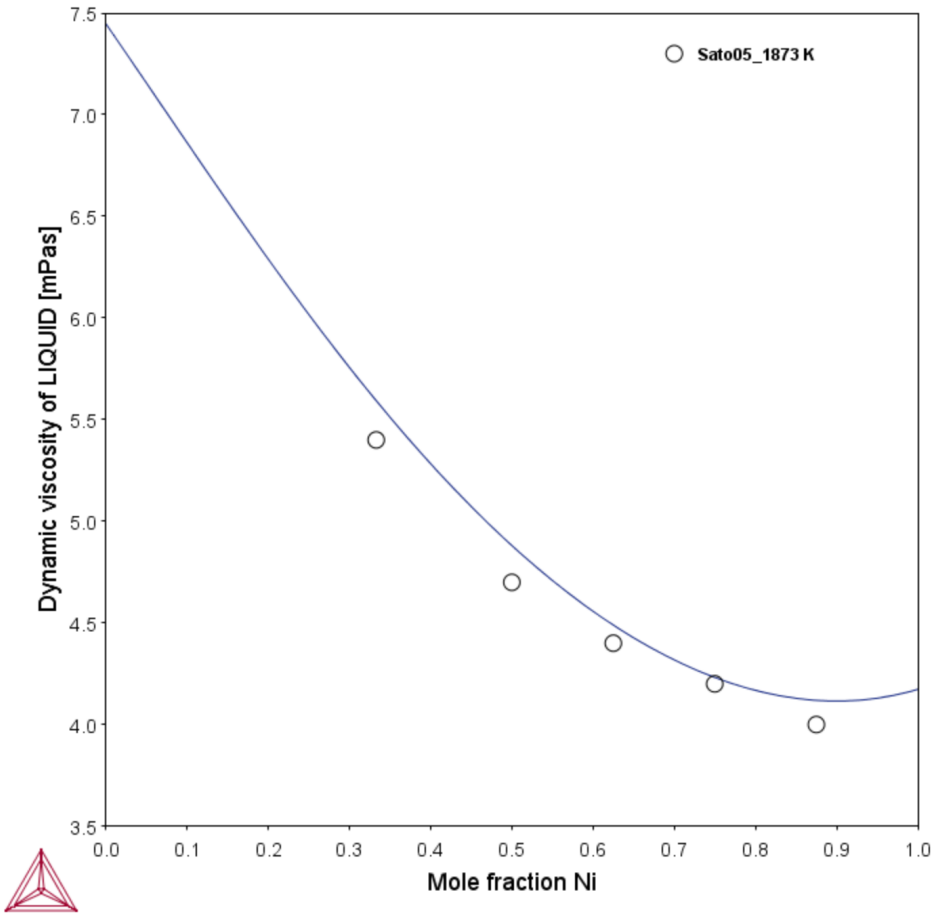
[2005, Sato] Y. Sato, K. Sugisawa, D. Aoki, T. Yamamura, "Viscosities of Fe–Ni, Fe–Co and Ni–Co binary melts," Meas. Sci. Technol. 16, 363–371 (2005).

You can learn more about the viscosity model by searching the help (press F1 when in Thermo-Calc).

The same example is also provided in Console Mode as `tcex55`.

Project File Information

- Folder: Thermo-Calc
- File name: *T_12_Viscosity_in_Cr-Ni.tcu*.



T_13: Scheil Solidification with Solute Trapping

In Graphical Mode, you use the **Scheil Calculator** to set up the various Scheil solidification simulations outlined in more detail in Scheil-Gulliver Solidification Calculations.

This example shows the use of the *Scheil with solute trapping* option with an Al-7.5Si-0.2Cu alloy as compared to a Classic Scheil calculation. The thermodynamic ALDEMO (Aluminum demo) database, available to all users, is selected for this calculation to simulate the effect of solute trapping in the primary phase. This type of simulation is useful for additive manufacturing applications.

This example shows how the alloy starts to solidify at a lower temperature compared to a classic Scheil simulation, an effect which increases with increasing solidification speed. The solidification speed is calculated from user supplied scanning speed and angle between the solid/liquid interface and the scanning direction.

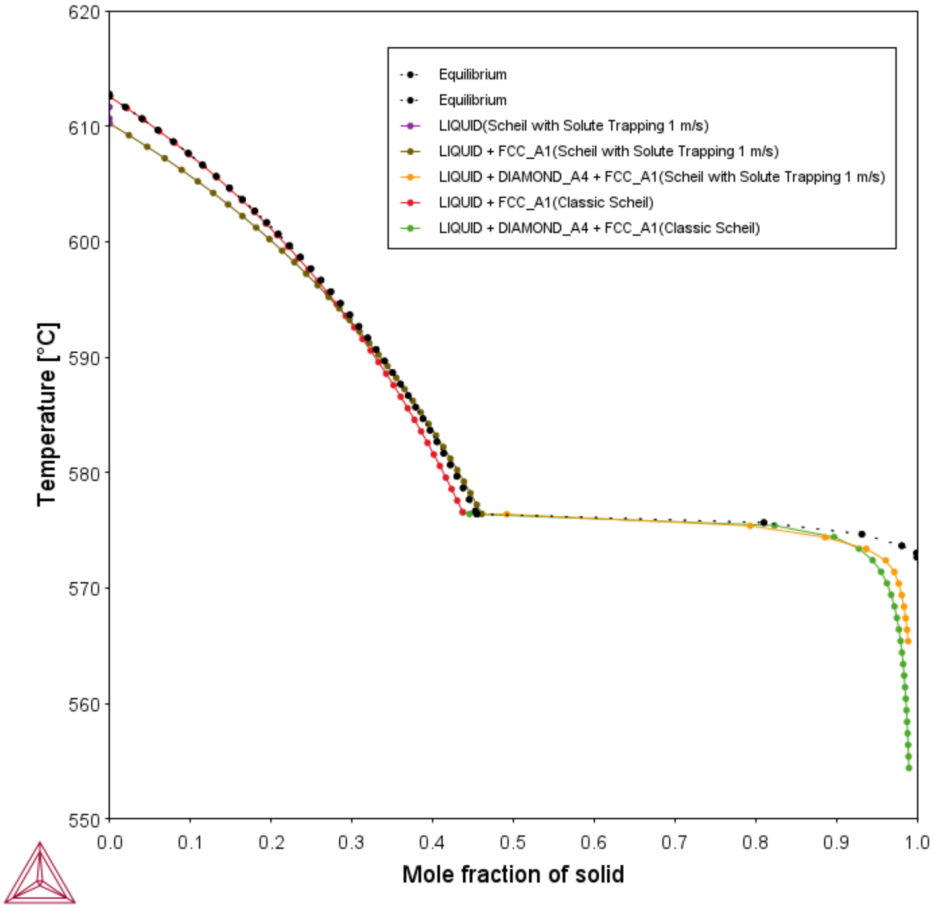


Figure 26: The effect of Scheil solidification with solute trapping of a Al-7.5Si-0.2Cu alloy compared to equilibrium and a Classic Scheil calculation.

Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T_13_Scheil_with_Solute_Trapping.tcu*.

For video tutorial examples using Scheil, see our website and YouTube channel.

Thermo-Calc General Property Model Examples Collection

The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc.

About the Examples

In this section:

PM_G_01: Phase Transition 440
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PM_G_03: Driving Force and Interfacial Energy 448
PM_G_04: Yield Strength 450
PM_G_05: Yield Strength NiAlCr 453
PM_G_06: Yield Strength HEA 455
PM_G_07: Hot Crack Susceptibility 457
PM_G_08: Spinodal 460
PM_G_09: T-Zero Temperature 462
PM_G_10: Freeze-in Thermal Conductivity 464
PM_G_11: Freeze-in Electric Conductivity 466
PM_G_12: Solidus and Liquidus Batch Calculation 468

PM_G_01: Phase Transition

The example uses the Property Model Calculator to predict the transition temperature to the unwanted brittle sigma phase. The example shows how the temperature is influenced by changes to a steel alloy's composition using the *uncertainty* calculation type and how to create either a *histogram* (frequency diagram) or *probability* plot.

This example is included as a tutorial on our website and our YouTube channel.

Phase Transition Property Model Settings in the *Thermo-Calc User Guide*.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_01_Phase_Transition.tcu*

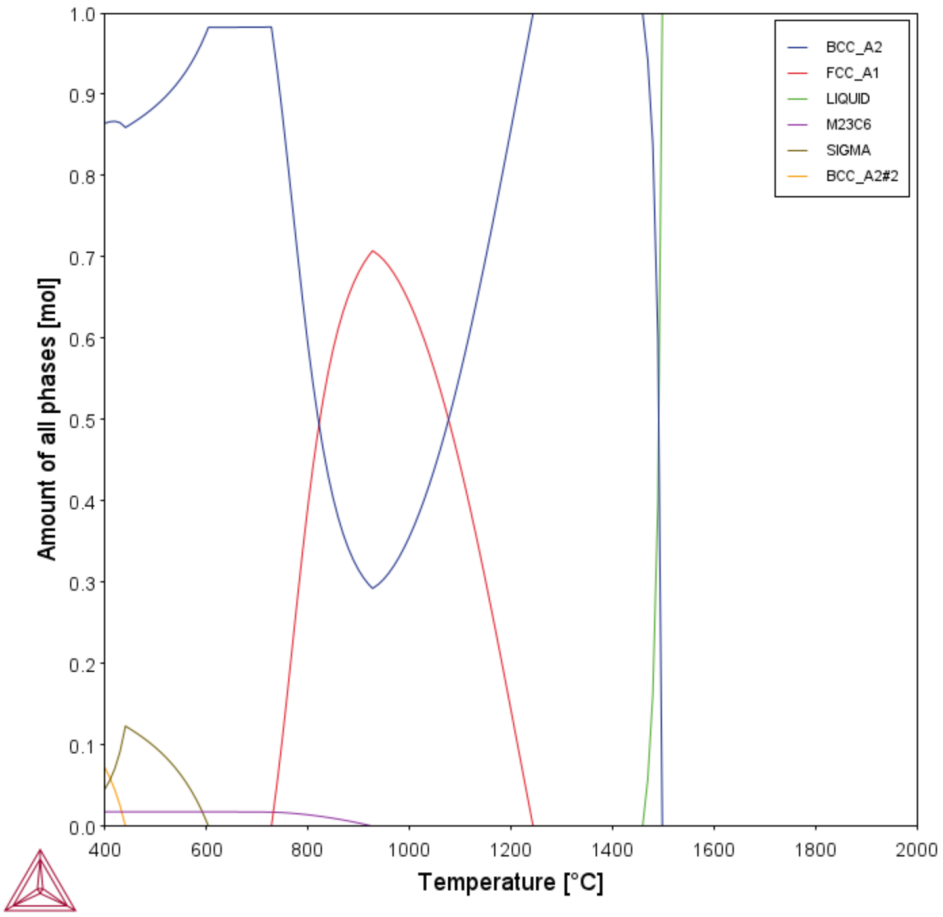


Figure 27: A property diagram as a result of using the Equilibrium Calculator with a One-axis calculation to determine a good starting temperature of the SIGMA phase.

Once you set up the Property Model Calculator, but before running a Grid calculation, it is recommended you run a Single calculation to make sure the calculation is valid. If `the subprocess completed normally` displays in the **Event Log**, it means it worked correctly. You will also see in the Log, the result "Relaxed Condition", which refers to the variable, in this case, temperature. If the calculation did not work, you will see `NAN` (not a number) display instead. Check your configurations and run it again before moving on to the more complicated calculation.

▶ About the Uncertainty Calculations

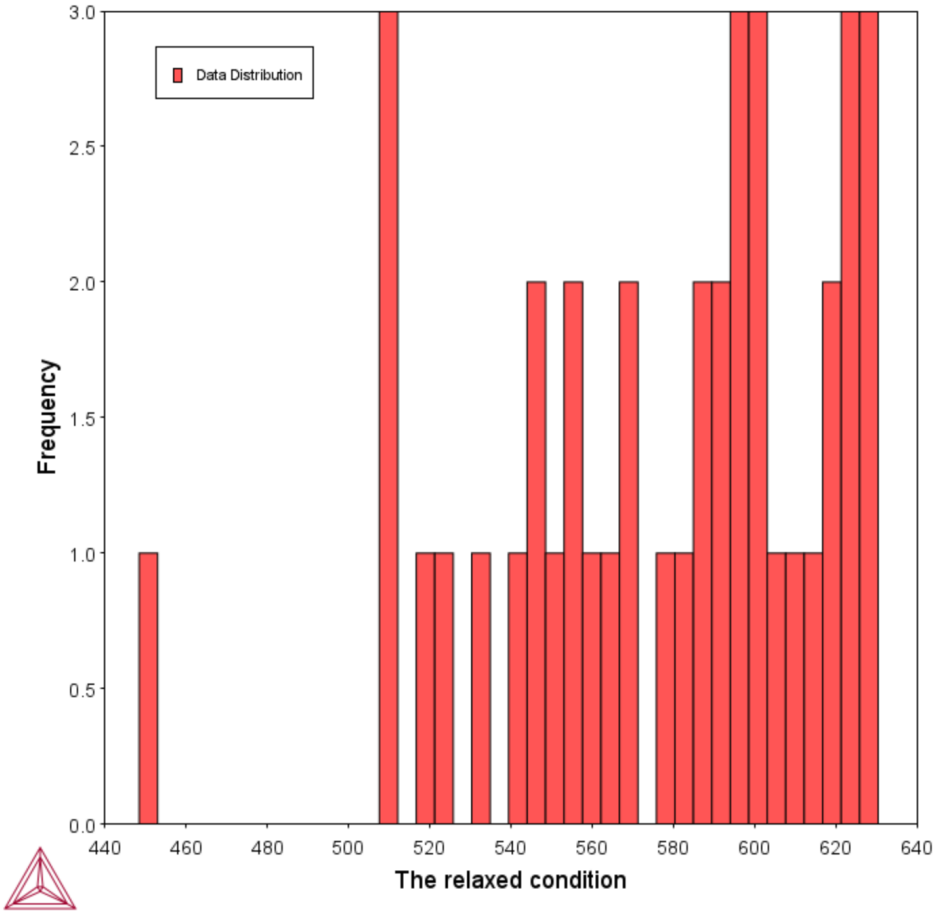


Figure 28: Using the Property Model Calculator with the Phase Transition Model to plot a histogram showing how the transition temperature of sigma varies when you vary the composition. The plot changes each time you run the calculation because it is taking a random sampling from the composition range set.

Note that the X-axis is labeled the **Relaxed Condition**, which you can see on the Configuration window it is **Temperature** for the **Condition to Vary** setting. The Y-axis shows the Frequency, which is the number of samples out of 40 where the composition transitions at each temperature. You can see that the transitions occur more frequently near the 600 degree starting point and less frequently at the edges.

PM_G_02: Coarsening and Interfacial Energy

The example uses the Property Model Calculator and both thermodynamic (FEDEMO) and kinetic (MFEDEMO) demonstration steel databases. Using a *Grid* calculation type it produces these plots: a *heat map*, a *contour plot* and a *cross plot with contour* (where both the interfacial energy and coarsening rate is shown). It also creates a diagram to show the phase fractions vs time and a 3D plot comparing the coarsening rate coefficient.

This example is included as a tutorial on our website and our YouTube channel.

Coarsening Property Model Settings and Interfacial Energy Property Model Settings

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_02_Coarsening_and_Interfacial_energy.tcu*

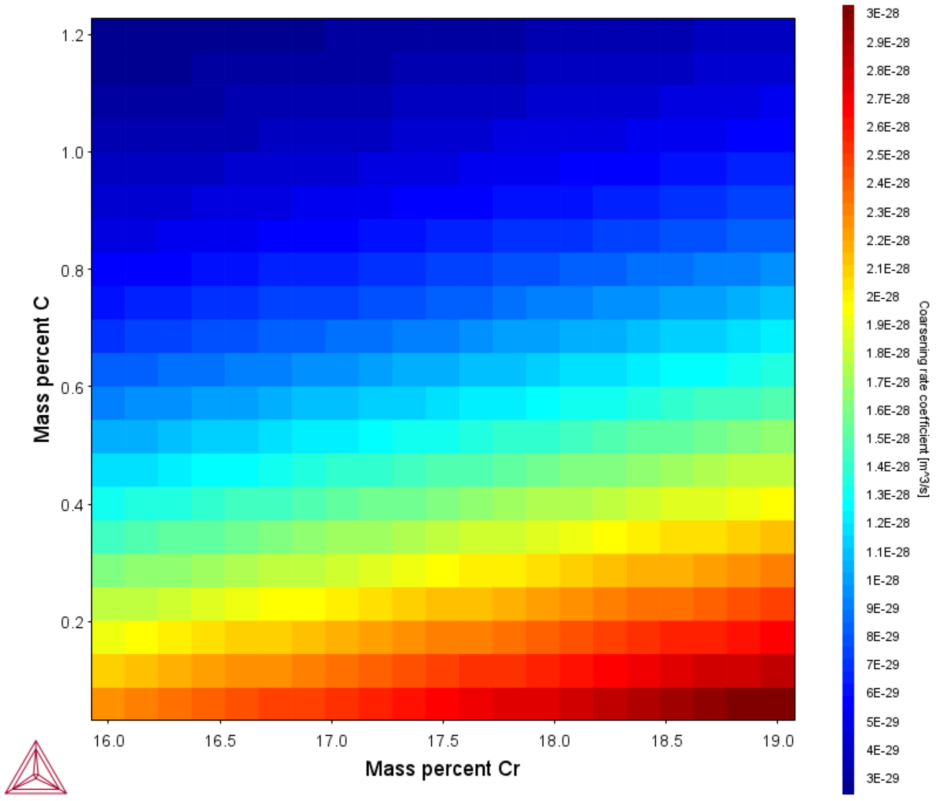


Figure 29: Coarsening rate coefficient (heat map plot).

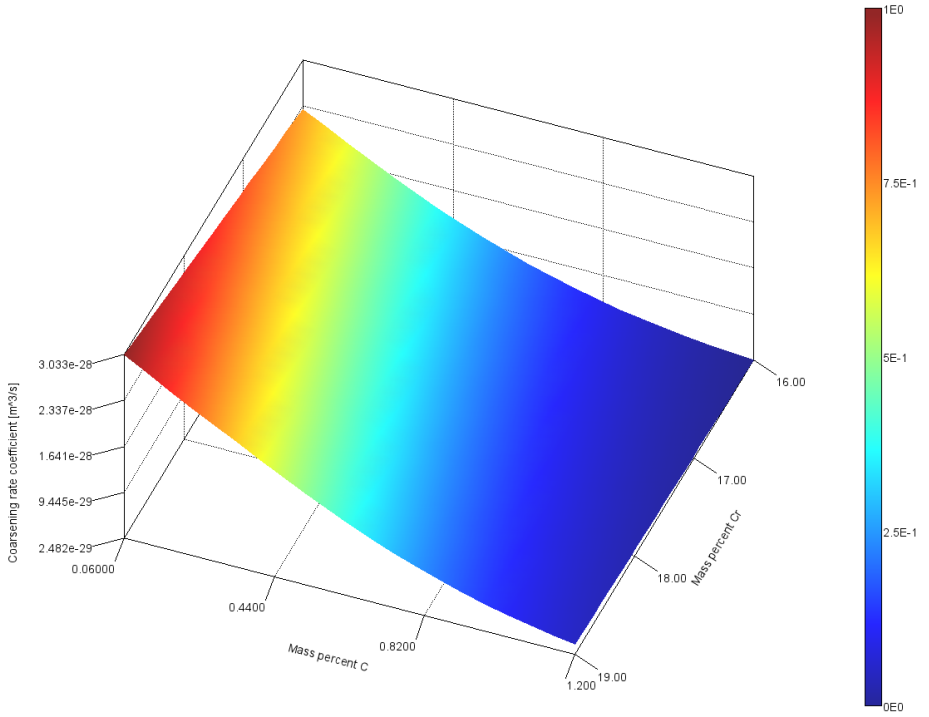


Figure 30: Coarsening rate coefficient (3D plot).

When in the Thermo-Calc help (press F1), go to Rotating 3D Plots to watch a short video showing you how to rotate this plot in the Results window.

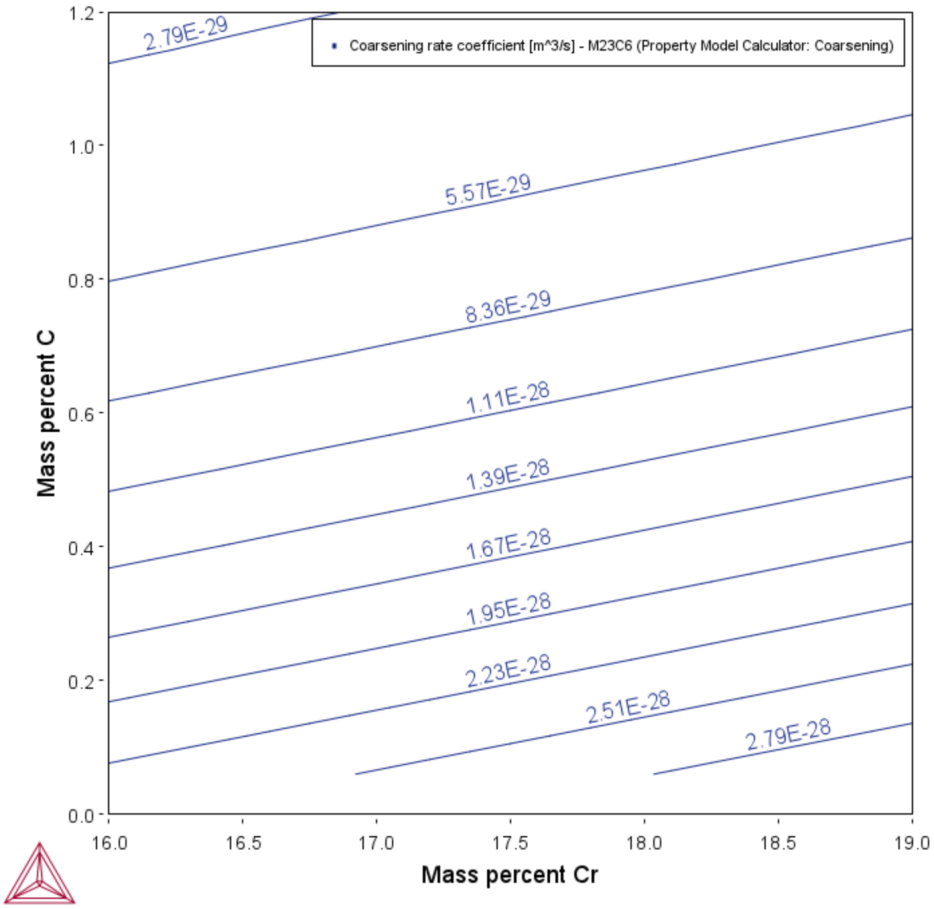


Figure 31: Coarsening rate coefficient (contour plot)

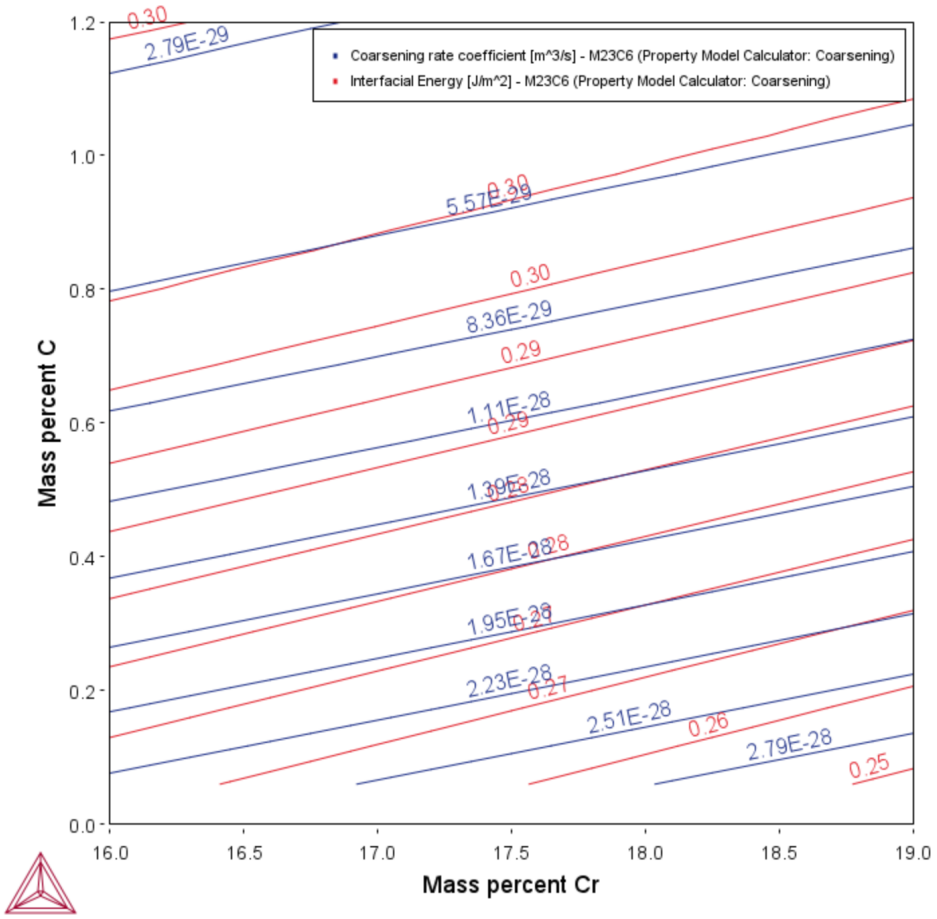


Figure 32: The coarsening rate coefficient and interfacial energy in overlayed plots.

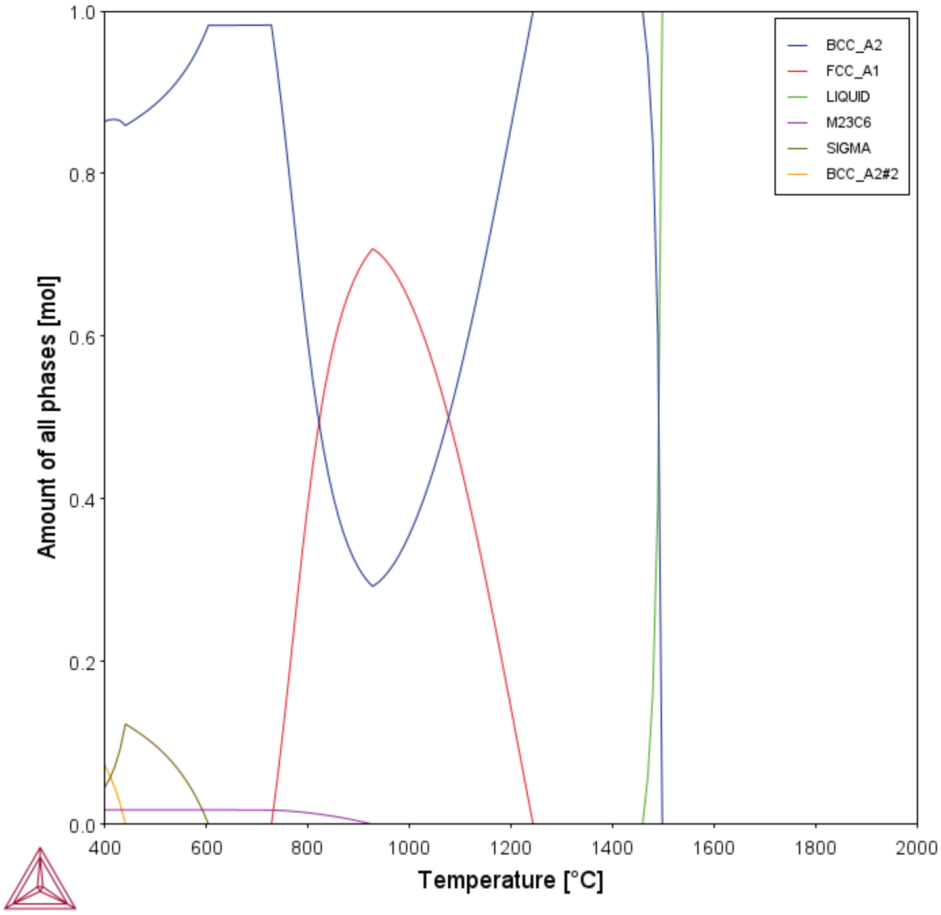


Figure 33: Phase fractions vs T (One axis).

PM_G_03: Driving Force and Interfacial Energy

The example uses the Property Model Calculator and a thermodynamic demonstration steel database (FEDEMO). Using a *grid* calculation type it produces a *contour* plot comparing the driving force and interfacial energy.

This example is included as a tutorial on our website and our YouTube channel.

Driving Force Property Model Settings and Interfacial Energy Property Model Settings in the *Thermo-Calc User Guide*.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_03_Driving_force_and_Interfacial_energy.tcu*

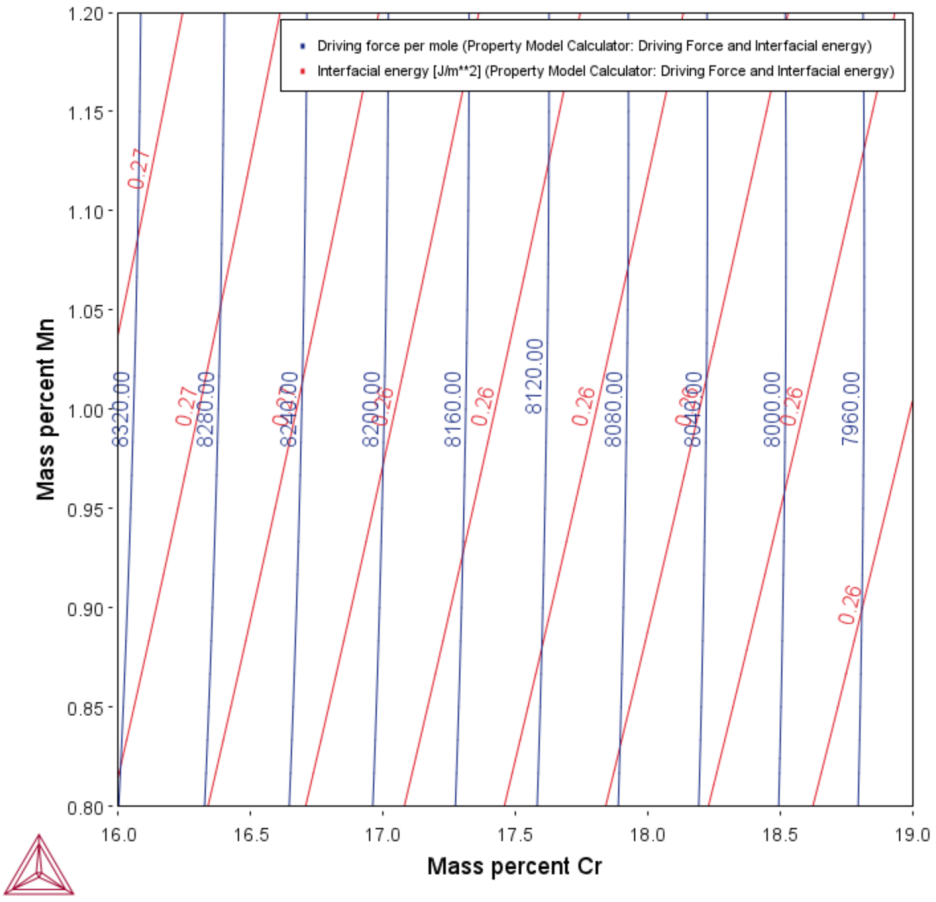


Figure 34: A contour plot.

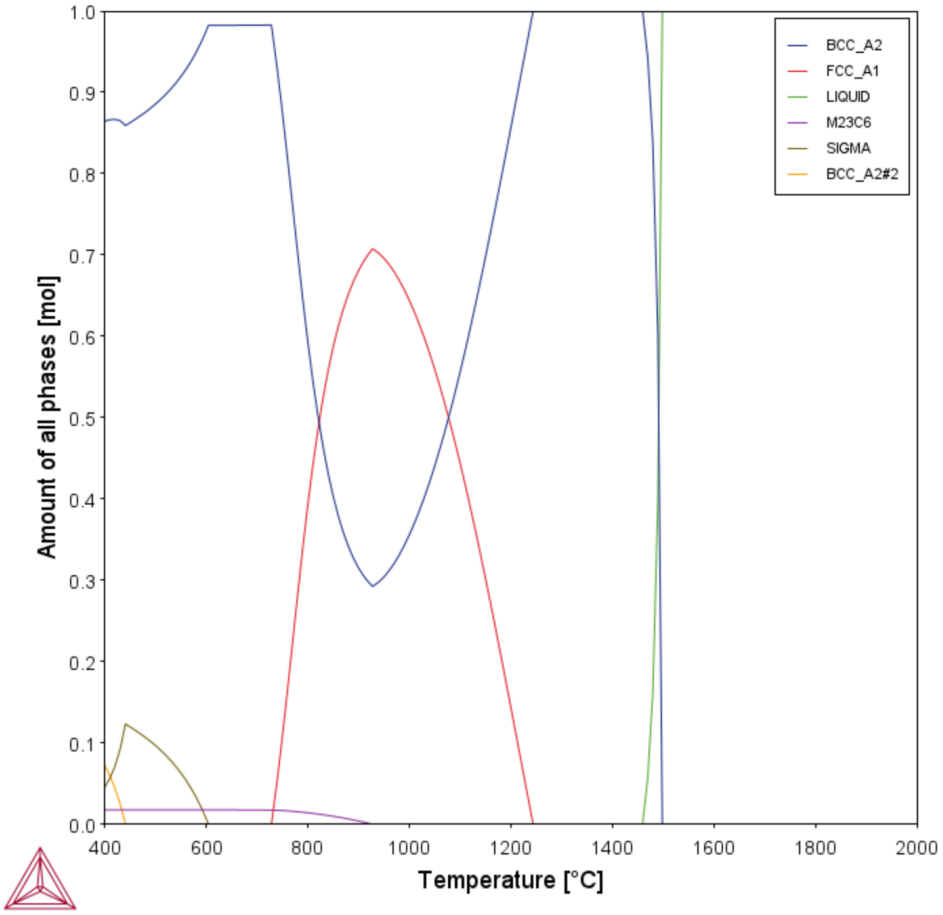


Figure 35: Phase fraction.

PM_G_04: Yield Strength

Yield Strength Property Model Settings and About the Yield Strength Property Model in the *Thermo-Calc User Guide*.

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic demonstration aluminum database (ALDEMO).

This example compares the **Simplified** and **Seidman** models yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C. Although the experimental set up is designed to eliminate grain boundary and solid solution strengthening, these are also included by optimizing the model parameters.

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_04_Yield_Strength.tcu*

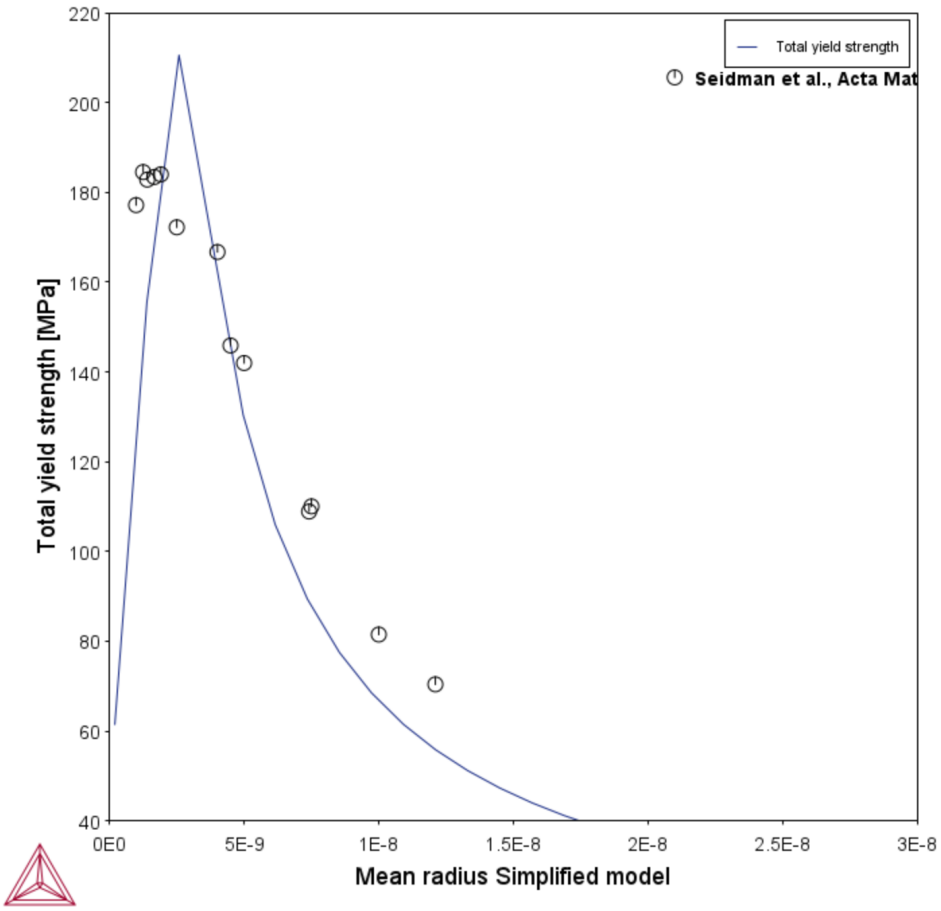


Figure 36: Strength vs Radius - Simplified.

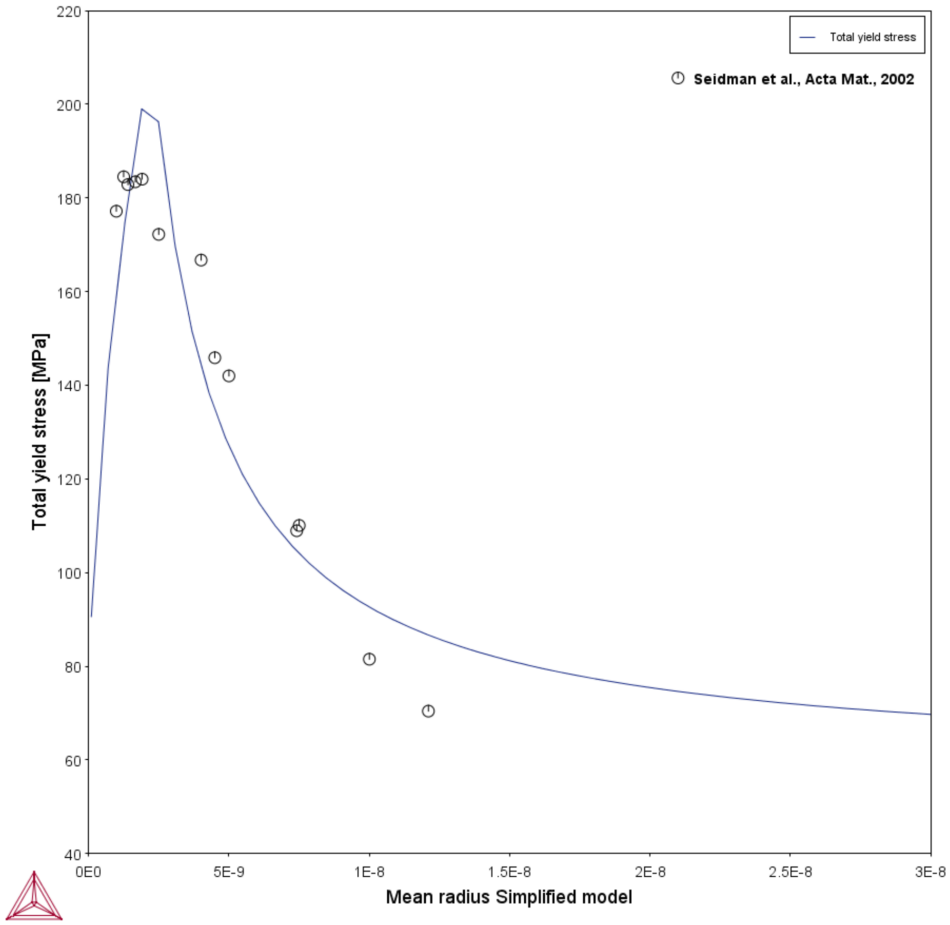


Figure 37: Strength vs Radius - Seidman.

PM_G_05: Yield Strength NiAlCr

Yield Strength Property Model Settings and About the Yield Strength Property Model in the *Thermo-Calc Graphical Mode User Guide*.

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic demonstration nickel database (NIDEMO).

The Reppich model is developed for calculation of precipitation strengthening in Ni-based super alloys consisting mainly of gammaprime precipitates in a gamma matrix. The example shows a calculation of the precipitation strengthening vs precipitate radius in a Ni-10at%Al-10at%Cr alloy.



Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_05_Yield_Strength_NiAlCr.tcu*

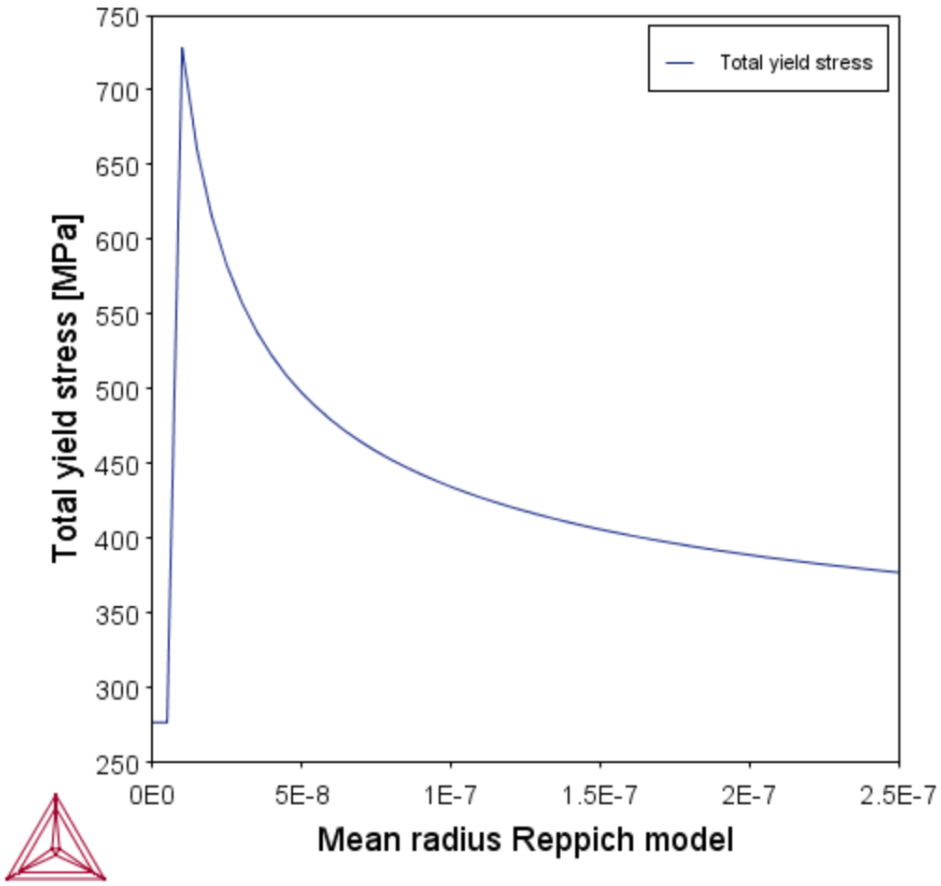


Figure 38: Reppich model plotted with results and experimental data for PE16, all data is normalized with the square root of the volume fraction of precipitate.

PM_G_06: Yield Strength HEA

Yield Strength Property Model Settings and About the Yield Strength Property Model in the *Thermo-Calc Graphical Mode User Guide*.



This example requires the use of the TCS High Entropy Alloy (TCHEA) database. A license is required to run the example.

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic high entropy alloy database (TCHEA). This is an example of solid solution strengthening, which is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. The example shows the solid solution strengthening over the full solubility range for the Mo-Ta system as compared to experimental data.



Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_06_Yield_Strength_HEA.tcu*

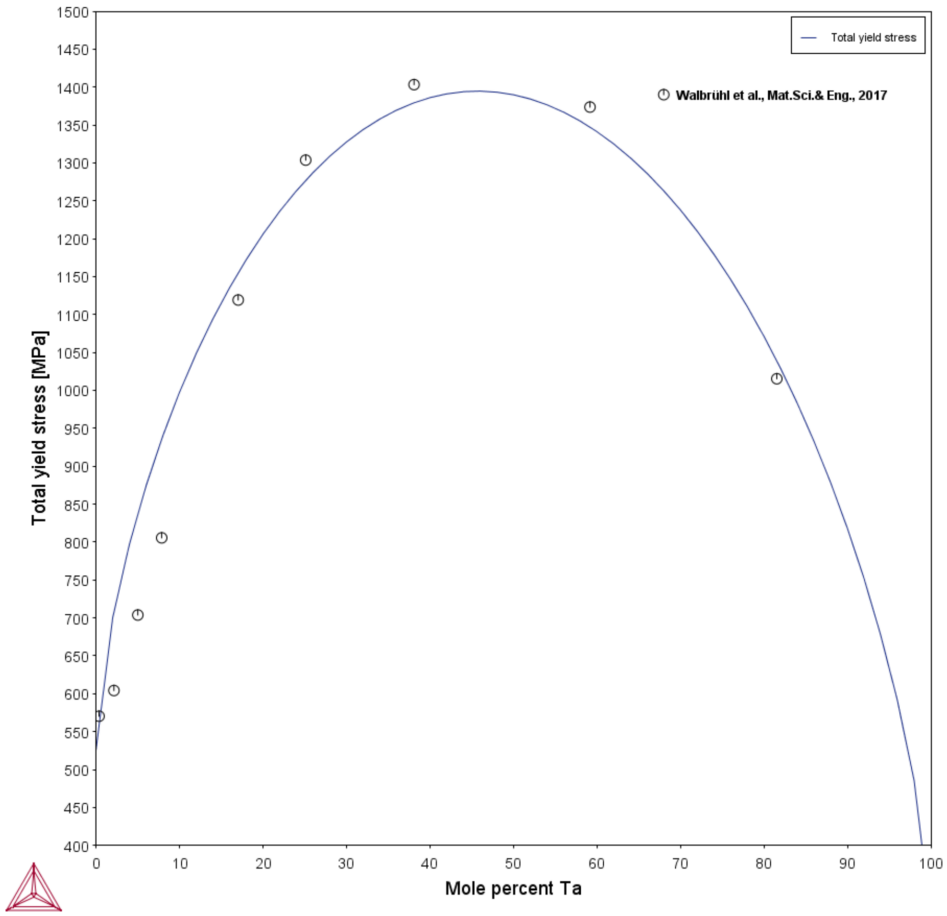


Figure 39: Strength vs at% Ta

PM_G_07: Hot Crack Susceptibility

See About the Crack Susceptibility Coefficient Property Model for background information about this Property Model.

The example uses the **Property Model Calculator** and the **Crack Susceptibility Coefficient** Property Model to calculate the hot tearing tendency during solidification for an Al-Si alloy.

The **ALDEMO: Aluminum Demo Database** is used and this example is available to all users.

Hot tearing is one of the most common and serious defects encountered during the casting of, for example, aluminum alloys. In general, it is defined by the formation of a macroscopic fissure in a casting as a result of stress and the associated strain, generated during cooling, at a temperature above the non-equilibrium solidus.

The Model is based on the publication by Yan and Lin [2006, Yan] and uses experimental data [1955, Pumphrey; 1976, Feurer; 2004 Barnett] from this paper.

The experimental hot cracking susceptibility of an alloy is defined as the ratio between the cracking length for that alloy and the maximum cracking length in the alloy system studied. Considering the uncertainties and difficulties in hot tearing measurements, the calculated hot tearing tendencies are in excellent agreement with the experimental data. The typical L-shaped curve is well reproduced in the current prediction. It rapidly increases at a low solute content and has a maximum at a composition of around 0.5 wt pct Si.

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_07_Hot_Crack_Susceptibility.tcu*

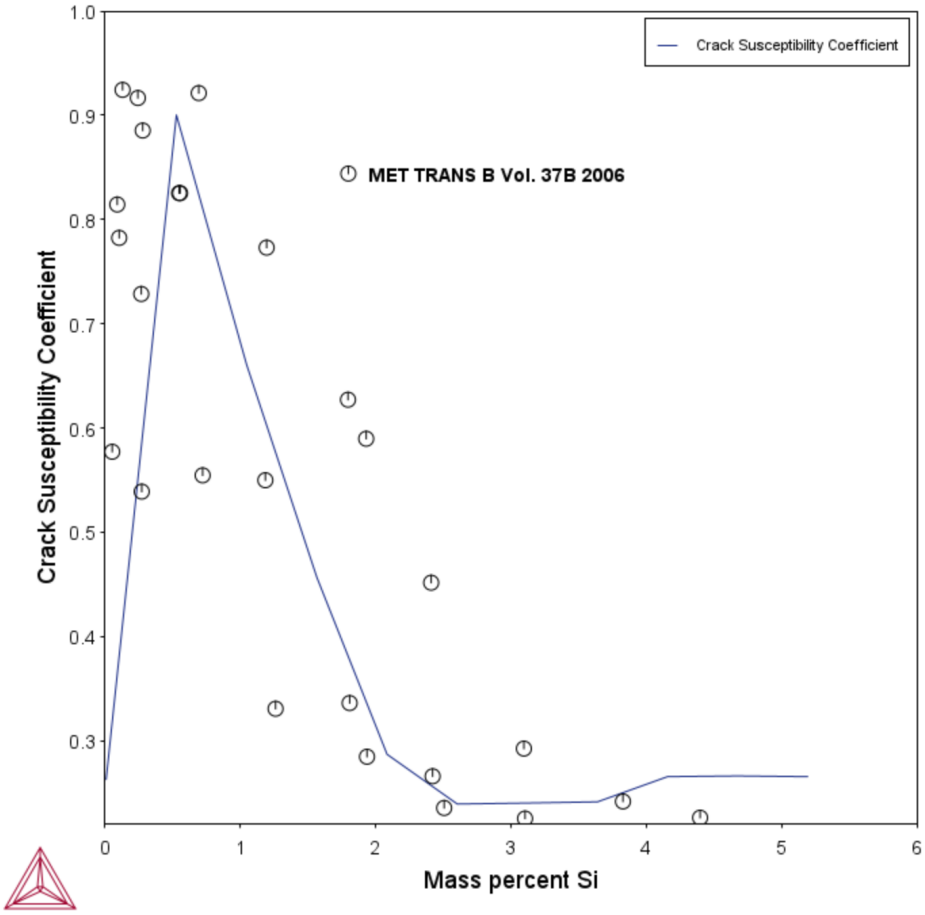


Figure 40: The plot compares the predicted cracking susceptibility/composition curve for the Al-Si system with the experimental hot tearing tendencies [1955, Pumphrey; 1976, Feurer; 2004 Barnett].

References

[1955 Pumphrey] W.I. Pumphrey: ‘‘The Aluminum Development Association Report No. 27,’’ Aluminum Development Association, London, 1955.

[1976 Feurer] V. Feurer: Giessereiforschung, 1976, vol. 28, pp. 75-80.

[2004 Barnett] S. R. Barnett, J. A. Taylor, and D. H. St. John: Solidification of Aluminum Alloys, M.G. Chu, D.A. Granger, and Q. Han, eds., TMS, Warrendale, PA, 2004, pp. 201-09.

[2006 Yan] X. Yan and J. C. Lin, “Prediction of hot tearing tendency for multicomponent aluminum alloys,” Metall. Mater. Trans. B, vol. 37, no. 6, pp. 913–918, Dec. 2006.

PM_G_08: Spinodal

About the Spinodal Property Model

The example uses the **Property Model Calculator** and the **Spinodal** Property Model to calculate the so-called spinodal curve for the BCC_A2 miscibility gap in the system Fe-Cr.

The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

Two Property Model Calculators are used in this example. The spinodal curve (a **One axis** calculation), is overlayed on top of a the Fe-Cr **Phase diagram** calculation. As can be seen in the plot, the spinodal curve for BCC goes through the one-phase region for Sigma. This is because the spinodal curve for a phase is calculated when all other phases are suspended.

Project File and Video Tutorial Information

- Folder: **Property Models>General**
- File name: *PM_G_08_Spinodal.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

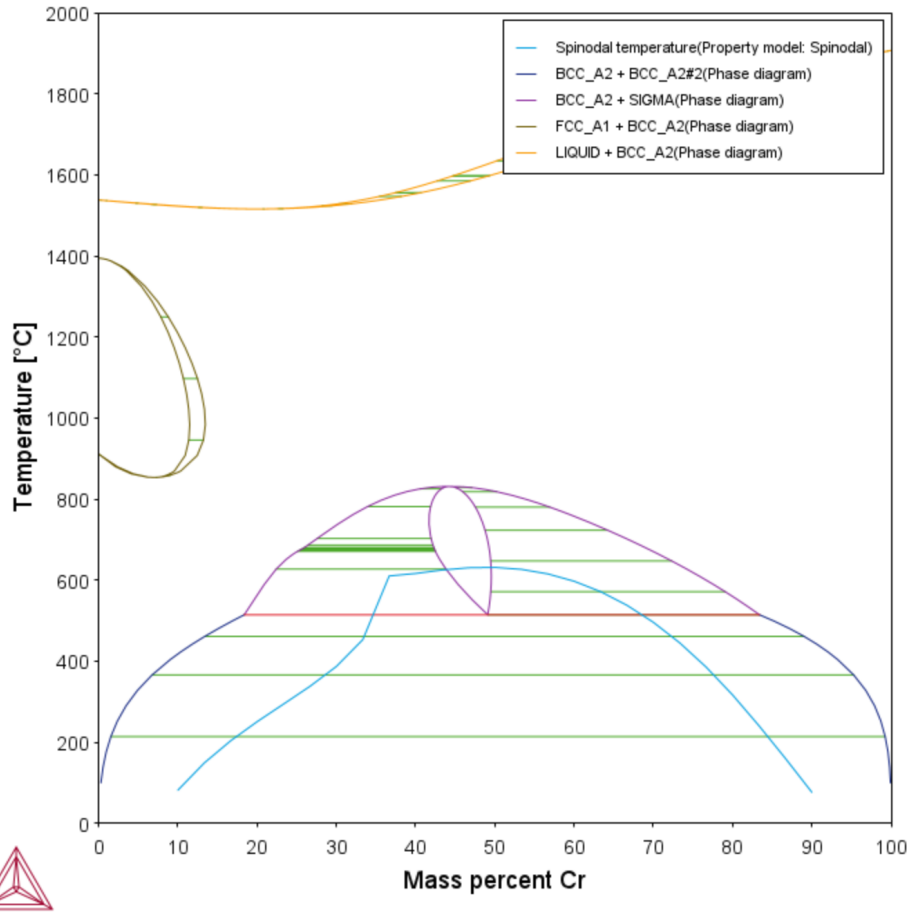


Figure 41: An Fe-Cr spinodal curve for BCC goes through the one-phase region for Sigma.

PM_G_09: T-Zero Temperature

About the T0 Temperature Property Model

The example uses the **Property Model Calculator** and the **T-Zero Temperature** Property Model to calculate the so-called T_0 line for the two-phase field FCC_A1 and BCC_A2 in the Fe-Ni system. The line is plotted together with the phase diagram for the same Fe-Ni system.

The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

The T_0 temperature is defined as the temperature where two phases of identical chemical composition have the same molar Gibbs free energy. This temperature is an important quantity in the field of diffusionless phase transformations, e.g. martensitic transformation, since it is the upper limit where diffusionless phase transformations can occur.

Two Property Model Calculators are used in this example. The T_0 line (a **One axis** calculation) for the two-phase field FCC_A1 and BCC_A2 is overlayed on top of a the Fe-Ni **Phase diagram** calculation.

Project File and Video Tutorial Information

- Folder: **Property Models>General**
- File name: *PM_G_09_T-Zero_temperature.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

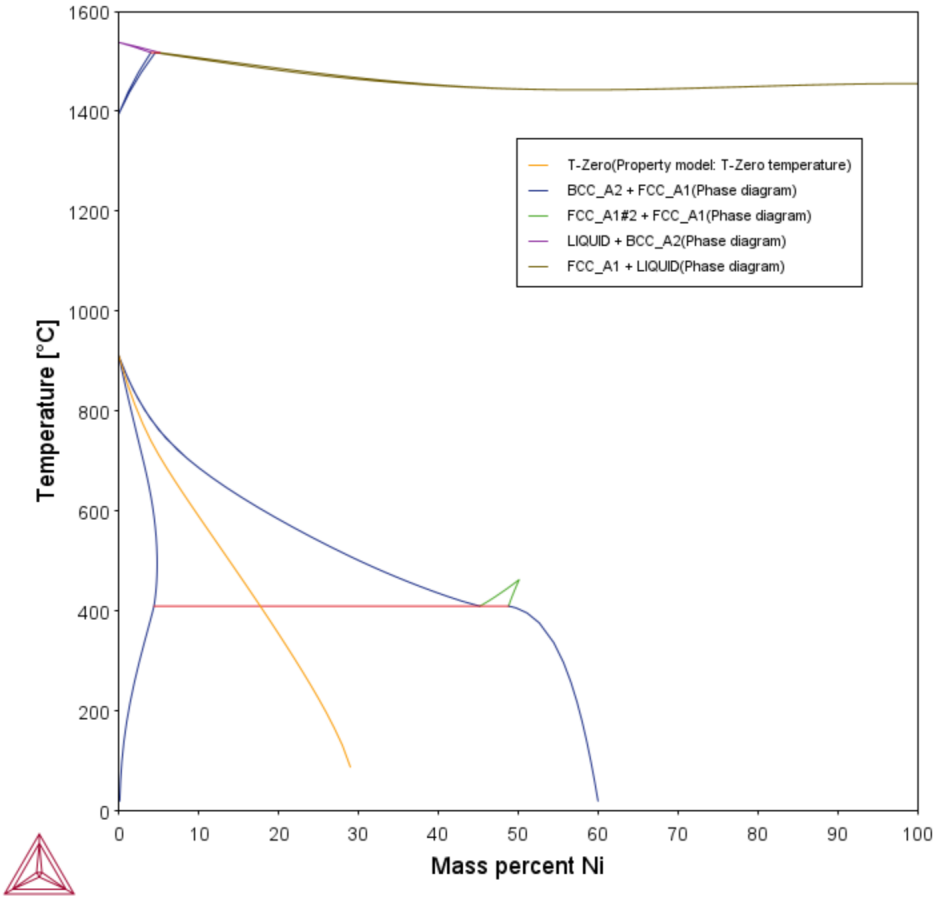


Figure 42: In this plot for the Fe-Ni system, the T_0 line for the FCC_A1 and BCC_A2 phases is located in the middle of the two-phase region. No solution for the T_0 temperature exists above about 30 mass% Ni.

PM_G_10: Freeze-in Thermal Conductivity

About the Equilibrium with Freeze-in Temperature Property Model

The **TCAL Al-Alloys** Database (version 7 and newer) is used in this example. A valid license is required to run the example.

The example uses the **Property Model Calculator** and the **Equilibrium with Freeze-in Temperature** Property Model to compare the use of the model with thermal conductivity with and without grain boundary (GB) phase scattering being included in the calculation.

The TCS Al-based Alloy Database (TCAL) is used to evaluate a 7075_T6 alloy (Al-1.6Cu-2.5Mg-5.6Zn-0.25Fe-0.15Mn-0.23Cr-0.2Ti-0.2Si) mass%. The "T6" in the alloy name means that the alloy has been artificially peak-aged, i.e. the matrix is almost depleted. The heating is assumed to be at a typical artificial aging temperature of 150 °C. The temperature has then been increased for measuring of the reported values thermal conductivity at 400, 500, and 532 °C.

The electrical resistivity due to grain boundary phase scattering is approximated as a scattering constant times the total volume fraction of the grain boundary phases. The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.

The calculation set up assumes that the alloy reaches equilibrium at the peak-age temperature, i.e. that the amounts of phases and their composition freeze-in at 150 °C and that these do not change for the evaluation of thermal conductivity at the temperatures 400, 500, and 532 °C. Calculations are compared between accounting and ignoring contributions from grain boundary (GB) phase scattering.

As can be seen in Figure 43, the calculation including the approximate effect of grain boundary phase scattering is close to the experimentally measured values. Excluding the effect of grain boundary phase scattering slightly overestimates the thermal conductivity. Experimental data is from [2008, ASM].

Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM_G_10_Freeze_In_Thermal_Conductivity.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

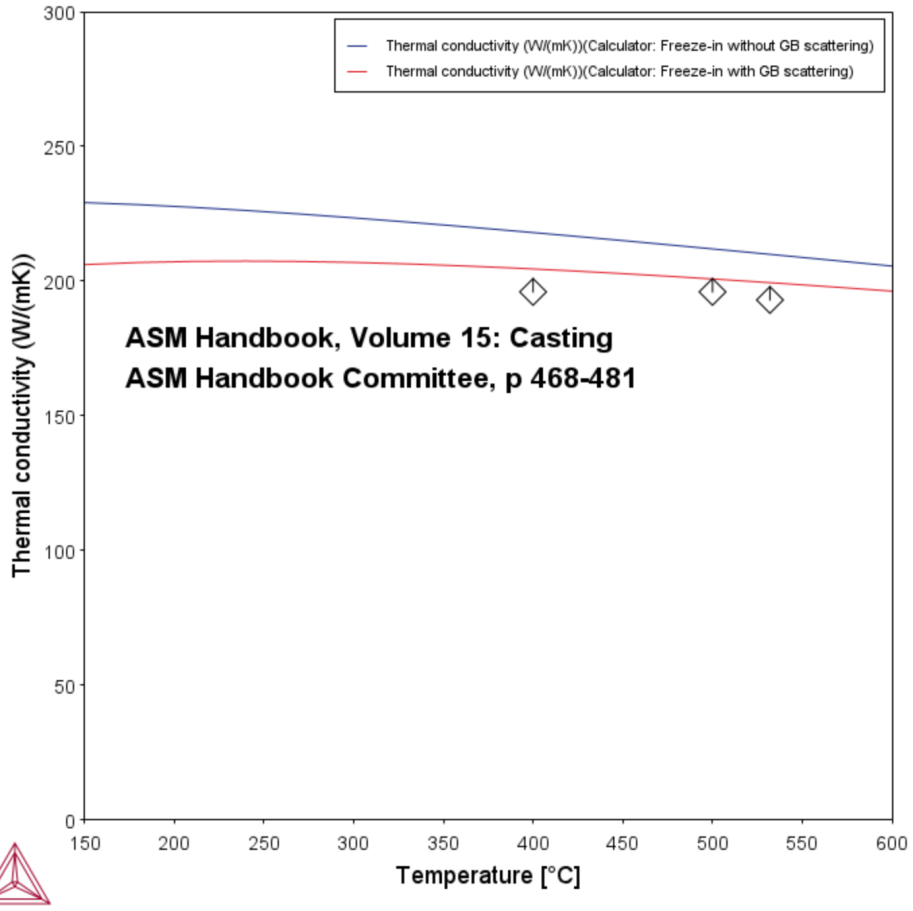


Figure 43: Comparing the freeze-in temperature for the 7075_T6 alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

[2008, ASM] ASM Handbook Committee, ASM Handbook Volume 15: Casting. ASM International, p. 468-481, 2008, ISBN 978-0-87170-711-6.

PM_G_11: Freeze-in Electric Conductivity

About the Equilibrium with Freeze-in Temperature Property Model

The **TCAL Al-Alloys** Database (version 7 and newer) is used in this example. A valid license is required to run the example.

The example uses the **Property Model Calculator** and the **Equilibrium with Freeze-in Temperature** Property Model to compare the use of the model for electric conductivity with and without grain boundary (GB) scattering being included in the calculation.

The TCS Al-based Alloy Database (TCAL) is used to evaluate a 4032-O alloy (Al-0.9Cu-1.0Mg-0.9Ni-12.2Si) mass%. The "O" in the alloy name means that the Al alloy has been heat-treated at a typical temperature of 350 °C. The measurement of electric resistivity is usually performed at room temperature.

The electrical resistivity due to grain boundary phase scattering is approximated as a scattering constant times the total volume fraction of the grain boundary phases.

The calculation set up assumes that the alloy reaches equilibrium at the "O" heat-treated temperature, i.e. that the amounts of phases and their composition freeze-in at 350 °C and that these do not change for the evaluation of electric resistivity at the room temperature. Calculations are compared between accounting and ignoring contributions from grain boundary (GB) scattering.

As can be seen from Figure 44, the calculated electric resistivity at room temperature, including grain boundary phase scattering, is very close to the experientially measured value (4.3E-8) for the alloy. Excluding the grain boundary phase scattering somewhat underestimates the electric resistivity for the alloy. Experimental data is from [1993, Davis].

Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM_G_11_Freeze_In_Electric_Conductivity.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

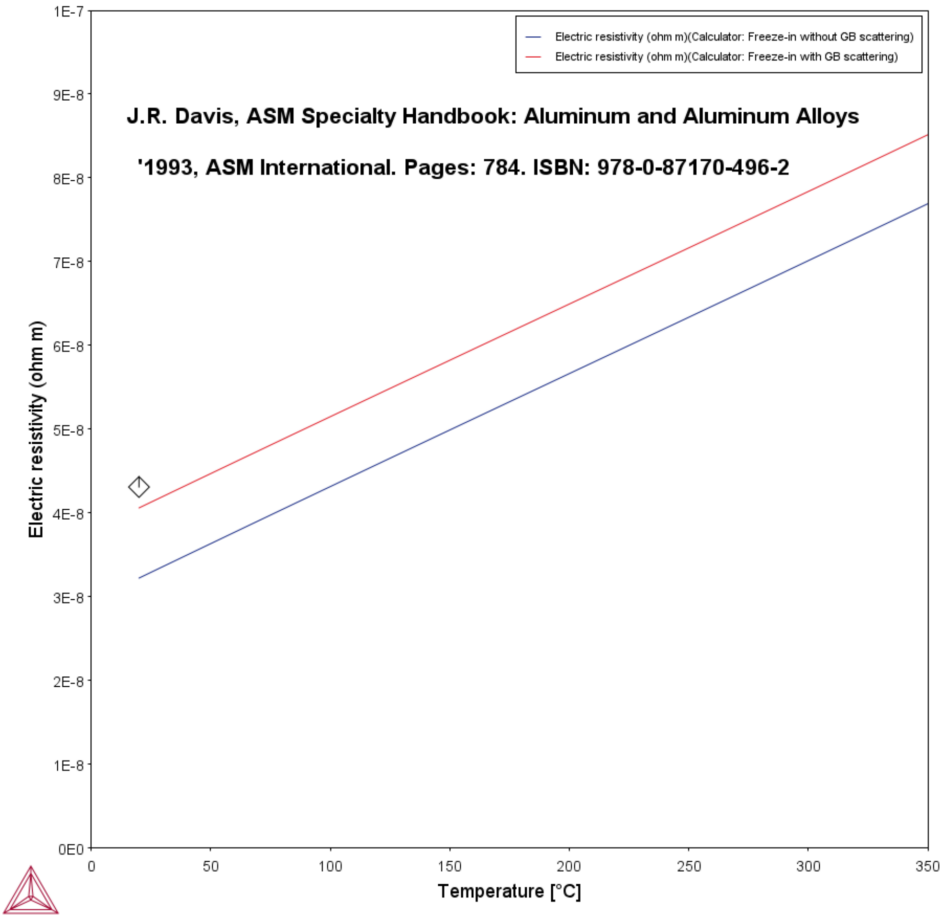


Figure 44: Comparing the freeze-in temperature for the 4032-O alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

[1993, Davis] J.R. Davis, ASM Specialty Handbook: Aluminum and Aluminum Alloys, 1993, ASM International. Pages: 784. ISBN: 978-0-87170-496-2.

PM_G_12: Solidus and Liquidus Batch Calculation

The example uses the **Property Model Calculator** and the **Liquidus and Solidus Temperature** Property Model to demonstrate the use of the **Batch** calculation type.

Working with Batch Calculations

The thermodynamic demonstration steel database (FEDEMO) is used along with a randomized set of experimental data points that are shown on the **Configuration** window in a table. The data showing in this example is imported from a data file prepared with specific data entry requirements.

A variety of compositions for an Fe-Cr-Mn-Ni-C alloy is used for the calculations; these compositions are also taken from the same data file. When the heading includes `Exp`, then these columns are considered experimental data by Thermo-Calc, where in this example it is the columns titled `Exp Liq temp C` and `Exp Sol temp C`. This experimental data can then be plotted as a function of the calculated solidus/liquidus temperature and compared on the plot using a **Cross plot mode**, which is selected on the Plot Renderer. The limits are shown using the setting RMS (root mean square).

The experimental data entered into the batch data file is unitless even though the actual experimental data unit is Celsius (as written in the header text). In order for the plot and calculations to match, Celsius is chosen as the temperature unit when defining the **Solidus/Liquidus** Property Model and all the axes manually scaled to the same limits (1360 → 1520).

Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM_G_12_Solidus_and_Liquidus_Batch_Calculation.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

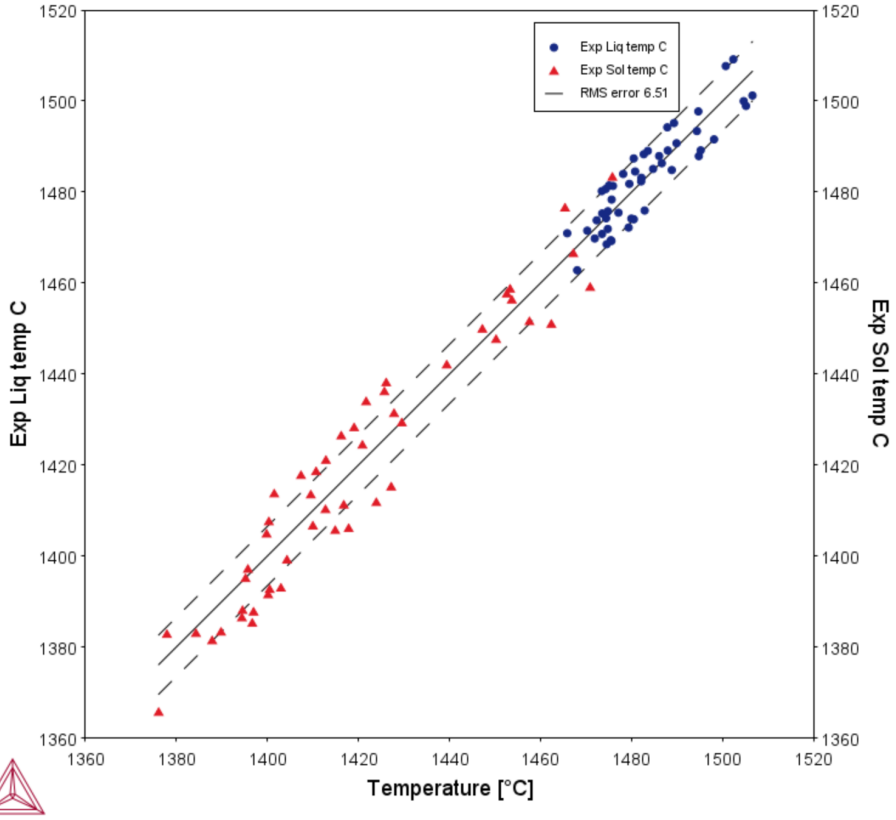


Figure 45: A comparison of experimental liquidus and solidus data using the Cross plot mode with a Batch calculation. A root mean square (RMS) setting shows the distribution of the data points.

Steel Model Library Examples Collection

The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus Property Models in the Steel Model Library.

About the Examples

In this section:

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing 471
PM_Fe_02: Fe-Mn Martensite Morphologies 474
PM_Fe_03: Fe-C-Mn Pearlite 476
PM_Fe_04: Critical Temperatures 480
PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite 483
PM_Fe_06: TTT Diagram Property Model 485
PM_Fe_07: Hardenability Design of Steel 487
PM_Fe_08: CCT Diagram Property Model 489

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

- Property Model Calculator, About the Martensite Temperatures Property Model, and About the Martensite Fractions Property Model

The example uses the **Property Model Calculator** with the **Martensite Fractions** and **Martensite Temperatures** Models to calculate martensite fractions and martensite temperatures [martensite start (Ms) and 90% transformation temperature (M90)].

The alloy is first intercritically annealed and then quenched. Austenite composition is determined by an equilibrium calculation at the annealing temperature. Martensite fraction is calculated as a function of temperature which the alloy is quenched to. The example also shows how Cr content in the alloy influences Ms and M90 after intercritical annealing.

Project File and Video Tutorial Information

- Folder: Property models >Steel
- File name: *PM_Fe_01_Fe-Cr-C_martensite_intercritical_annealing.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

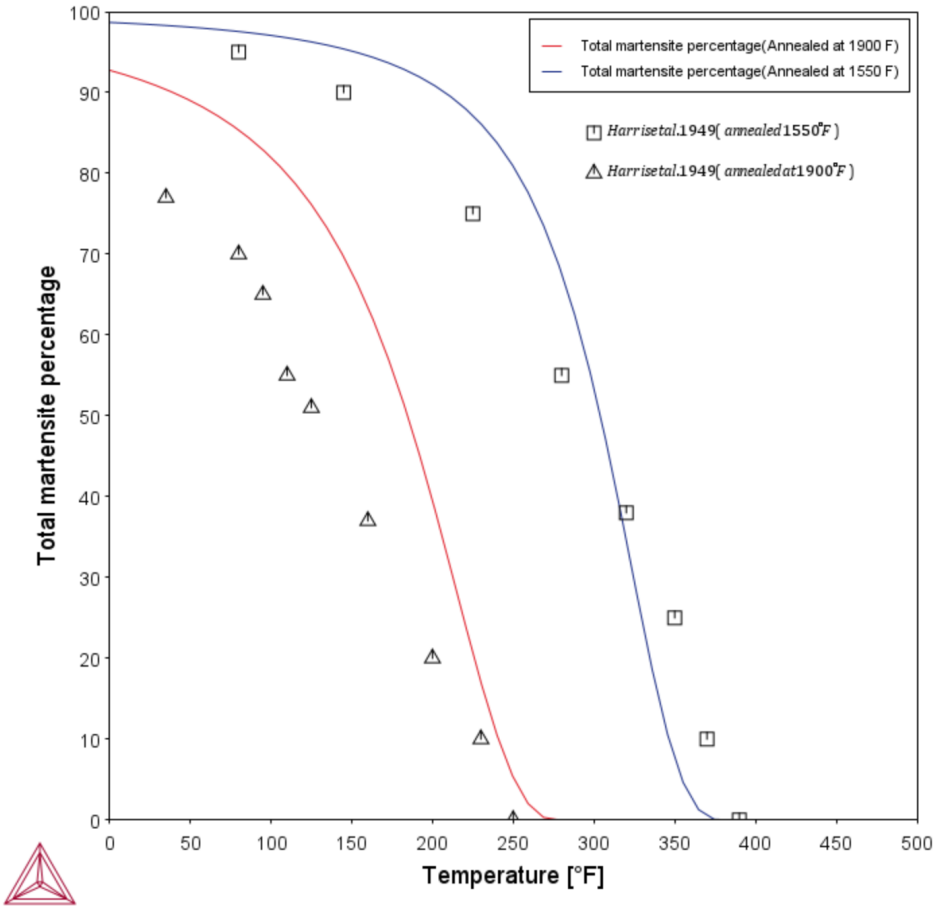


Figure 46: The transformation curves plot showing Fe-Cr-C martensite with intercritical annealing.

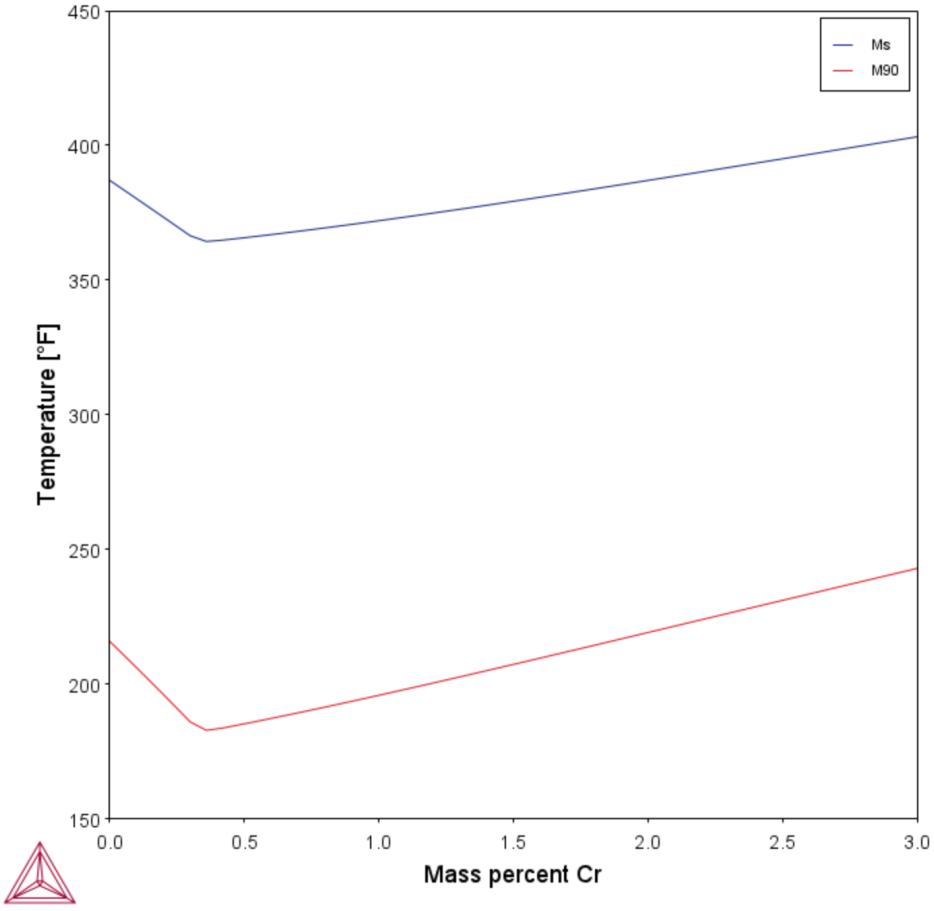


Figure 47: Comparing Martensite start (Ms) to Martensite finish (Mf).

Reference

[1949, Harris] Harris, William J, and Morris Cohen. 1949. “Stabilization Of The Austenite-Martensite Transformation.” Trans. AIME 180: 447–70.

PM_Fe_02: Fe-Mn Martensite Morphologies

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

- Property Model Calculator and About the Martensite Temperatures Property Model

The example uses the **Property Model Calculator** with the **Martensite Temperatures** Property Model to calculate the Ms temperatures of different types of martensites: lath, plate, and ε (hcp), compared with experimental ε Ms values taken from several sources.

Project File and Video Tutorial Information

- Folder: Property Models>Steel
- File name: *PM_Fe_02_Fe-Mn_martensite_morphologies.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

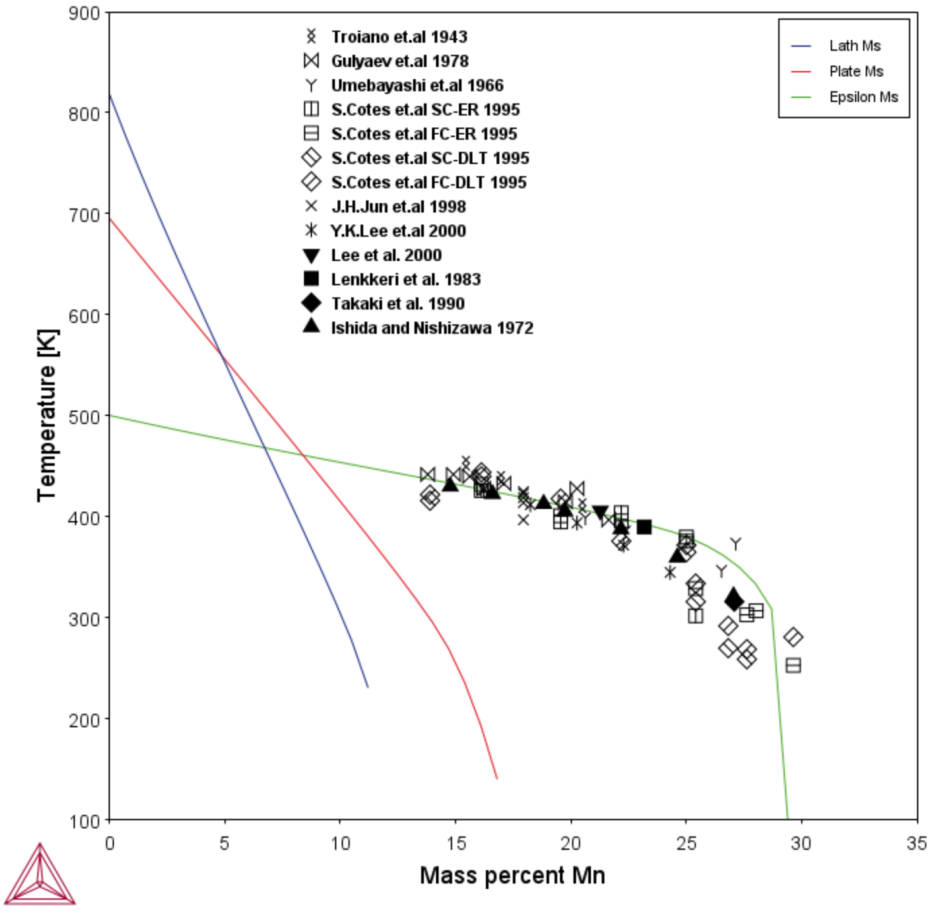


Figure 48: A diagram showing all the Ms temperatures of different types of martensite morphologies (lath, plate and epsilon (hcp) compared with experimental epsilon Ms values.

PM_Fe_03: Fe-C-Mn Pearlite

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Property Model Calculator and About the Pearlite Property Model

The example uses the **Property Model Calculator** and with the **Pearlite** Property Model and shows how to calculate pearlite growth rate, lamellar spacing, and times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %). With *maximize growth rate* set as the *criterion*, the model gives maximal growth rate and minimal lamellar spacing. With *optimal pearlite* as the *pearlite mode*, the model optimizes partitioning of substitutional alloying element(s) (Mn in this example) according to the criterion, which realizes a smooth transition between ortho-pearlite at high temperature and para-pearlite at low temperature.

Project File and Video Tutorial Information

- Folder: Property Models>Steel
- File name: *PM_Fe_03_Fe-C-Mn_Pearlite.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

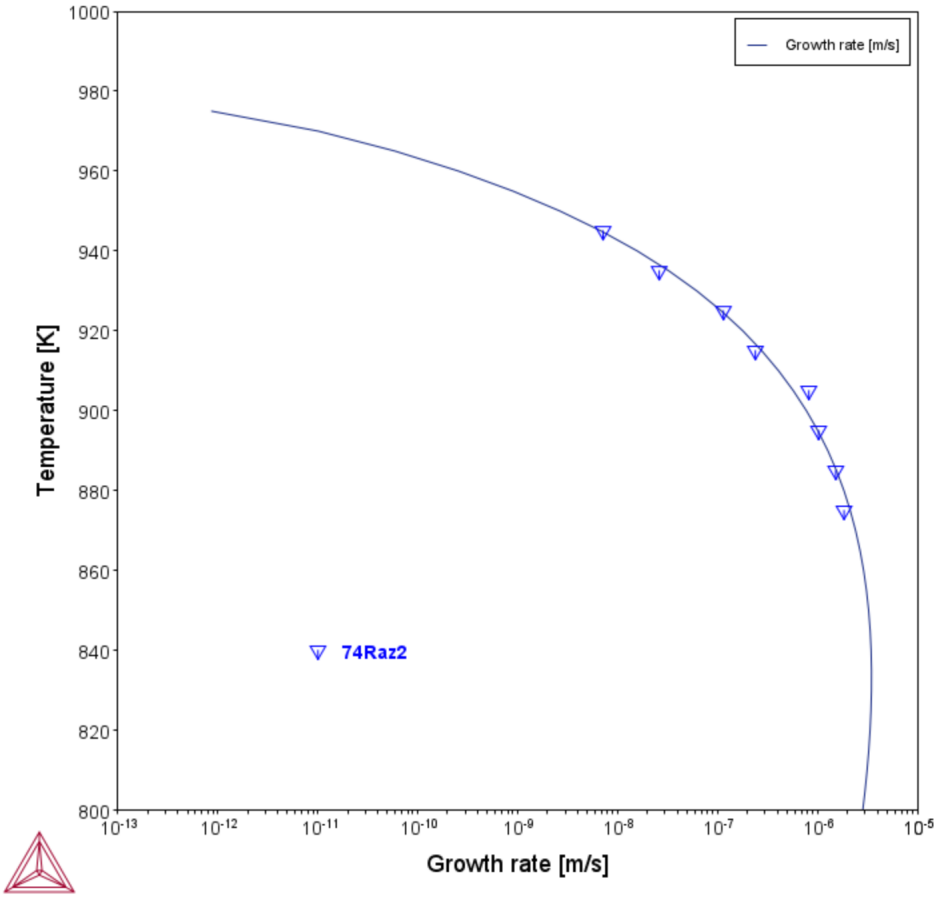


Figure 49: Growth rate as a function of temperature.

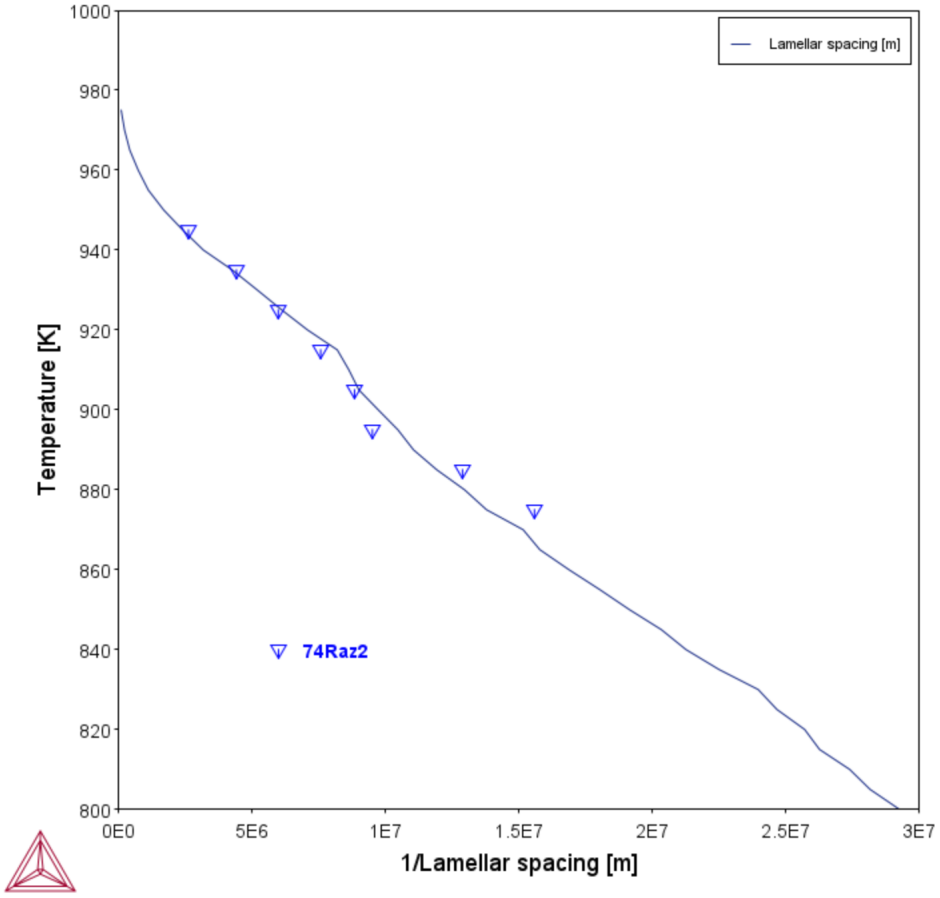


Figure 50: Lamellar spacing as a function of temperature.

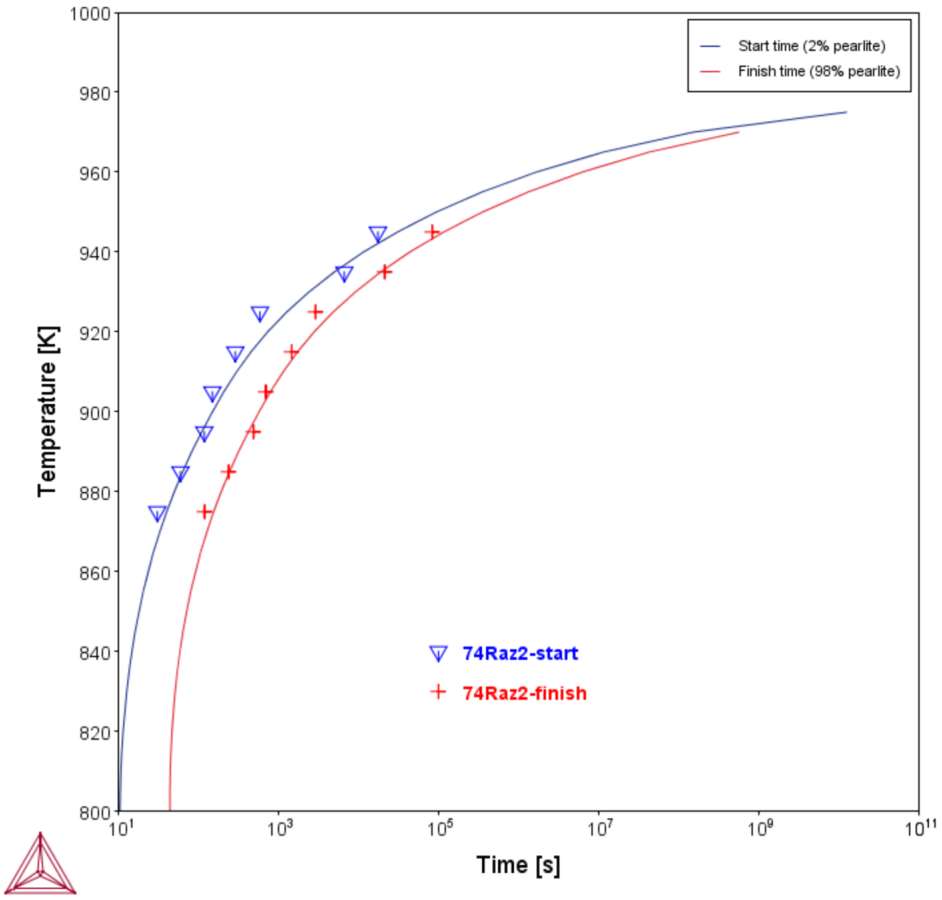


Figure 51: The TTT (time-temperature-transformation) diagram showing times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %).

Reference

[1974 Razik] Razik, N.A, G.W. Lorimer, and N Ridley. 1974. “An Investigation of Manganese Partitioning during the Austenite-Pearlite Transformation Using Analytical Electron Microscopy.” Acta Metallurgica 22 (10): 1249–58.

PM_Fe_04: Critical Temperatures

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Property Model Calculator and About the Critical Transformation Temperatures Property Model

The example uses the **Property Model Calculator** and the **Critical Transformation Temperatures** Model to calculate the distribution of the typical phase transition temperatures for a low alloy steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification for the alloy.

The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

In the set up of the example, the **Critical Transformation Temperatures** model is used with a Property Model Calculator **Uncertainty** calculation to plot a histogram showing the distribution of A1- and A3-temperatures (Figure 52). As a comparison, an Equilibrium Calculator, **One axis** calculation results in a property diagram showing the phase transitions for the nominal composition (Figure 53).

The phase transition temperatures are defined as:

- Liquidus: First austenite or ferrite transformation from the liquid
- Solidus: Liquid fully transformed to solid
- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)

Project File and Video Tutorial Information

- Folder: Property **Models>Steel**
- File name: *PM_Fe_04_Critical_Temperatures.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

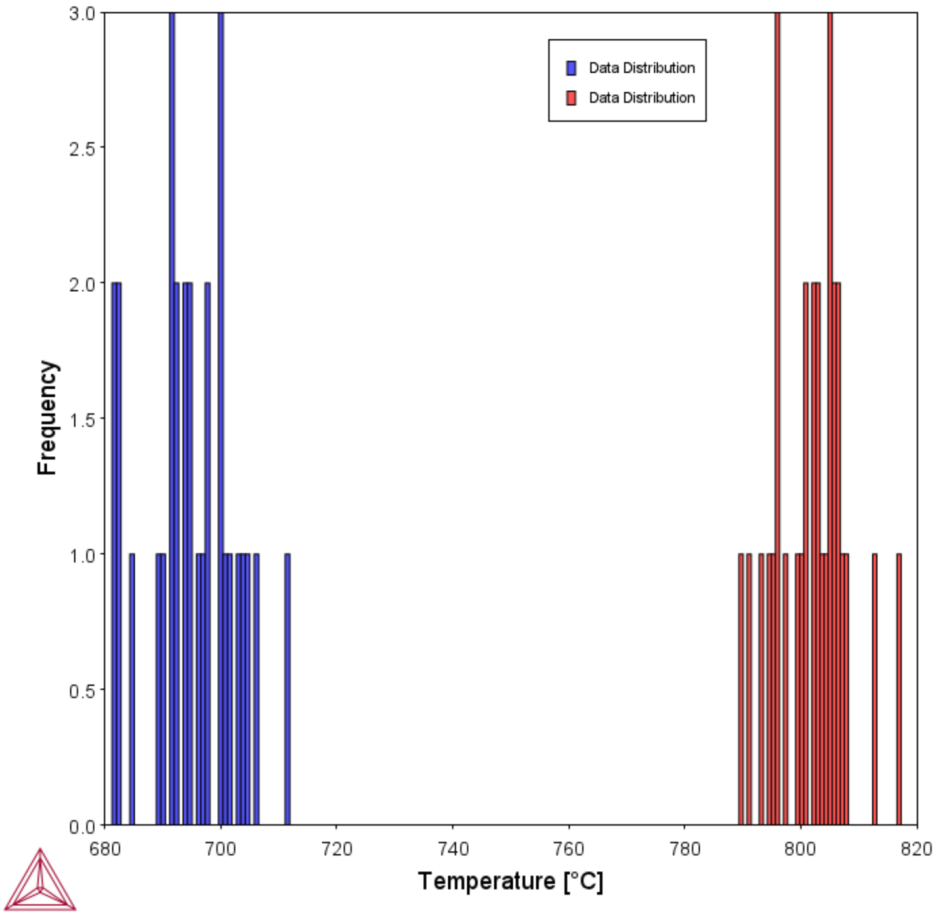


Figure 52: The distribution of the A1 and A3 phase transition temperatures for a low alloyed steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification. This plot uses the Critical Transformation Temperatures model with the Property Model Calculator.

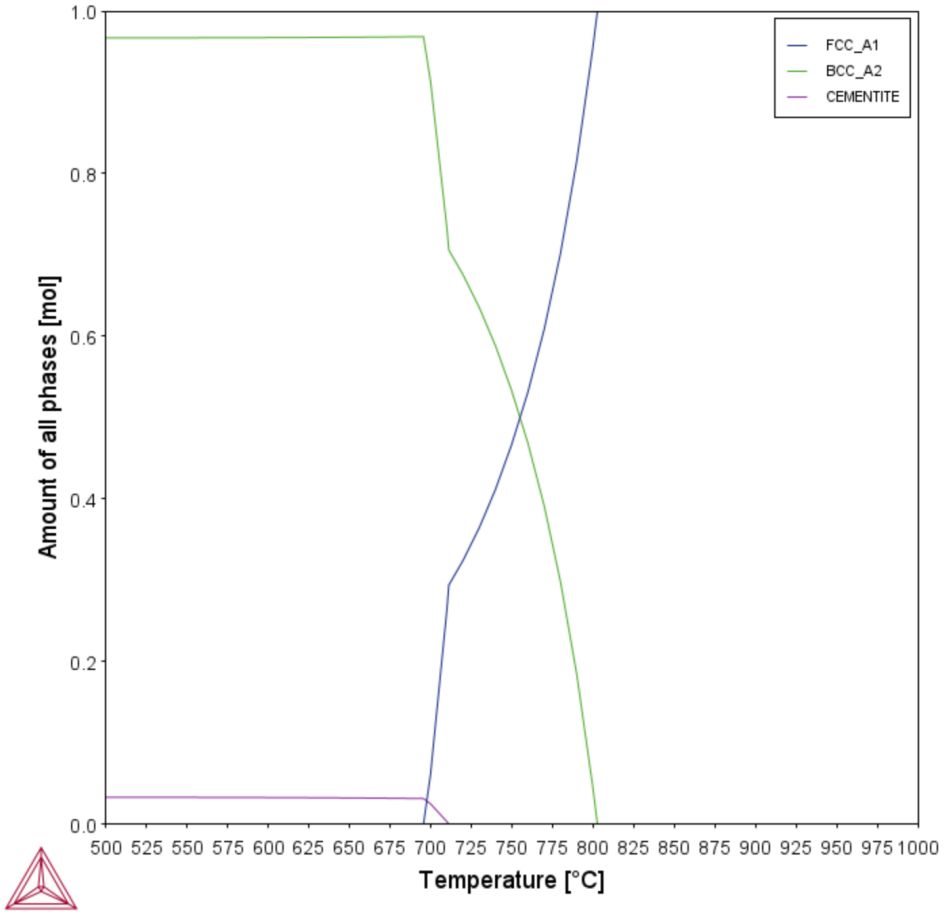


Figure 53: This plot uses an Equilibrium Calculator to show an alternate visualization of the phase transitions in a property diagram for the nominal composition.

PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The example uses the **Property Model Calculator** and the **Bainite** Steel Model to calculate a Time-Temperature-Transformation (TTT) diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy. The result is compared to experimental results from [1948, Jaffe]. Other elements with low amount in the experimental alloy are omitted for the calculation.

Considered elements: Fe, C, Mn, Si, Cr, Ni, Mo. Other elements in the system are neglected for bainite by mass percent.

A Property Model Calculator is used with a *One axis* calculation and the *TTT mode* selected on the Plot Renderer to plot the TTT diagram.

For more information see About the Bainite Property Model, Plot Settings: TTT Mode, and Plotting Modes.

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_05_Fe-C-Mn-Si-Ni-Cr-Mo_Bainite.tcu*

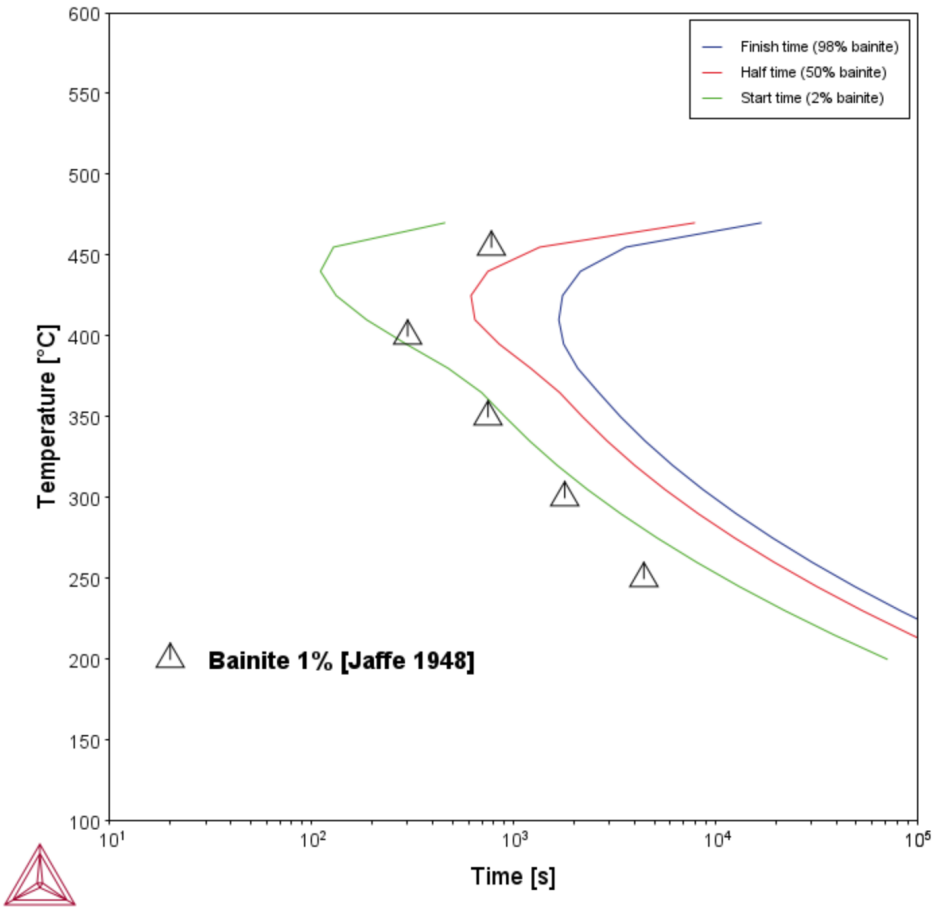


Figure 54: The bainite TTT diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy.

Reference

[1948, Jaffe] L. D. Jaffe, “Anisothermal formation of bainite and proeutectoid constituents in steels,” Trans. AIME, vol. 176, pp. 343–383 (1948).

PM_Fe_06: TTT Diagram Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The example uses the **Property Model Calculator** and the **TTT Diagram** Property Model to calculate a Time-Temperature-Transformation (TTT) diagram for an Fe-C-Mn-Si-Cr-V alloy (Steel 42CrV6). The calculation is compared to an experimental TTT diagram for the same steel (with some other impurities) from data in [1958Wev].

A *One axis* calculation is selected on the Property Model Calculator and then the *TTT mode* selected on the Plot Renderer in order to plot the final TTT diagram shown in the figure below.

For more information see About the TTT Diagram Property Model, TTT Diagram Property Model Settings, and Plot Settings: TTT Mode.

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu*

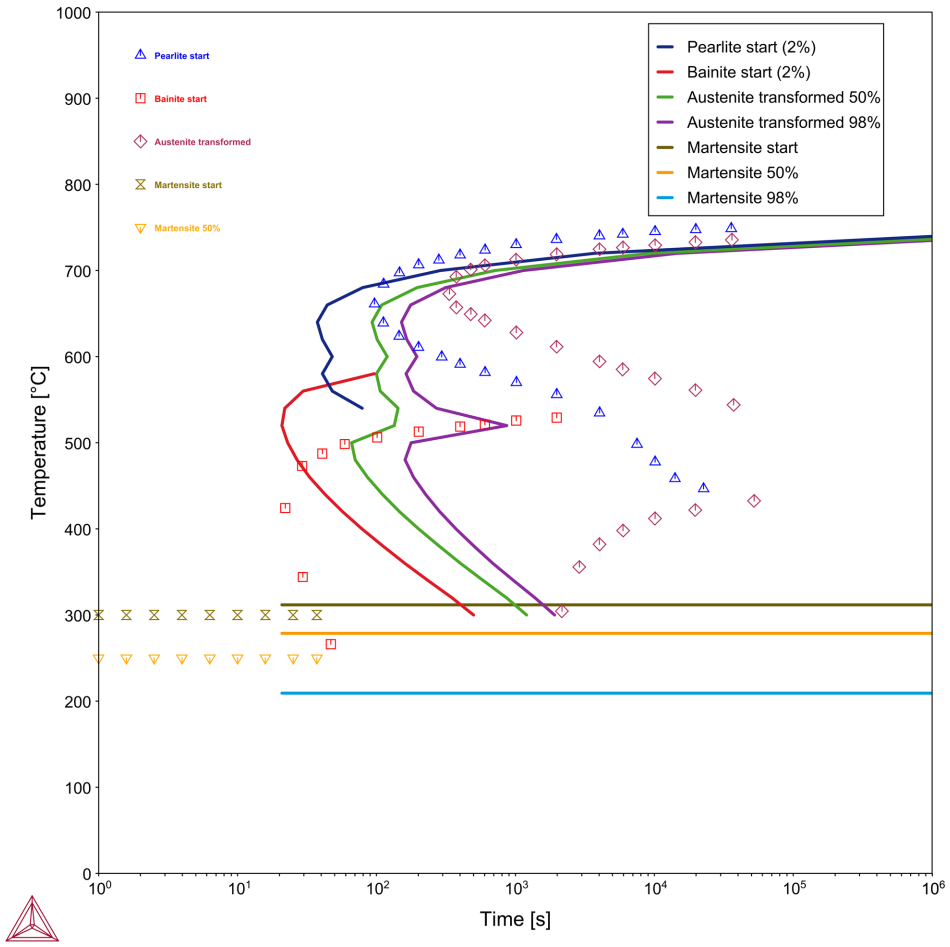


Figure 55: The TTT diagram for an Fe-C-Mn-Si-Cr-V alloy comparing the calculation with experimental data from [1958Wev].

Reference

[1958Wev] F. Wever, A. Rose, Atlas zur Wärmebehandlung der Stähle: 1954/56/58 (Verlag Stahleisen, Düsseldorf, 1958), p. II-112.

PM_Fe_07: Hardenability Design of Steel

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

This application example, which is showcased on our website, shows how the Steel Model Library in Thermo-Calc can be used to find the optimal compositions for an Fe-Mn-C steel to achieve high hardenability for the purpose of strength.

This example focuses on the hardenability design of steel using the Steel Model Library in Thermo-Calc. It shows how to find the optimal compositions for Fe-Mn-C steel to achieve high hardenability for the purpose of strength. Hardenability refers to the ability of steel to form martensite on quenching. It is a measure of the capacity of a steel to be hardened in depth when quenched from its austenitizing temperature. Among various factors, composition is one of the most important factors which has great influence on the hardenability of the steel. In this example, we use the Steel Model Library to investigate the possible composition ranges of Fe-C-Mn alloys to reach a fully martensitic microstructure.

To fulfil the requirement, room temperature martensite fraction should be large and the amount of retained austenite should be small. Meanwhile, other products of austenite decomposition should be avoided during continuous cooling. Such transformation products can be suppressed by fast quenching, yet the cooling rate is usually limited by the capacity of facilities or other problems such as cracking. Therefore, for hardenability purposes, it is desirable to achieve a fully martensitic structure with a relatively low cooling rate. This is done by promoting martensite formation while retarding other transformations through adjusting the steel composition.

Open the example project file and click **Perform Tree** to generate the plots associated with this application example.

Although this example uses the FEDEMO and MFEDEMO databases, running the calculation requires a license for Thermo-Calc 2021b or newer and for the Steel Model Library.

The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_07_Hardenability_Design_of_Steel.tcu*

PM_Fe_08: CCT Diagram Property Model

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The example uses the **Property Model Calculator** and the **CCT Diagram** Property Model to calculate a Continuous-Cooling-Transformation (CCT) diagram for an Fe-C-Mn-Si-Cr-V alloy (Steel 42CrV6). The calculation is compared to an experimental CCT diagram for the same steel (with some other impurities) from data in [1958Wev].

A *One axis* calculation is selected on the Property Model Calculator and then the *CCT mode* selected on the Plot Renderer in order to plot the final CCT diagram shown in the figure below.

For more information see About the CCT Diagram Property Model, CCT Diagram Property Model Settings, and Plot Settings: CCT Mode.

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu*

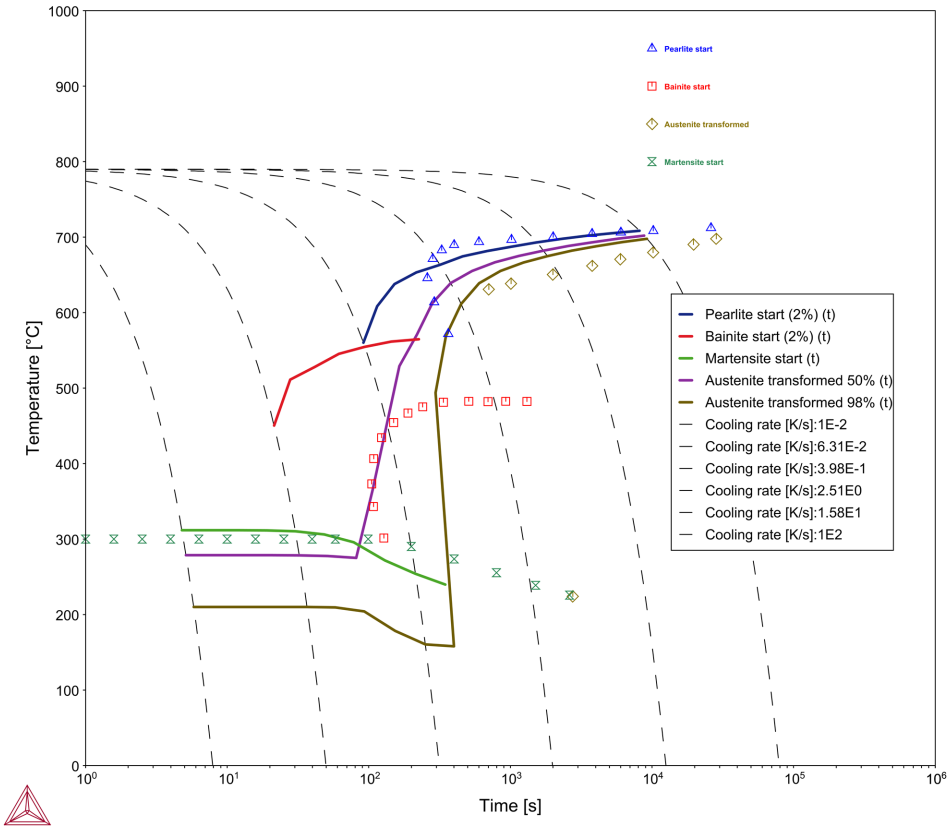


Figure 56: The CCT diagram for an Fe-C-Mn-Si-Cr-V alloy comparing the calculation with experimental data from [1958Wev].

Reference

[1958Wev] F. Wever, A. Rose, Atlas zur Wärmebehandlung der Stähle: 1954/56/58 (Verlag Stahleisen, Düsseldorf, 1958), p. II-112.

Process Metallurgy Module Examples Collection

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

- The Process Metallurgy Module
- About the Examples

In this section:

PMET_01: Basic Oxygen Furnace (BOF) 492
PMET_02: Desulphurization in a Ladle Furnace (LF) 494
PMET_03: Argon Oxygen Decarburization (AOD) 496
PMET_04: Basic Oxygen Furnace (BOF) Kinetics 503
PMET_05: Lab Scale Ladle Furnace (LF) Kinetics 505
PMET_06: Ladle Furnace (LF) Kinetics 511
PMET_07: Vacuum Oxygen Decarburization Kinetics 514
PMET_08: Steel Deoxidation on Tapping 516

PMET_01: Basic Oxygen Furnace (BOF)

The example uses the **Process Metallurgy Calculator** to demonstrate a simplified steelmaking process in a Basic Oxygen Furnace (BOF).

> One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

This application example in its various forms is showcased on our website. There are two application examples (one equilibrium, one kinetic) showing how the Process Metallurgy Module can be used to calculate the BOF process.

This example uses equilibrium calculations to gain a general understanding of your BOF process and help you determine optimal operation conditions and predict and optimize costs of raw materials and recycling. The other set of examples gives detailed instructions on how to simulate the kinetics of the BOF process using the kinetic process simulation.

For information about the kinetic examples, see PMET_04: Basic Oxygen Furnace (BOF) Kinetics.

Project Files

Open the example project file(s) from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_01_Basic_Oxygen_Furnace.tcu**. Choose a, b, or c versions of the example based on whether you have the relevant licenses listed below.

- **PMET_01a_Basic_Oxygen_Furnace** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. This is a highly simplified example and uses the OXDEMO database, and only considers the elements Fe, C, and O.
- **PMET_01b_Basic_Oxygen_Furnace** is also a simplified calculation but uses the OXDEMO database. It requires a full license of Thermo-Calc 2021b or newer.
- **PMET_01c_Basic_Oxygen_Furnace** requires the TCOX11 database or newer and a full license of Thermo-Calc 2021b or newer.

This example is included as a tutorial on our website and our YouTube channel.

The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

PMET_02: Desulphurization in a Ladle Furnace (LF)

The example, which is also showcased on our website, uses the **Process Metallurgy Calculator** to demonstrate the use of a Ladle Furnace (LF) with the Process Metallurgy Module.

> One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

The ladle furnace fulfils many purposes in the steelmaking process. Desulphurization, which we will focus on in this example, is merely one of them.

Desulphurization is usually performed by transferring S that is dissolved in the liquid metal to a CaO-rich slag phase. For this process to be successful, two conditions need to be fulfilled:

1. The slag must be fully liquid (liquid fraction > 0.9). This is required for kinetic reasons. The slag phase must be fluid so that it can emulsify with the liquid steel and form a large surface area where the reaction between steel and slag can take place.
2. The slag must take up a large amount of S from the liquid steel (have a “high sulphur capacity”) so that a significant amount of sulphur will move from the liquid steel to the slag phase.

It is difficult to decrease the S content in the liquid steel during steelmaking in a basic oxygen converter (BOF) or an electric arc furnace (EAF) because conditions are predominantly very oxidizing. Desulphurization is therefore usually performed in a subsequent step, during steel refining in a ladle furnace or a vacuum degasser after the steel has been fully killed by a suitable deoxidizing agent and the oxygen activity is low.

The following example explores these two conditions for an equilibrium between liquid steel and slag in a ladle furnace, trying to find good slag compositions.

> The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

This example is included as a tutorial on our website and our YouTube channel.

Project Files

Open the example project files from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_02a_Ladle_Furnace.tcu** or **PMET_02b_Desulphurization_in_Ladle_Furnace.tcu**. Choose a or b versions of the example based on whether you have the relevant licenses listed below.

- **PMET_02a_Ladle_Furnace.tcu** can be run with OXDEMO database but requires the full license for Thermo-Calc 2021b.
- **PMET_02b_Desulphurization_in_Ladle_Furnace.tcu** requires the TCOX11 database and a full license for Thermo-Calc 2021b.

PMET_03: Argon Oxygen Decarburization (AOD)

Visit the website Application Examples→Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

The example uses the **Process Metallurgy Calculator**.

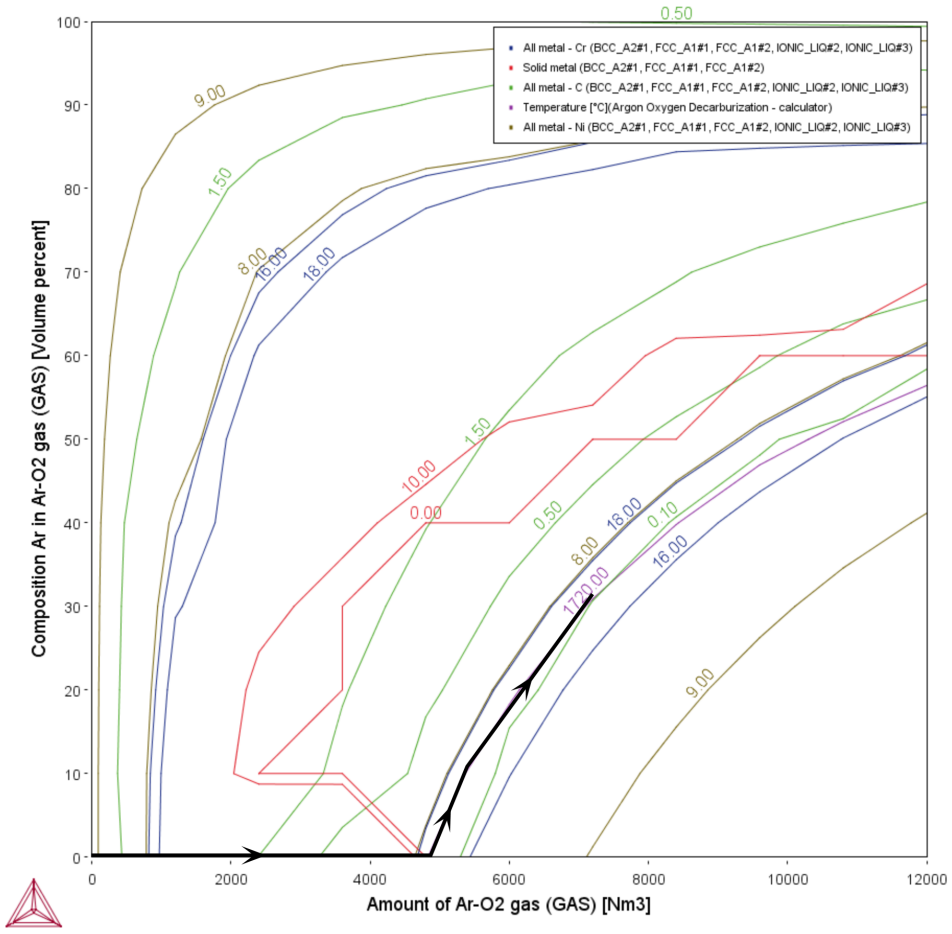
Open the Project File

This example does not require a license to run the simulation. It works with both the TCS Metal Oxide Solutions Database (TCOX versions 8 and newer) as well as the free OXDEMO database.

You can open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_03_Argon_Oxygen_Decarburization.tcu**.

The example takes several minutes to run.

The Argon Oxygen Decarburization (AOD) process is a converter process applied in stainless steel making. In this process the oxidation of chromium in the steel melt needs to be prevented while carbon is oxidized. This is achieved by reducing the oxygen partial pressure by having a high Ar-content in the blowing gas. It is a highly exothermic process that requires adiabatic modeling. In this example the conversion of carbon-rich steel scrap is modeled together with additions of Ferronickel and Ferrochrome to a stainless steel.



The AOD-process is characterized by an initially high O_2-content of the blowing gas, which is gradually replaced by Ar. The maximum temperature of the process is typically around 1720 °C. A grid plot of an adiabatic calculation is well suited to model the required simultaneous change of amount of gas and its composition during this process. The black line in the plot above indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

In principle, this plot could be used to control the blowing gas flow in a plant process. However, note that the simulation only considers a global gas phase, i.e. additional gas is added but never removed. This means that the given gas phase composition is an average one and not identical to the composition of the gas flowing in at each point in time. Additionally there is a certain impact on the resulting equilibria from the fact that all gas remains in the system and is not removed.

Slag Basicity

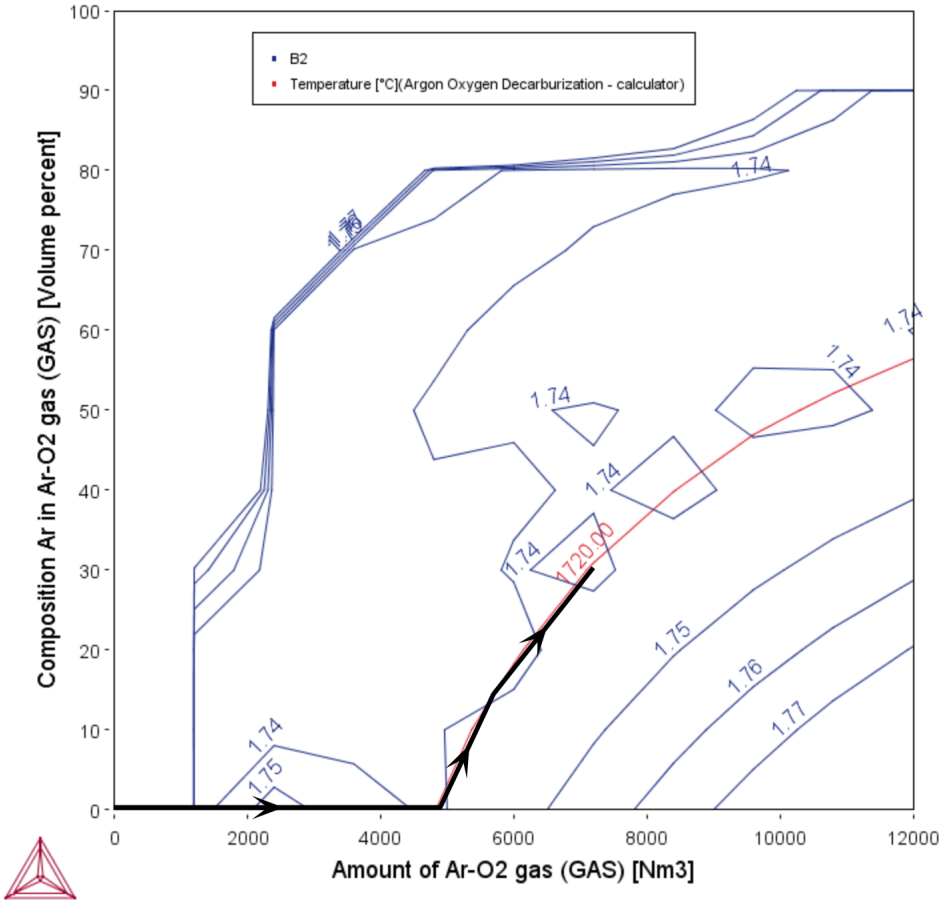


Figure 57: The Slag Basicity plot shows the basicity of the slag (which is a measure for the sulphur capacity of the slag). The process achieves a final basicity of 1.74 which is typical for an AOD-process. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

S Content in Steel

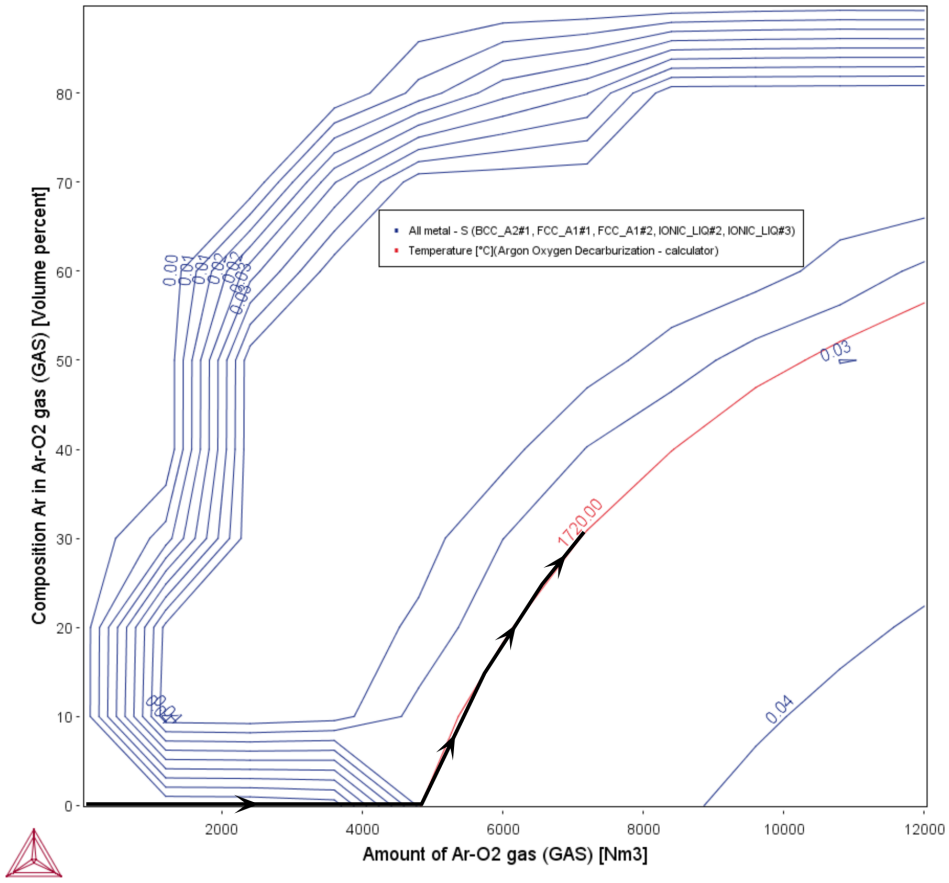


Figure 58: In the S Content in Steel plot, the sulphur content in the steel melt is slightly reduced during the process from 0.056% in the initial steel scrap to finally ca. 0.035%. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Cr Content in Slag

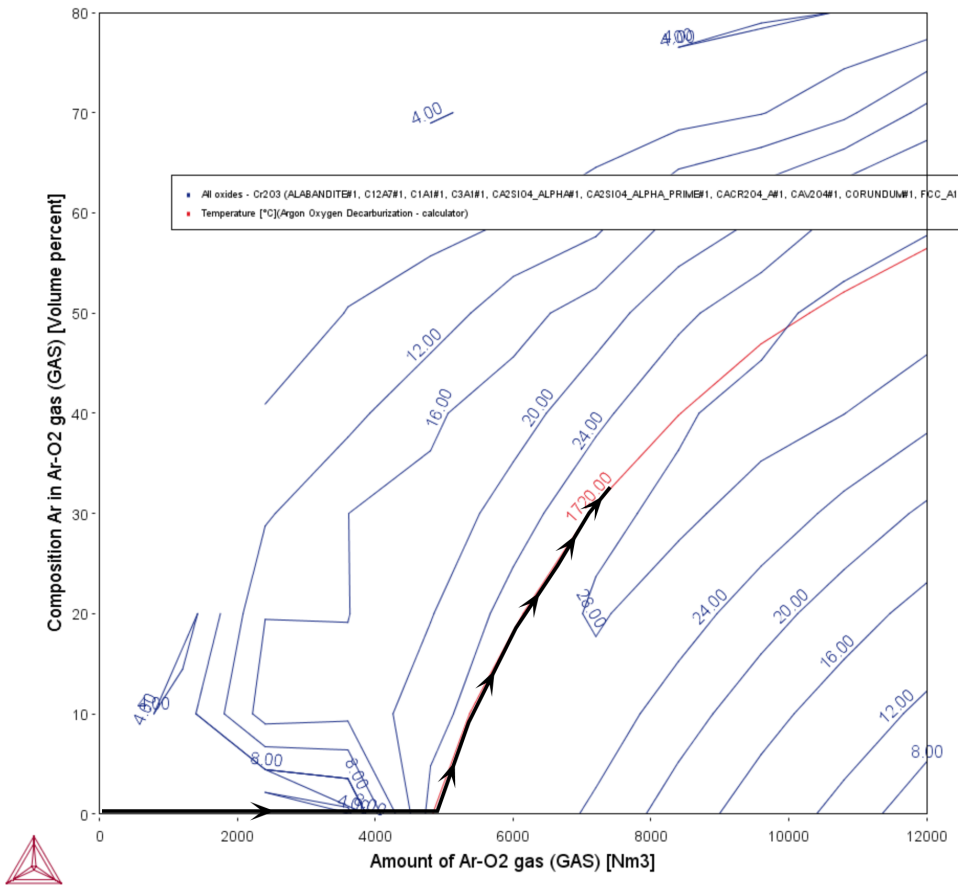


Figure 59: In the Cr Content in Slag plot, the Cr2O3-content in the slag reaches at the end of the process ca. 26 wt-%. This is typical for the AOD-process and requires an additional Cr-recovery step after the conversion to reduce the loss of chromium. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Amount of Slag

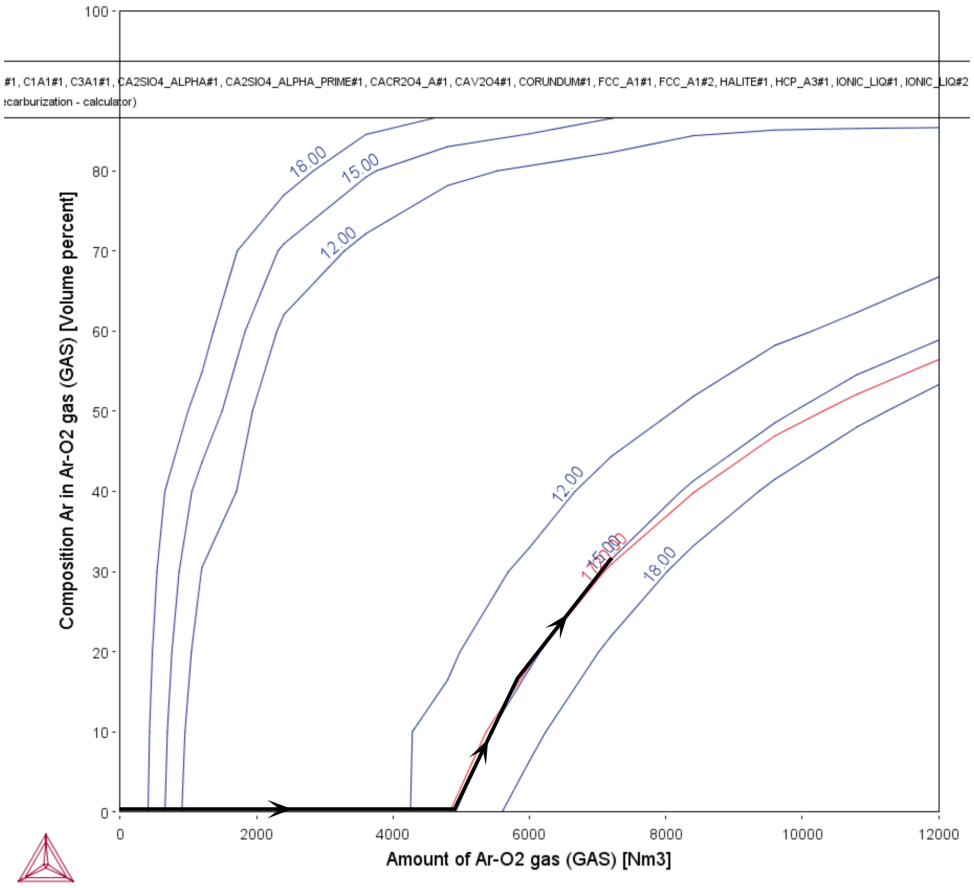


Figure 60: In the Amount of Slag plot, you can see that the process generates about 15 tons of slag in the total. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Liquid Slag Fraction

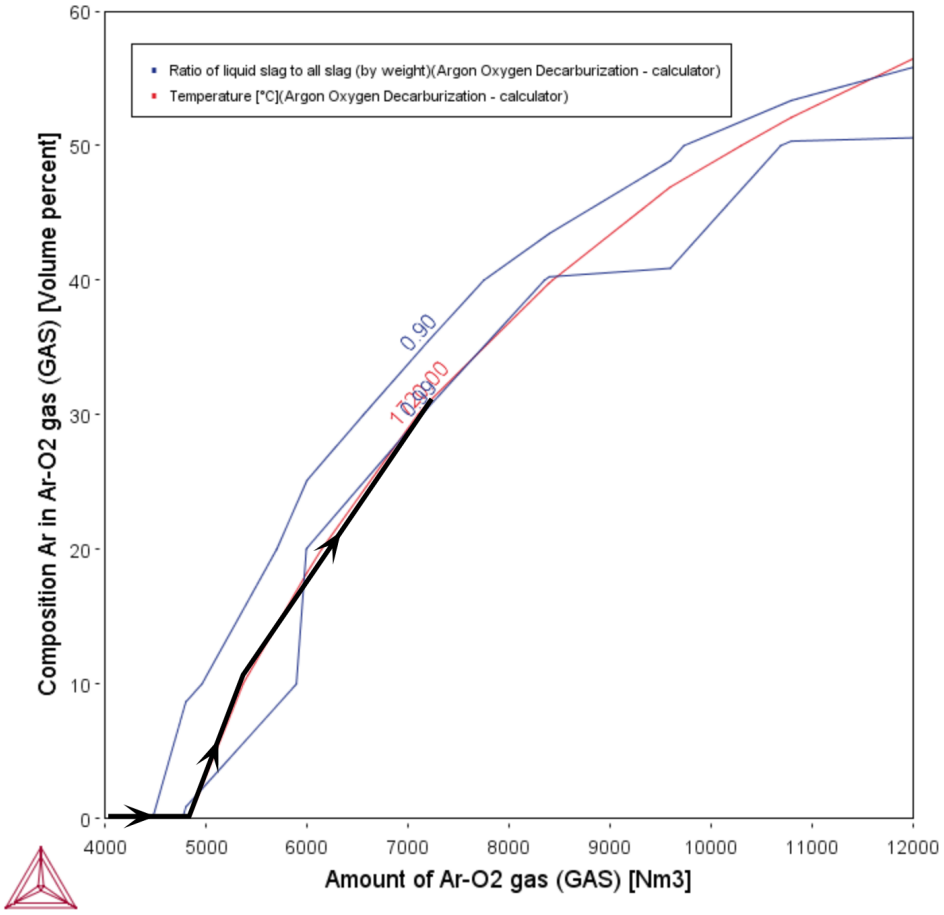


Figure 61: In the Liquid Slag Fraction plot, you can see that towards the end of the process the slag is calculated to be mostly liquid. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

PMET_04: Basic Oxygen Furnace (BOF) Kinetics

The example uses the **Process Metallurgy Calculator** to demonstrate the steelmaking process in a Basic Oxygen Furnace (BOF).

> One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

This application example in its various forms is showcased on our website. There are two application examples (one equilibrium, one kinetic) showing how the Process Metallurgy Module can be used to calculate the BOF process.

This example simulates the kinetics of the BOF process, whereas the other only considers equilibrium.

- For information about the equilibrium examples, see PMET_01: Basic Oxygen Furnace (BOF).

> The kinetic model is available starting with Thermo-Calc 2020b. However, this example requires Thermo-Calc 2021b or newer.

Project Files

Open the example project file(s) from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_04_Basic_Oxygen_Furnace_Kinetics.tcu**. Choose a, b, or c versions of the example based on whether you have the relevant licenses listed below.

- **PMET_04a_Basic_Oxygen_Furnace_Kinetics** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. This only considers the elements Fe, C, and O.
- **PMET_04b_Basic_Oxygen_Furnace_Kinetics** needs a full license of Thermo-Calc 2021b or newer, but uses the free OXDEMO database. It considers the elements Fe, C, O, Ca, Al, Si, and S.

- **PMET_04c_Basic_Oxygen_Furnace_Kinetics** requires both a full license of Thermo-Calc 2021b or newer and a license for the TCOX11 database or newer. This simulation corresponds pretty much to a real BOF process with the elements Fe, Mn, C, O, Ca, Al, Mg, Si, S, and P considered.

The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

A variety of video tutorials are available for many of our products and features on our website and our YouTube channel. The library keeps growing so be sure to check back on a regular basis.

PMET_05: Lab Scale Ladle Furnace (LF) Kinetics

Visit the website Application Examples→Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

Open the Project File

This example requires a license to run the simulation. It works with TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer.

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

To open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_05_Lab_Scale_Ladle_Furnace_Kinetics.tcu**.

Once you open the project file, click **Perform Tree** at the bottom center of the **Configuration** window.

About the Plot Results

Many different aspects of the reactions taking place in the LF can be plotted and analyzed. After you run the project file and obtain the plots, you can experiment by adjusting the settings on each Plot Renderer to see what happens in each case. There is more analysis about this and other examples available at the links to our website.

Setting Up the LF Process Simulation

Using the **Process Metallurgy Calculator** and the **Process simulation** branch, this example is based on the publication by Piva et al [2017, Piva] where a lab scale sample of pure iron is

first deoxidized with Si-Mn and then a synthetic top slag is added to the steel. Generally, by using the project file and the information below, you can get an idea about how to set up a ladle furnace simulation using the Process Metallurgy Module.

- Setting Up a Process Metallurgy Simulation
- Defining the Process Simulation

In the paper by Piva et al. [2017], it is experimentally investigated how the steel and inclusion composition changes in function of time as the Si-Mn killed steel reacts with the slag. This experiment can serve as a model for the production of SiMn killed steel with subsequent top-slag deoxidation.

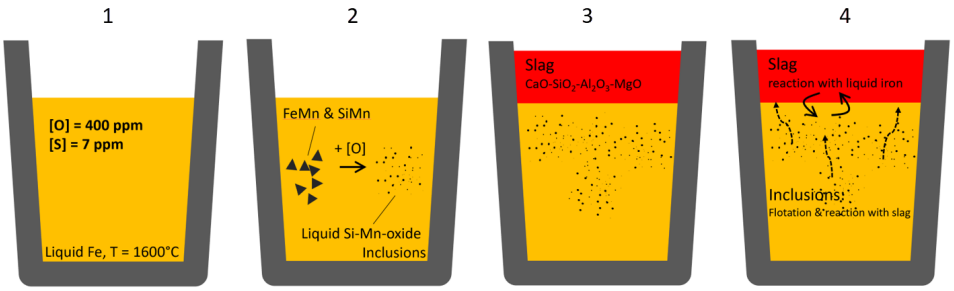


Figure 62: Diagram of the experiment performed by Piva et al. [2017]. The sequence as described in the text is: (1) liquid Fe with dissolved oxygen; (2) FeMn and SiMn added to deoxidize Fe; (3) top slag added after 360s; and (4) gradual reaction between steel, slag and inclusions.

According to the publication the following reaction sequence is expected as shown in the diagram:

1. The deoxidizing agents dissolve and react with the oxygen in the steel forming oxide inclusions, thereby reducing the amount of dissolved oxygen (“killing” the steel). The kinetics are fast, and it can be assumed that the reaction proceeds to thermodynamic equilibrium.
2. The inclusions formed in (1) slowly start to float upwards and are removed out of the liquid steel.
3. After adding the slag (360 s after killing the steel in (1) the liquid steel starts reacting with the slag.
4. The inclusions continue to float up out of the liquid steel and combine with the slag.

   According to the authors the most important reaction that takes place is the dissolution of Al out of the slag and its transferal into the liquid steel, where it reacts with the inclusions and changes the chemistry.

In this example only the last reaction is simulated after adding the slag. The kinetic parameters, compositions of all materials and process schedule are all taken from the publication.

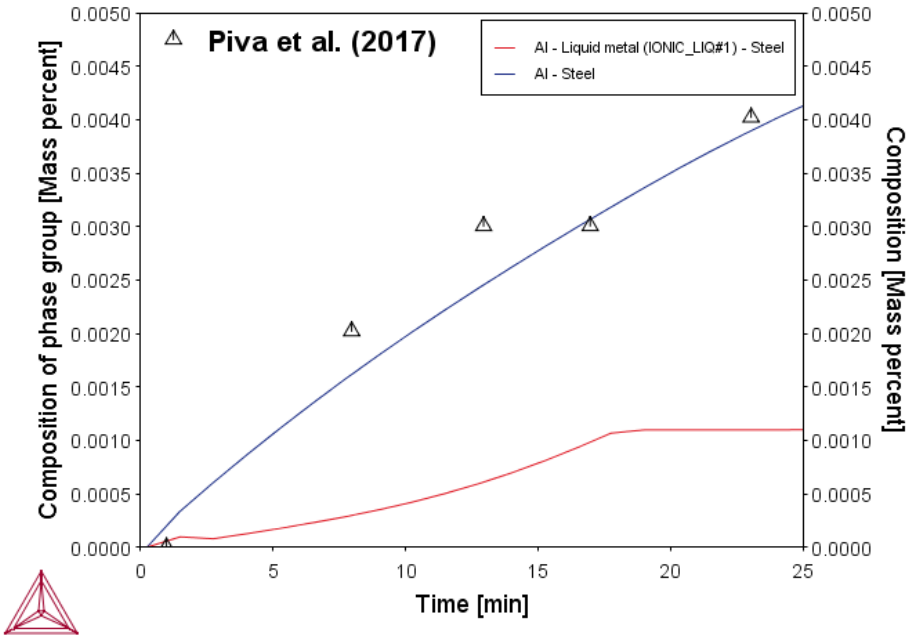
Results and Experimental Analysis

The plots below compare the Al content in the liquid steel with the experimentally determined amount. The bottom plot shows how the Al_2O_3 from the slag phase is gradually reduced to metallic Al that dissolves in the liquid steel.

In this example, only part of the Al in the liquid steel is dissolved as metallic Al. With the Process Metallurgy Module, it is possible to plot both dissolved Al and also total Al.

In the steel industry this fraction of Al in the liquid steel is often termed *dissolved Al*. The rest of the Al reacts with the oxygen in the liquid steel and forms oxide inclusions. The amount of dissolved Al plus the Al bound up in oxide inclusions is often termed *total Al*. The difference between total Al minus dissolved Al is an important measure for the steel cleanness.

Total Al is what was measured by Piva et al. [2017] and their experimental data are compared to the calculated values below.



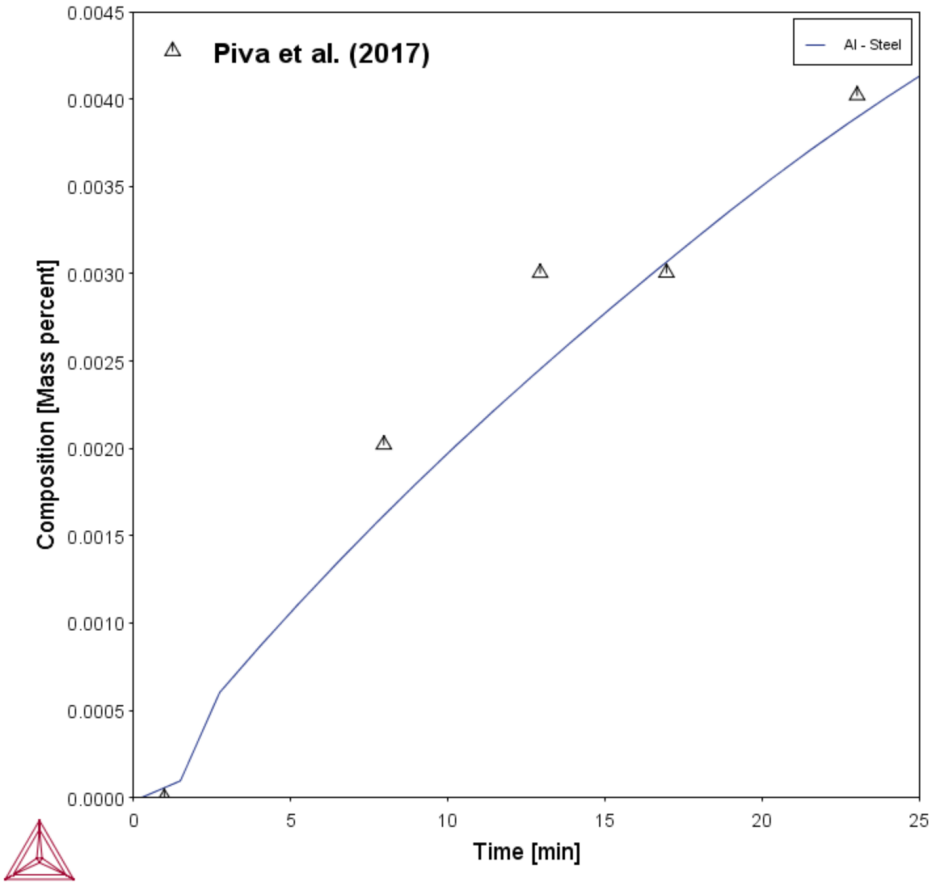


Figure 63: Total Al in the steel compared with experimental data (blue/top curve). If only the fraction of dissolved Al is to be plotted (red/bottom curve), this is done by selecting "Composition of phase group" and "Liquid metal". The bottom figure is available with the example.

Immediately after killing the steel with SiMn and FeMn, the liquid steel contains liquid Si-Mn-oxide inclusions only. As the liquid steel picks up Al from the slag phase in function of time, the inclusions get richer and richer in Al. This experimentally verified change in inclusion chemistry is well reproduced by this simulation.

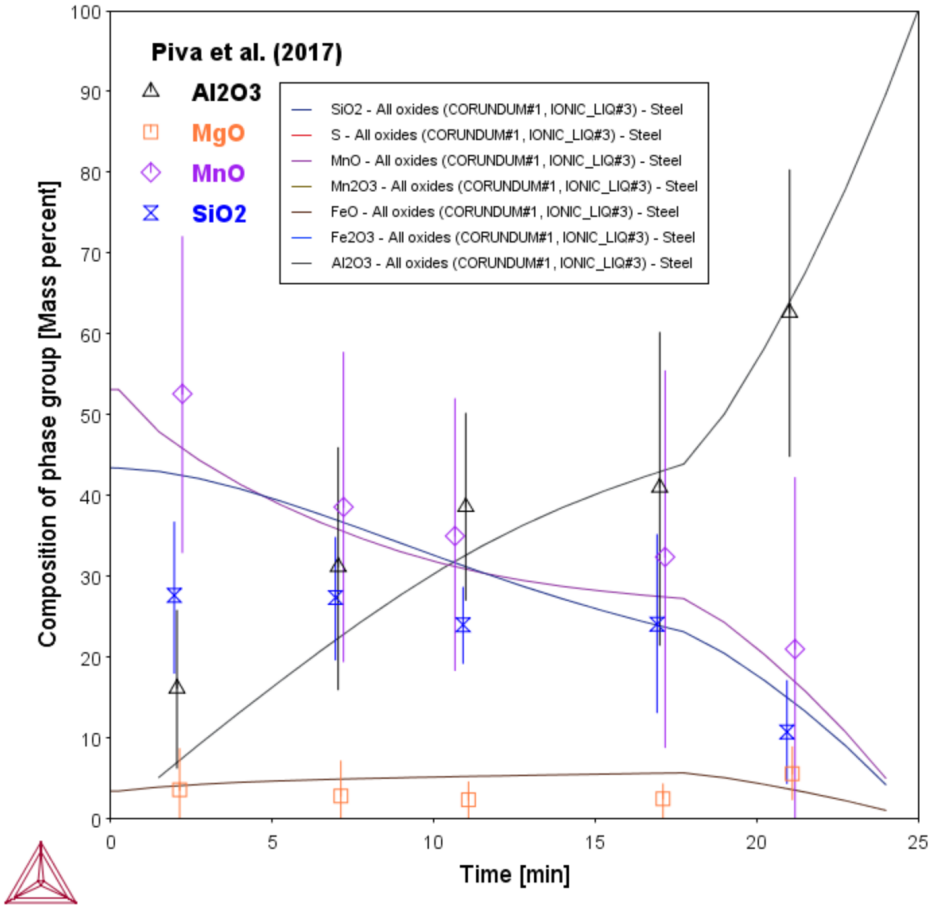


Figure 64: Calculated composition of non-metallic inclusions in function of processing time compared to experimental data [2017, Piva].

It is also possible to calculate the amount and type of inclusions present in the liquid steel. At the beginning of the process all the inclusions are liquid oxides. After about 20 minutes processing time, the first solid corundum (Al_2O_3) inclusions start appearing. After 25 minutes almost no liquid inclusions remain. The total amount of inclusions decreases in function of time as they float up out of the liquid steel and combine with the slag floating on top of the steel.

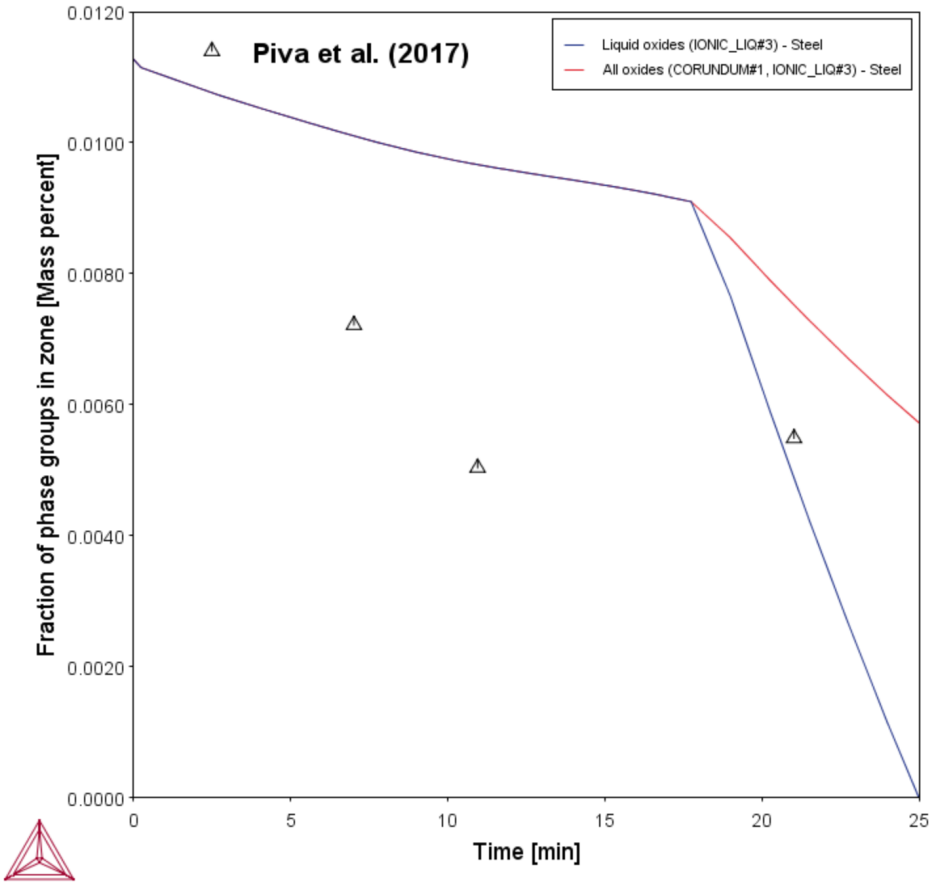


Figure 65: Amount of inclusions in the liquid steel in function of processing time. The total amount of inclusions (red line) and liquid oxide inclusions (blue line) are plotted. Up to about 20 min all inclusions are liquid oxide type, then they are replaced by solid corundum (Al_2O_3) inclusions. Experimental data from Piva et al. [2017].

Reference

[2017, Piva] Piva, S. P. T., Kumar, D. & Pistorius, P. C. "Modeling Manganese Silicate Inclusion Composition Changes during Ladle Treatment Using FactSage Macros," Metall. Mater. Trans. B 48, 37–45 (2017).

PMET_06: Ladle Furnace (LF) Kinetics

This in-depth example, which is also showcased on our website, uses the **Process Metallurgy Calculator** to show how to set up a full kinetic simulation of steel refining in a ladle furnace using the Process Metallurgy Module in Thermo-Calc. The Process Metallurgy Module uses the Effective Equilibrium Reaction Zone model (EERZ) to simulate the kinetics of the process.

> One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

After steelmaking, which is mostly performed in a basic oxygen furnace (BOF) or electric arc furnace (EAF), the steel is usually tapped into a ladle where certain additions are made (deoxidation agents, slag formers, certain alloying elements) and then transferred to the ladle furnace (LF). The LF fulfils many purposes in the steel refining process, the most important being:

- Temperature control / heating by an electrical arc.
- Mixing by Ar or N2 bubbling through porous plugs in the bottom of the ladle to achieve homogeneous temperature and composition throughout the ladle.
- Removal of unwanted non-metallic phases / inclusions such as corundum (Al2O3), liquid oxide inclusions, spinel, on so on, by flotation, aided by Ar or N2 bubbling.
- Modification / engineering of non-metallic inclusions so that they are not detrimental for the downstream processing and/or the final product.
- Removal of unwanted volatile elements such as Pb, Zn, Sn, and so on. Due to their high vapor pressure, these elements are enriched in the rising Ar or N2 bubbles. After the gas escapes out of the ladle and cools, they condense, forming copious amounts of dust.
- Removal of unwanted elements such as sulphur by liquid steel / slag reactions.
- Lowering of the dissolved gas content. In the LF this is mainly achieved through chemical reactions. For direct removal of dissolved gas, vacuum degassing (VD) is usually required.
- Alloying and trimming of the steel to achieve the exact alloy composition required by the specification of the steel that is to be produced.

The reactions taking place in a LF are a complex interplay between equilibrium thermodynamics that define the direction of chemical reactions, and kinetics that define how fast the equilibrium state is approached.

In this example, a full kinetic simulation of the LF refining process is set up using the Process Metallurgy Module.

The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

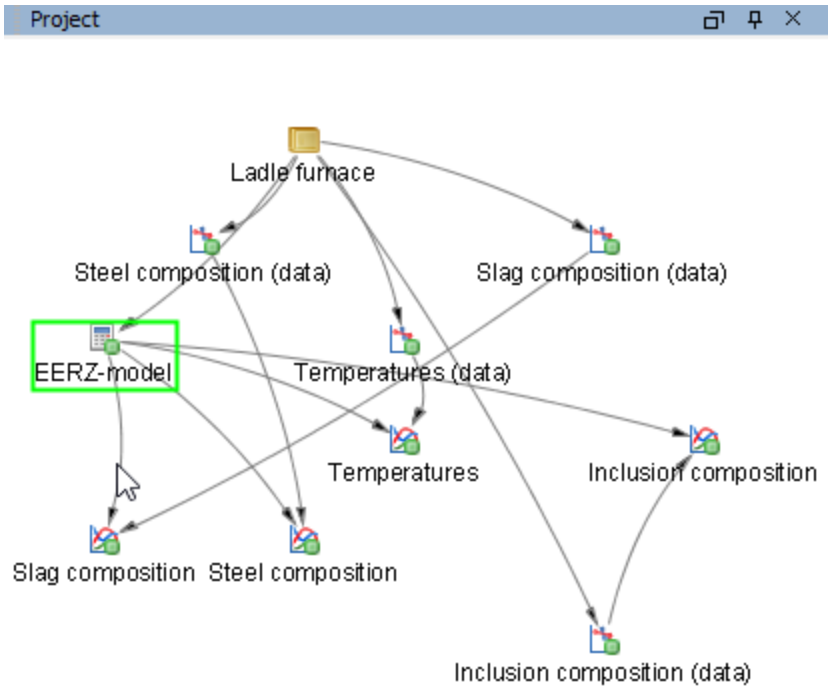
Project File

To open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_06_Ladle_Furnace_Kinetics.tcu**.

- This example requires the database TCOX10 or newer, a full license of Thermo-Calc 2020b or newer, and a license for the Process Metallurgy Module.

This example is included as a tutorial on our website and our YouTube channel.

Once you open the project file, and if you have the required licenses, click **Perform Tree** at the bottom center of the **Configuration** window. It takes several minutes to run the simulation.



The nodes in the Project window for this example. The Process Metallurgy Calculator is renamed to EERZ model. If you click this node the Configuration window opens, which is where all the settings for the process simulation are located. This advanced example also uses three Experimental Data Reader nodes to read the experimental data that is included in the simulation results. After setting up the system and accessing the experimental data, you then add Plot Renderers to the calculator to generate the output in the Results window.

PMET_07: Vacuum Oxygen Decarburization Kinetics

This application example, which is showcased on our website and uses the **Process Metallurgy Calculator**, shows how the Process Metallurgy Module in Thermo-Calc can be used to simulate the Vacuum Oxygen Decarburization (VOD) process for a stainless steel.

> One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

This example, based on data of a real VOD process published by Ding et al. [2000Din], shows how to set up the VOD process in Thermo-Calc's Process Metallurgy Module. Use of the following features in the Process Metallurgy Module are highlighted in this example:

- Change of pressure as a function of time during the process
- Change of reaction kinetics as a function of time during the process
- Selection of zone where degassing is allowed

Project File

Open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_07_Vacuum_Oxygen_Decarburization_Kinetics.tcu**.

This example requires a license for Thermo-Calc 2021a or newer, the database TCOX10 or newer, and a license for the Process Metallurgy Module.

> The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Reference

[2000Din] R. Ding, B. Blanpain, P. T. Jones, P. Wollants, Modeling of the vacuum oxygen decarburization refining process. Metall. Mater. Trans. B. 31, 197–206 (2000).

PMET_08: Steel Deoxidation on Tapping

This application example, which is showcased on our website and uses the **Process Metallurgy Calculator**, shows a few of the ways the Process Metallurgy Module in Thermo-Calc can be used to investigate steel deoxidation (killing) on tapping.

> One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

About Deoxidation or "Killing" of Steel

Deoxidation of steel, also known as killing of steel, occurs toward the end of the steelmaking process, but before desulphurization. After primary steelmaking, for example in a basic oxygen furnace (BOF) or electric arc furnace (EAF), the liquid steel contains a large amount of dissolved oxygen [O] (400 to over 1000 ppm, see PMET_04: Basic Oxygen Furnace (BOF) Kinetics). This oxygen must be removed from the liquid steel for several reasons, including:

- Desulphurization is not effective with high oxygen content in the steel (see example on desulphurization)
- Continuous casting of un-killed steel is not possible and will result in "boiling" of the steel in the mould and massive porosity, as shown in the figure.

The two most widely applied methods of deoxidizing or killing the steel are adding Al (Al-killed steel) to the steel and adding Si (Si-killed steel) to the steel. These elements readily react with oxygen to form oxides that precipitate within the liquid steel. This does not reduce the total amount of oxygen in the liquid steel; it simply transforms the dissolved oxygen into an oxide precipitate. This oxide precipitate then needs to be removed from the steel by flotation during secondary metallurgy in the ladle furnace (LF).

In this example we look at how the Process Metallurgy Module can be used to investigate these two widely applied methods of deoxidizing or killing the steel: adding Al (Al-killed steel) or adding Si (Si-killed steel). This, however, can result in the formation of damaging inclusions that cause problems during further processing, so we go on to look at two simple and very common processes that are used to transform the solid SiO_2 and Al_2O_3 inclusions into liquid oxides so that they are less damaging.

Project Files

Open the project files, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_08_Steel_Deoxidation_on_Tapping.tcu**. Choose a or b versions of the example based on whether you have the relevant licenses listed below.

- **PMET_08a_Steel_Deoxidation_on_Tapping.tcu** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. It is a simplified version that uses the OXDEMO database.
- **PMET_08b_Steel_Deoxidation_on_Tapping.tcu** requires a full license of Thermo-Calc version 2021b or newer and database TCOX11 or newer.



The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Diffusion Module (DICTRA) Graphical Mode Examples

Examples using up to three elements are available to all users. The other examples require a Diffusion Module (DICTRA) license to calculate and plot results.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

These examples use the **Diffusion Calculator**. All examples use demonstration database packages included with your installation no matter what licenses you have.

About the Examples

In this section:

D_01: Homogenization of a Binary Fe-Ni Alloy 519
D_02: Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy 521
D_03: Evolution of an Fe-Cr-Ni Diffusion Couple 523
D_04: Fe-C Moving Boundary: Austenite to Ferrite 525
D_05: γ/α/γ Diffusion couple of Fe-Ni-Cr alloys 527
D_06: Diffusion Through a Tube Wall 534
D_07: Multiphase Carburization of an Alloy 536
D_08: Microsegregation During Solidification 539

D_01: Homogenization of a Binary Fe-Ni Alloy

The single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K in a planar domain. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase. Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

This example is available as a video tutorial on our website and YouTube channel. In previous versions of the software (prior to 2017b) it is example 19.

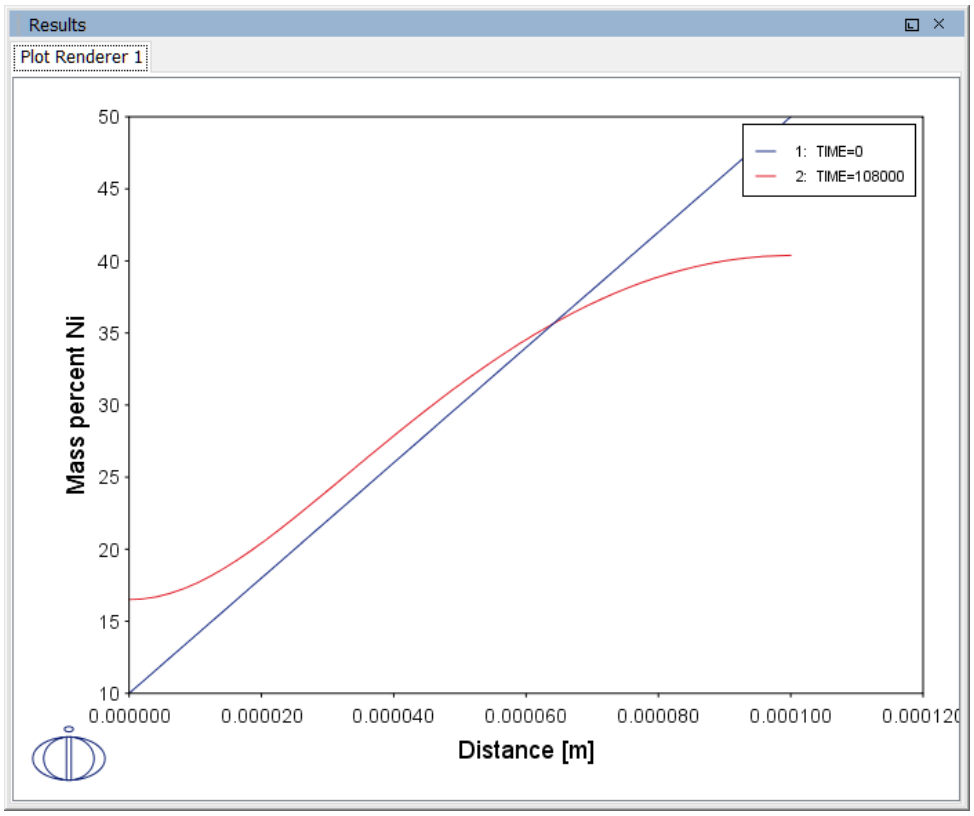


Figure 66: Composition of Ni vs Distance.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_01_Diffusion_Single_Phase.tcu*



This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

D_02: Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy

The moving phase boundary example simulates the growth of ferrite (bcc) into austenite (fcc). The austenite is assumed to be initially homogeneous with the composition Fe-0.15 mass-% C. The transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation.

This example is available as a video tutorial on our website and YouTube channel.

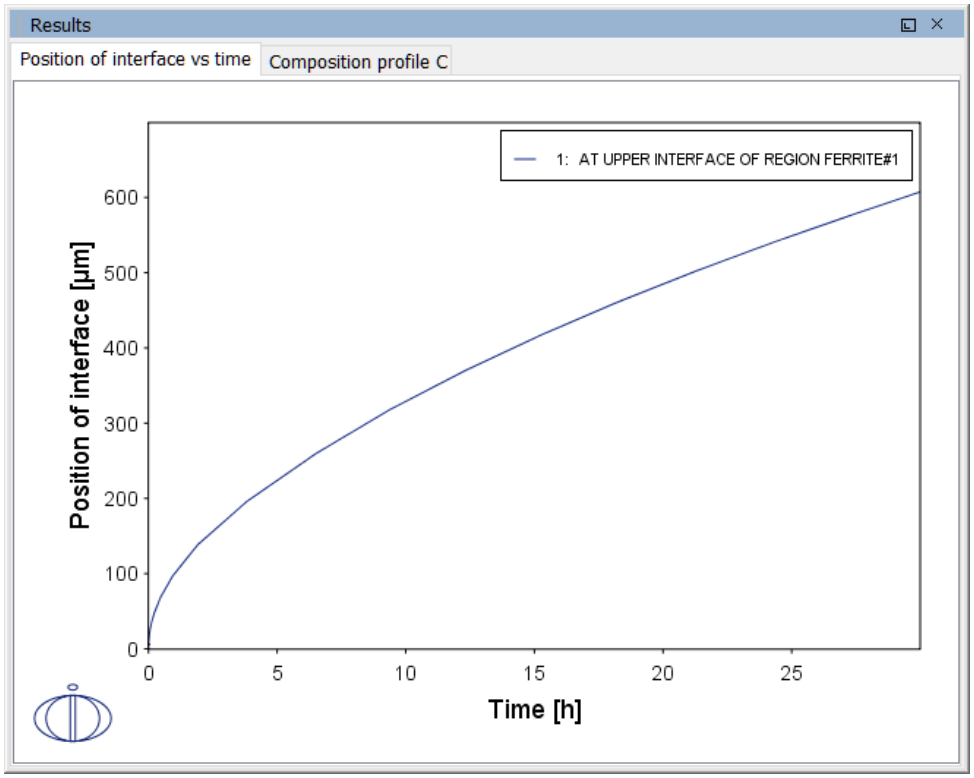


Figure 67: Position of interface vs time.

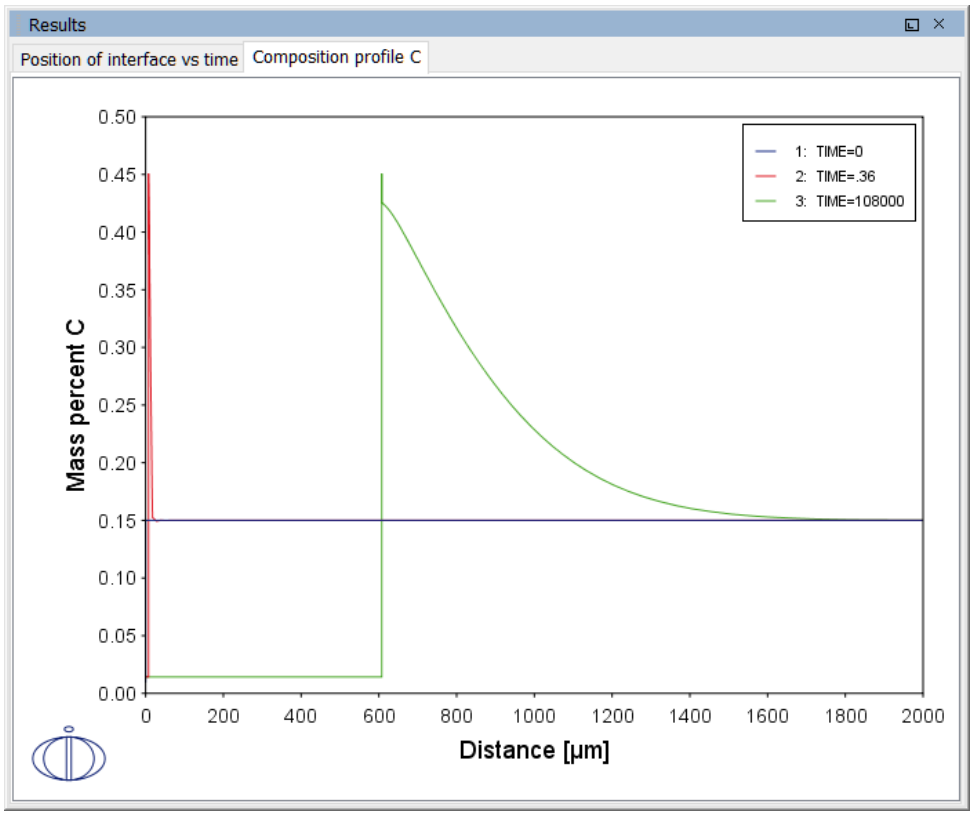


Figure 68: Composition profile C.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_02_Diffusion_Moving_Boundary.tcu*

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

D_03: Evolution of an Fe-Cr-Ni Diffusion Couple

The multiphase example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström [2006Lar] and Larsson and Höglund [2009Lar]. Experimental data is from Engström [1995Eng].

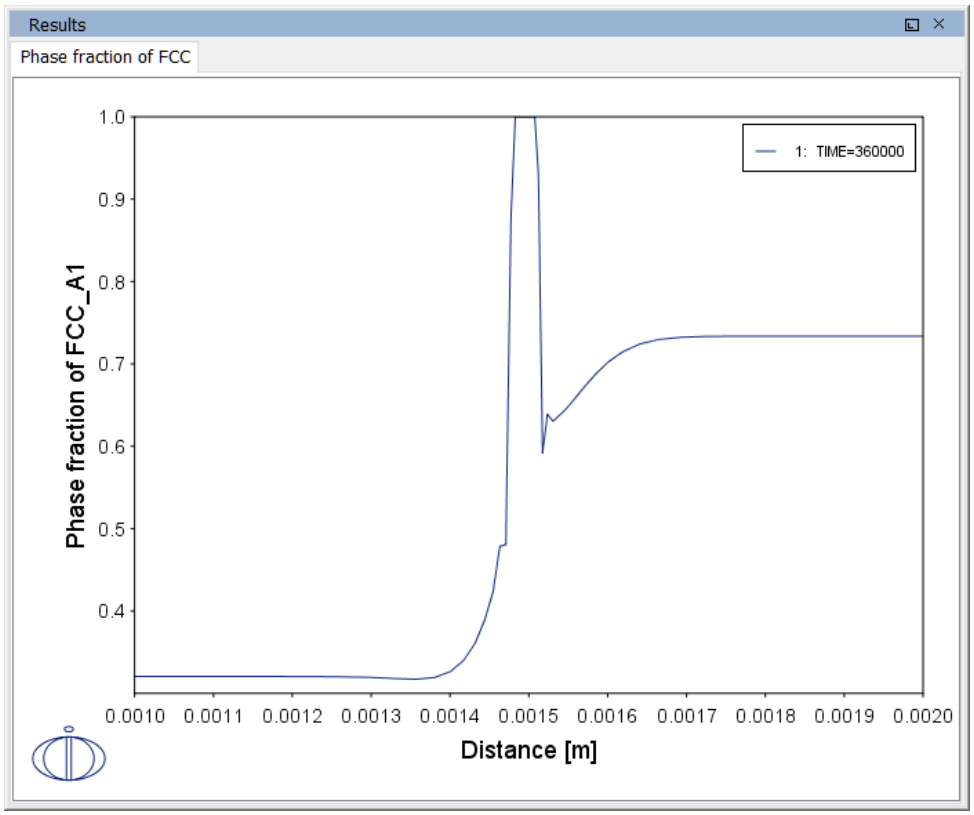


Figure 69: Phase fraction of FCC.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_03_Diffusion_Multiphase.tcu*



This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

References

[1995Eng] A. Engström, Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples. Scand. J. Metall. 24, 12–20 (1995).

[2006Lar] H. Larsson, A. Engström, A homogenization approach to diffusion simulations applied to α+γ Fe–Cr–Ni diffusion couples. Acta Mater. 54, 2431–2439 (2006).

[2009Lar] H. Larsson, L. Höglund, Multiphase diffusion simulations in 1D using the DICTRA homogenization model. Calphad. 33, 495–501 (2009).

D_04: Fe-C Moving Boundary: Austenite to Ferrite

This example simulates the austenite to ferrite transformation in a Fe-0.01 mass% C steel during continuous cooling. The simulation starts at a temperature where only austenite is stable, ferrite nucleates and grows into the austenite during cooling in the two phase region. Plots of thermal and carbon composition profiles are generated.

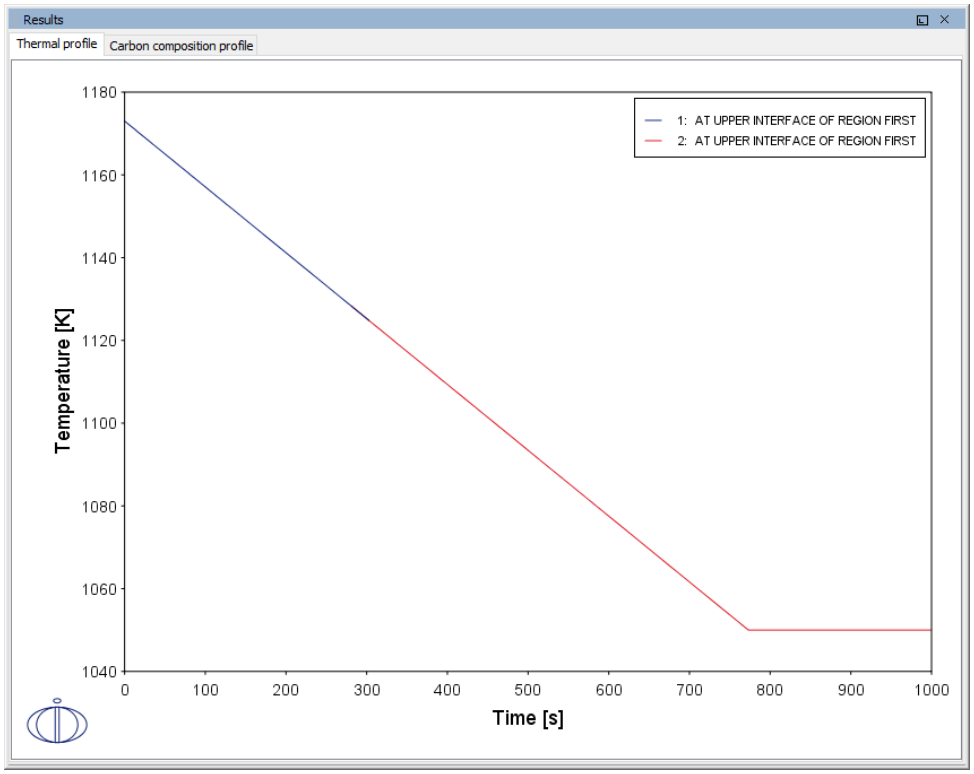


Figure 70: Thermal profile.

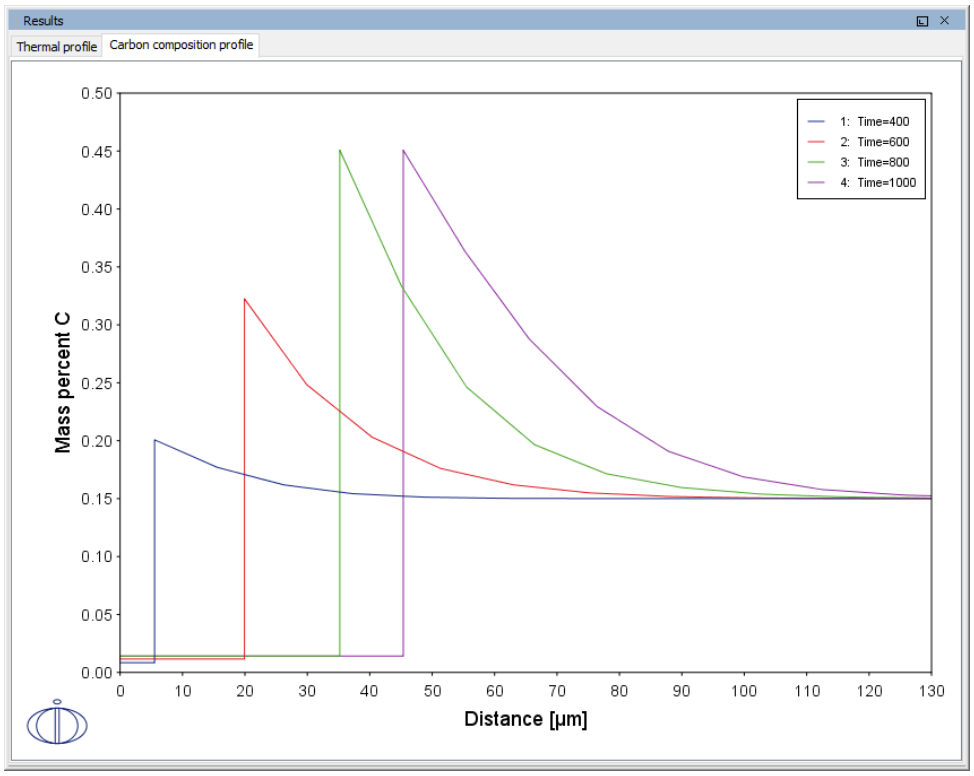


Figure 71: Carbon composition profile.

Project File Name

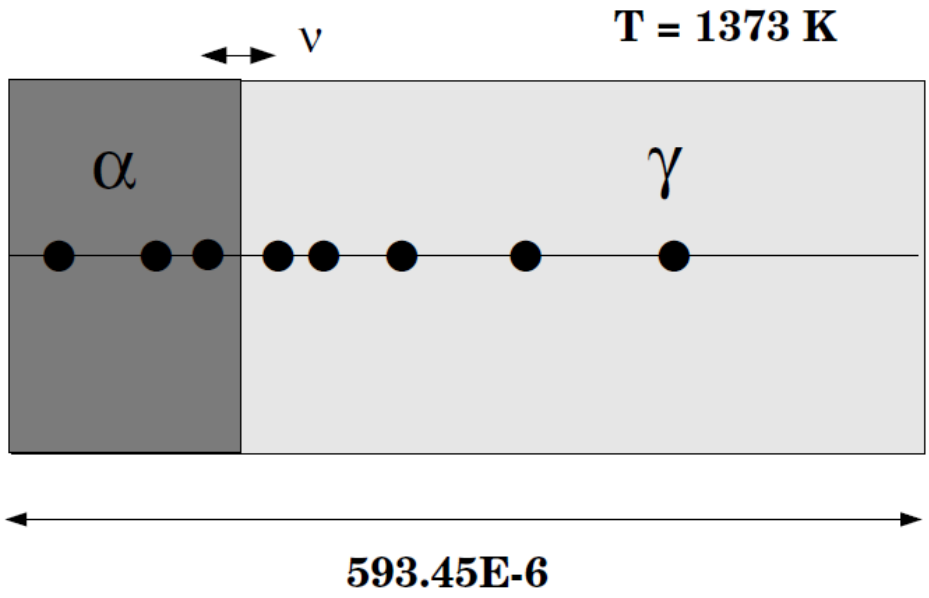
- Folder: Diffusion Module - DICTRA
- File name: *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite.tcu*

This example is available to all users.

D_05: γ/α/γ Diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evolution of a ternary Fe-Cr-Ni diffusion couple. A thin slice of ferrite (α phase) (38%Cr,0%Ni) is clamped between two thicker slices of austenite (γ phase) (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373 K.

This set up corresponds to diffusion couple in Kajihara et al. [1993aKaj] and Kajihara and Kikuchi [1993bKaj].



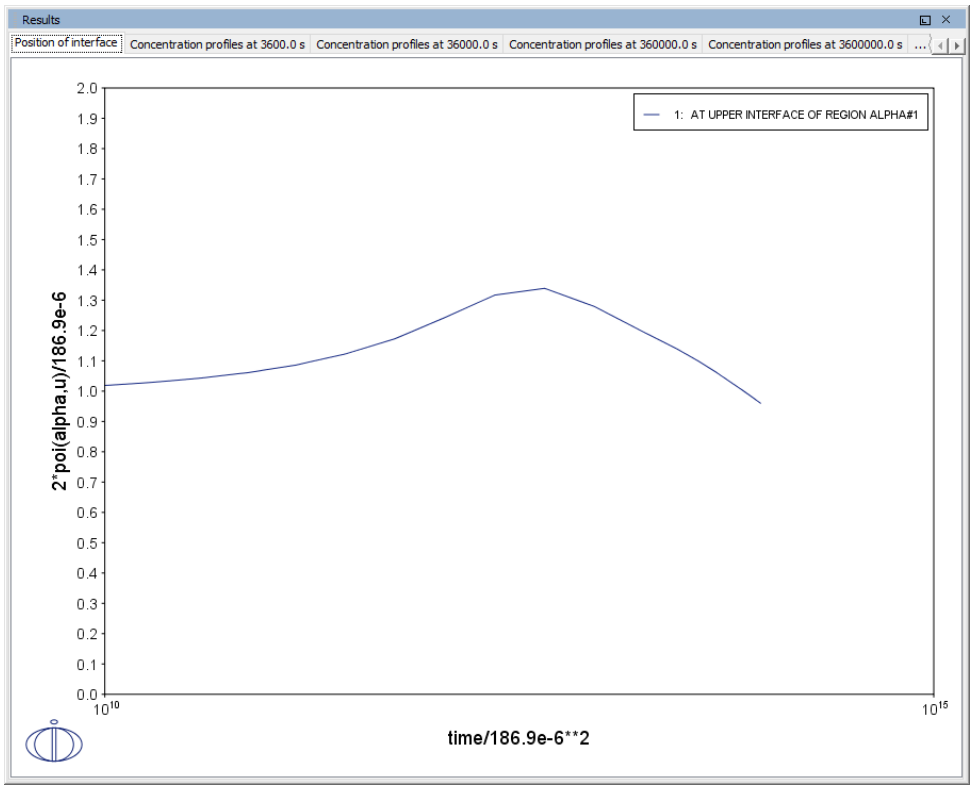


Figure 72: Interface position.

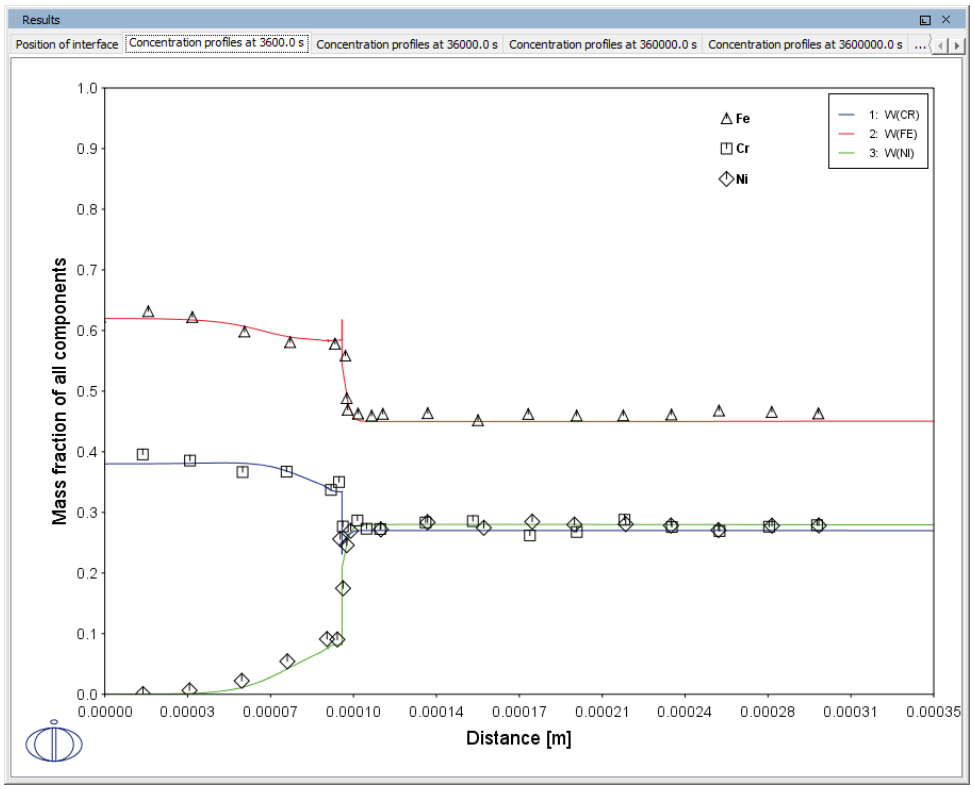


Figure 73: Concentration profiles at 3600 s.

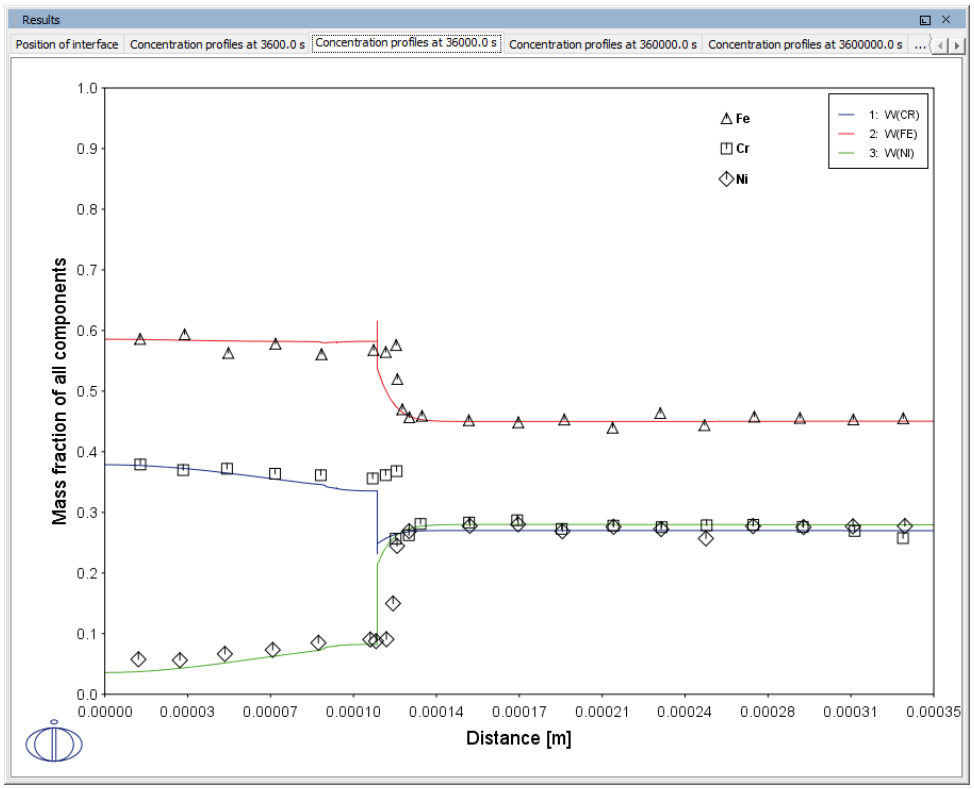


Figure 74: Concentration profiles at 36 000 s.

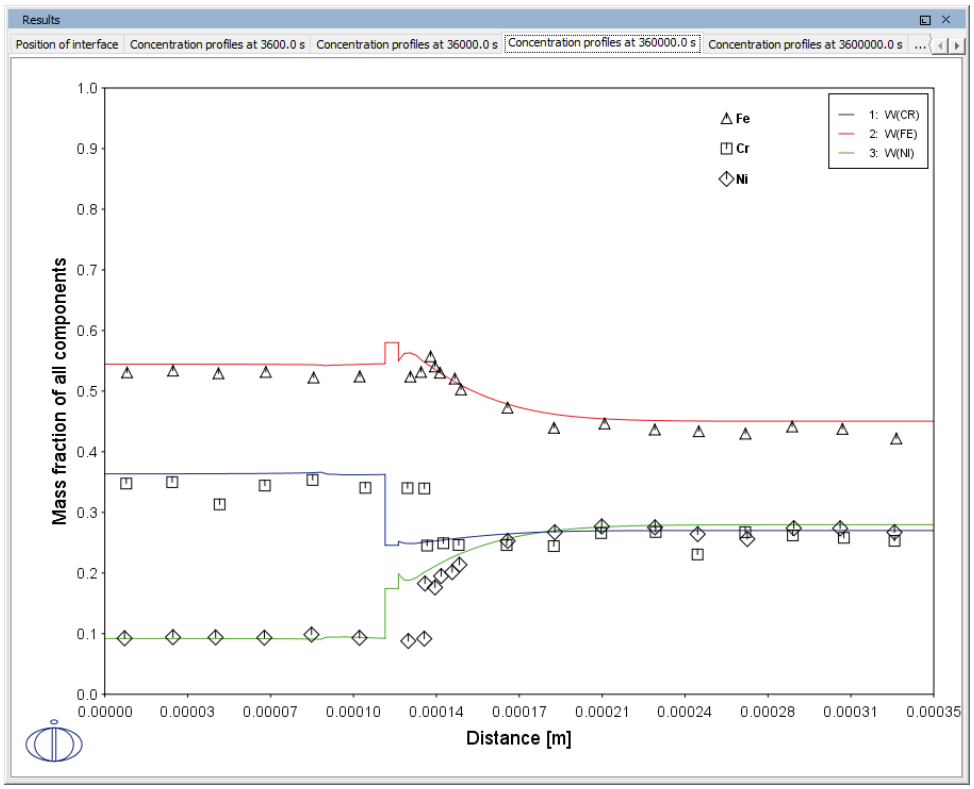


Figure 75: Concentration profiles at 360 000 s.

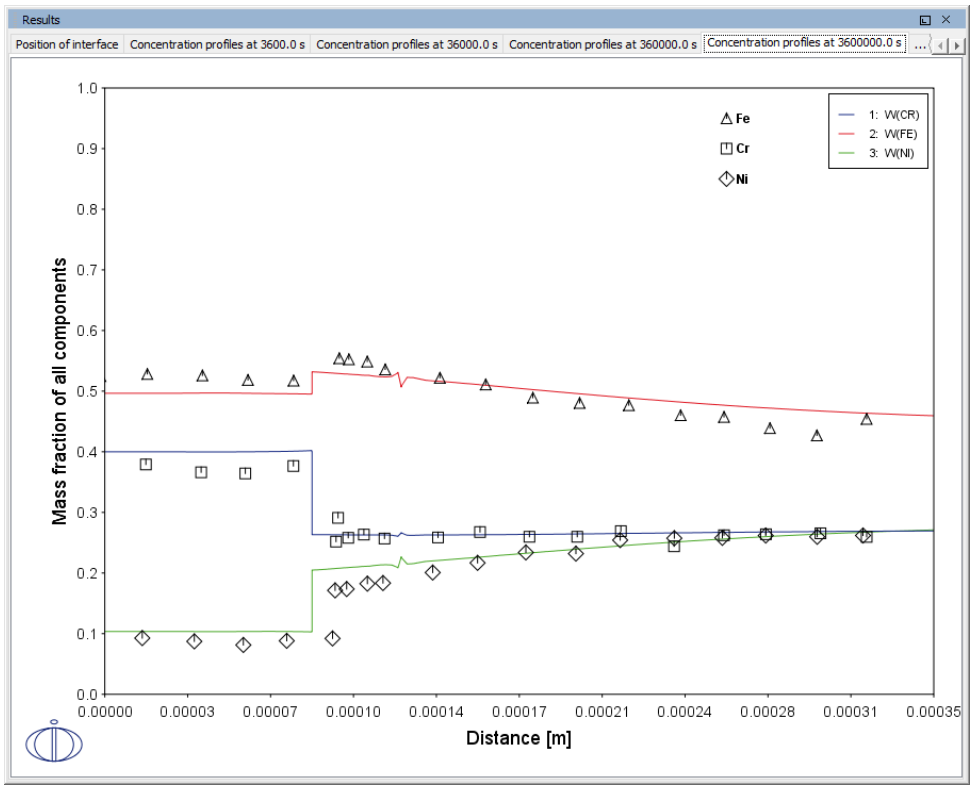


Figure 76: Concentration profiles at 3 600 000 s.

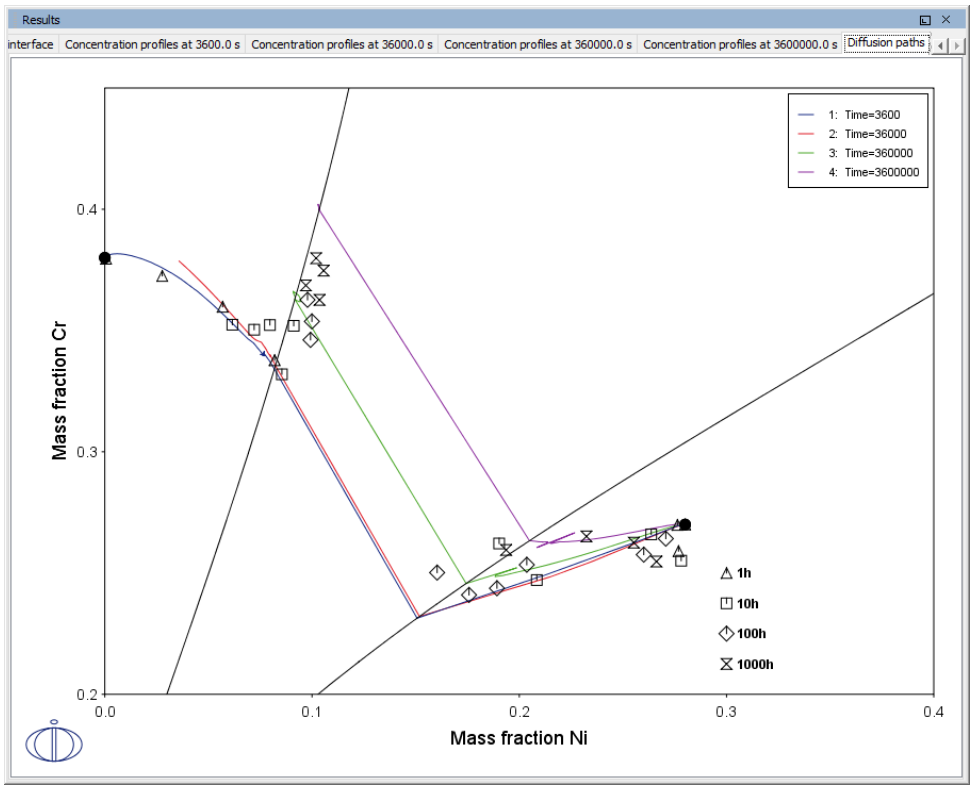


Figure 77: Diffusion paths.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_05_Diffusion_Fe_Ni_Cr_Moving_Boundary_Diffusion_Couple.tcu*

This example is available to all users.

References

[1993aKaj] M. Kajihara, C.-B. Lim, M. Kikuchi, Experimental Study on Dissolution of ALPHA Phase in GAMMA/ALPHA/GAMMA Diffusion Couples of the Fe-Cr-Ni System. ISIJ Int. 33, 498–507 (1993).

[1993bKaj] M. Kajihara, M. Kikuchi, Numerical analysis of dissolution of α phase in γ/α/γ diffusion couples of the Fe-Cr-Ni system. Acta Metall. Mater. 41, 2045–2059 (1993).

D_06: Diffusion Through a Tube Wall

This is a simple example of diffusion through a tube wall. The tube material is an Fe-0.06Mn-0.05C alloy. Two plots comparing distance to the U-fraction of manganese and composition of carbon are generated to visualize the austenite region. A *cylindrical* geometry is used with *mixed zero flux and activity* boundary conditions.

On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the carbon activity is very low. This example demonstrates the use of boundary conditions, advanced plotting and tables.

This example is based on Console Mode exab6. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).

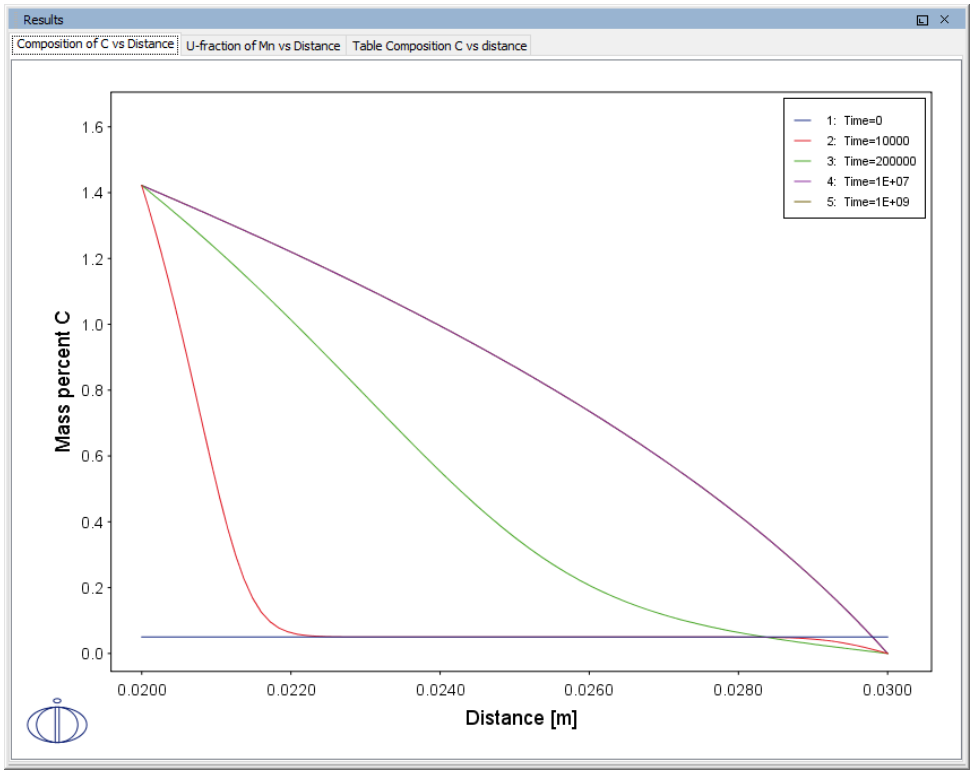


Figure 78: Composition of C vs Distance.

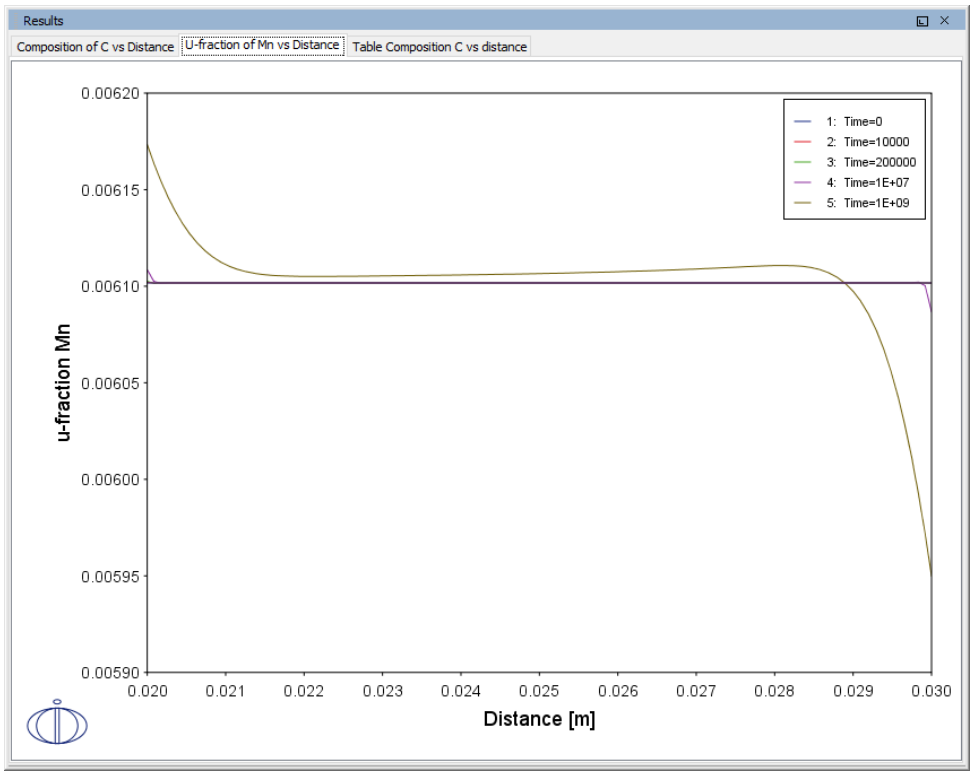
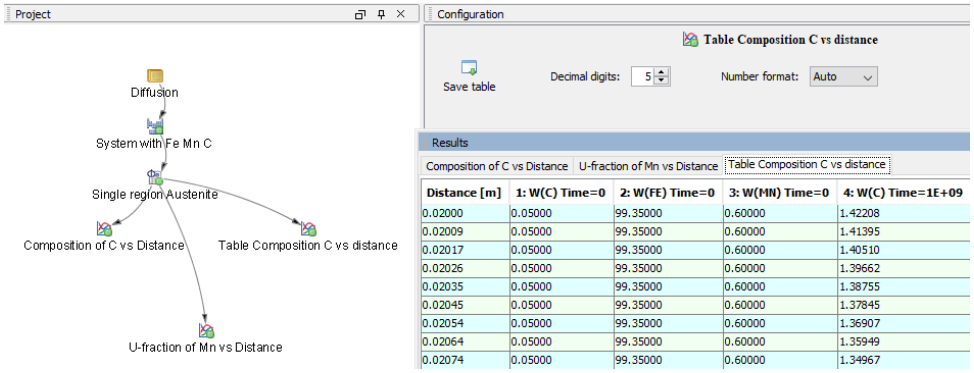


Figure 79: U-fraction of Mn vs Distance.



Distance [m]	1: W(C) Time=0	2: W(FE) Time=0	3: W(MN) Time=0	4: W(C) Time=1E+09
0.02000	0.05000	99.35000	0.60000	1.42208
0.02009	0.05000	99.35000	0.60000	1.41395
0.02017	0.05000	99.35000	0.60000	1.40510
0.02026	0.05000	99.35000	0.60000	1.39662
0.02035	0.05000	99.35000	0.60000	1.38755
0.02045	0.05000	99.35000	0.60000	1.37845
0.02054	0.05000	99.35000	0.60000	1.36907
0.02064	0.05000	99.35000	0.60000	1.35949
0.02074	0.05000	99.35000	0.60000	1.34967

Figure 80: Table: Composition C vs Distance.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_06_Diffusion_Carburization_Tube.tcu*

This example is available to all users.

D_07: Multiphase Carburization of an Alloy

This example is based on Engström et al. [1994Eng] and is about carburization of a Ni-25Cr-0.0001C alloy. In this case the M7C3 and M3C2 carbides are entered as spheroid phases in an FCC_A1 matrix. It is similar to Graphical Mode example D_06 except the default simulation condition is automatically set to use the homogenization model.

The isothermal calculation is run for 1000 hours at a temperature of 1123 K using the mixed zero flux and activity left boundary condition. Results are plotted using two Plot Renderers and a Table Renderer.

This example is based on Console Mode exd1b. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).

This example is available as a video tutorial on our website and YouTube channel.

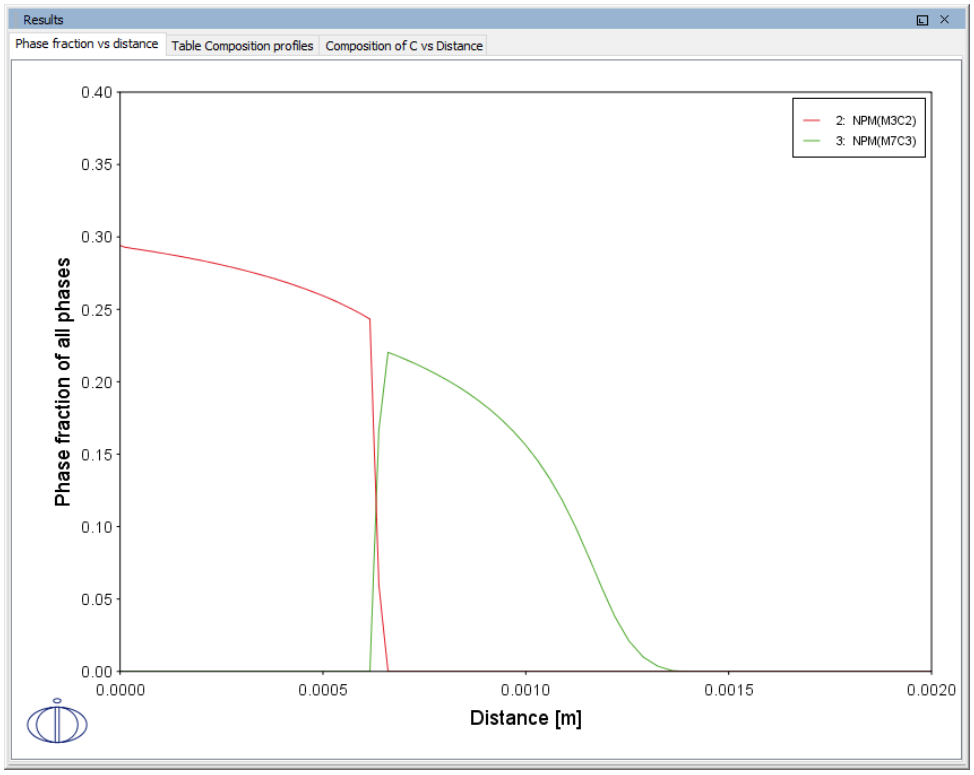
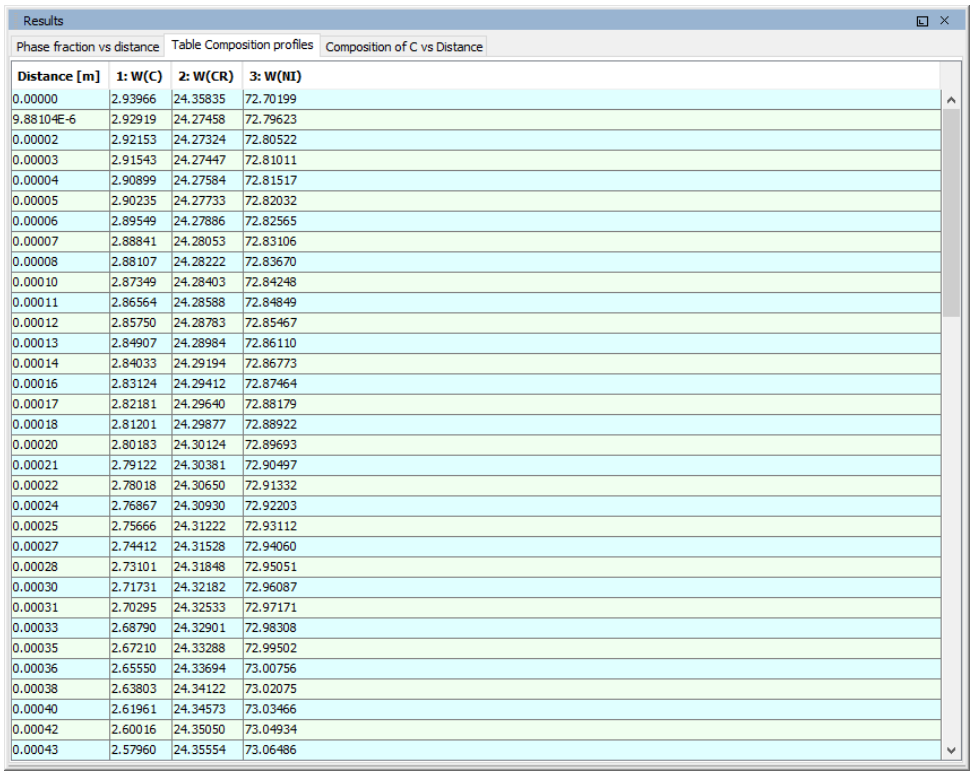


Figure 81: Phase fraction vs distance.


Results

Phase fraction vs distance | Table Composition profiles | Composition of C vs Distance

Distance [m]	1: W(C)	2: W(CR)	3: W(NI)
0.00000	2.93966	24.35835	72.70199
9.88104E-6	2.92919	24.27458	72.79623
0.00002	2.92153	24.27324	72.80522
0.00003	2.91543	24.27447	72.81011
0.00004	2.90899	24.27584	72.81517
0.00005	2.90235	24.27733	72.82032
0.00006	2.89549	24.27886	72.82565
0.00007	2.88841	24.28053	72.83106
0.00008	2.88107	24.28222	72.83670
0.00010	2.87349	24.28403	72.84248
0.00011	2.86564	24.28588	72.84849
0.00012	2.85750	24.28783	72.85467
0.00013	2.84907	24.28984	72.86110
0.00014	2.84033	24.29194	72.86773
0.00016	2.83124	24.29412	72.87464
0.00017	2.82181	24.29640	72.88179
0.00018	2.81201	24.29877	72.88922
0.00020	2.80183	24.30124	72.89693
0.00021	2.79122	24.30381	72.90497
0.00022	2.78018	24.30650	72.91332
0.00024	2.76867	24.30930	72.92203
0.00025	2.75666	24.31222	72.93112
0.00027	2.74412	24.31528	72.94060
0.00028	2.73101	24.31848	72.95051
0.00030	2.71731	24.32182	72.96087
0.00031	2.70295	24.32533	72.97171
0.00033	2.68790	24.32901	72.98308
0.00035	2.67210	24.33288	72.99502
0.00036	2.65550	24.33694	73.00756
0.00038	2.63803	24.34122	73.02075
0.00040	2.61961	24.34573	73.03466
0.00042	2.60016	24.35050	73.04934
0.00043	2.57960	24.35554	73.06486

Figure 82: Table of Composition profiles.

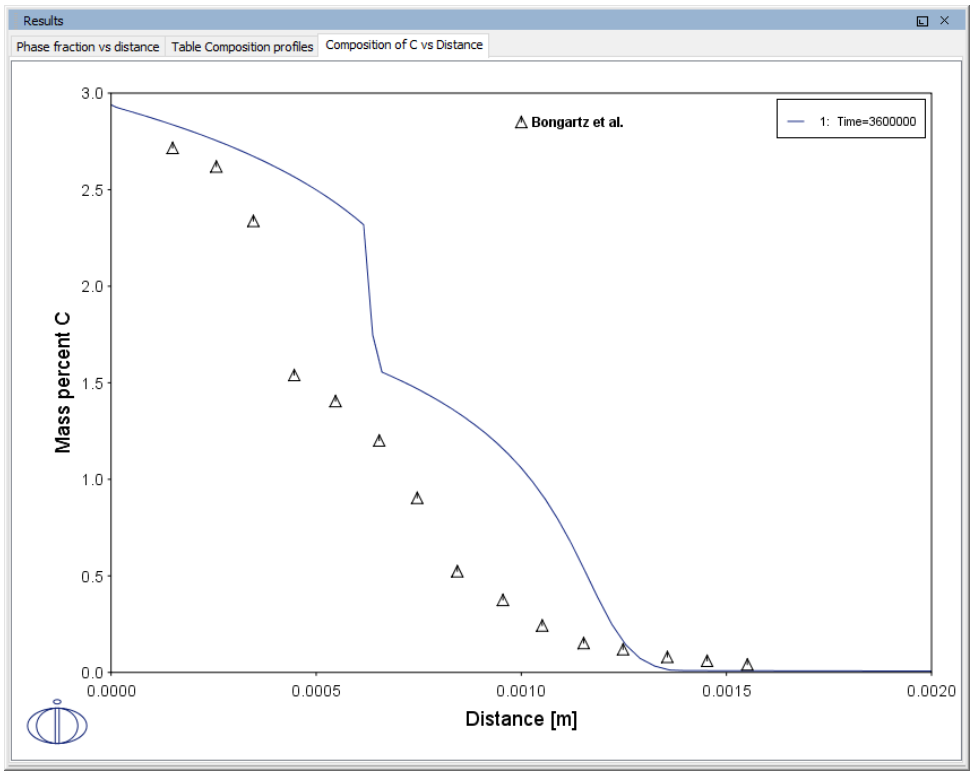


Figure 83: Composition of C vs distance.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_07_Diffusion_Carburization_Multiphase.tcu*

This example is available to all users.

Reference

[1994Eng] A. Engström, L. Höglund, J. Ågren, Computer simulation of diffusion in multiphase systems. Metall. Mater. Trans. A. 25, 1127–1134 (1994).

D_08: Microsegregation During Solidification

This application example, which is showcased on our website, shows how Thermo-Calc together with the Diffusion Module (DICTRA) can be used to investigate and predict microsegregation during solidification, also known as solute redistribution during solidification. The example uses a steel with composition Fe – 0.8% Mn – 0.7%Si – 0.03%P – 0.4%C.

The example is based on a real case where the elemental distribution of a continuously cast steel was measured revealing the concentration of the elements Si, Mn, and P. The profile results from the well-known segregation across secondary dendrite arms. The interesting point is that the elements Si and Mn show the expected positive segregation (higher concentrations) in the interdendritic regions. The peak of the P content, on the other hand, is shifted compared to Si and Mn, and, in fact, shows negative segregation in the interdendritic region. This is unexpected and counterintuitive.

The example also touches on some very basic concepts for metallurgy and using Thermo-Calc, such as stable and meta-stable phase diagrams, Scheil and para- or partial-equilibrium Scheil solidification simulations.

Open the example project file and click **Perform Tree** to generate the plots associated with this application example.



Running this calculation requires licenses for the Add-on Diffusion Module (DICTRA) plus the steels thermodynamic database (TCFE9 or newer) and mobility database (MOBFE4 or newer).



The result plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D_08_Diffusion_Microsegregation_During_Solidification.tcu*

Precipitation Module (TC-PRISMA) Graphical Mode Examples

Examples that use up to three elements are available to all users. The other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results.

All examples use demonstration database packages included with your installation. You can open the examples from the main menu: **File** → or **Help** → **Examples Files**.

Unless specified in tables for each example, all the numerical parameters are assumed default values.

In this section:

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P_10: Initial Particle Size Distribution of Fe-Cr-C 605

P_11: Interfacial Energy Function 609

P_12: Comparing Growth Rate Models for an Al-Zr System 612

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr 615

P_01: Isothermal Precipitation of Al_3Sc

This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The simulation results can be compared with experimental data collected from Marquis and Seidman [2001, Marquis] and Novotny and Ardell [2001, Novotny].

This example also includes a plot using the **Yield strength** Property Model. This demonstrates how you can use the results from a Precipitation Module (TC-PRISMA) simulation as input to the Yield Strength Model, i.e. the calculated precipitate radius/radii for each time step is used to calculate the precipitation strengthening, and similarly, the matrix composition for each time step is used to calculate the solid solution strengthening when this is selected in the **Configuration** on the Plot Renderer. The experimental data for the Yield Strength Model is from Seidman et al. [2002, Seidman].

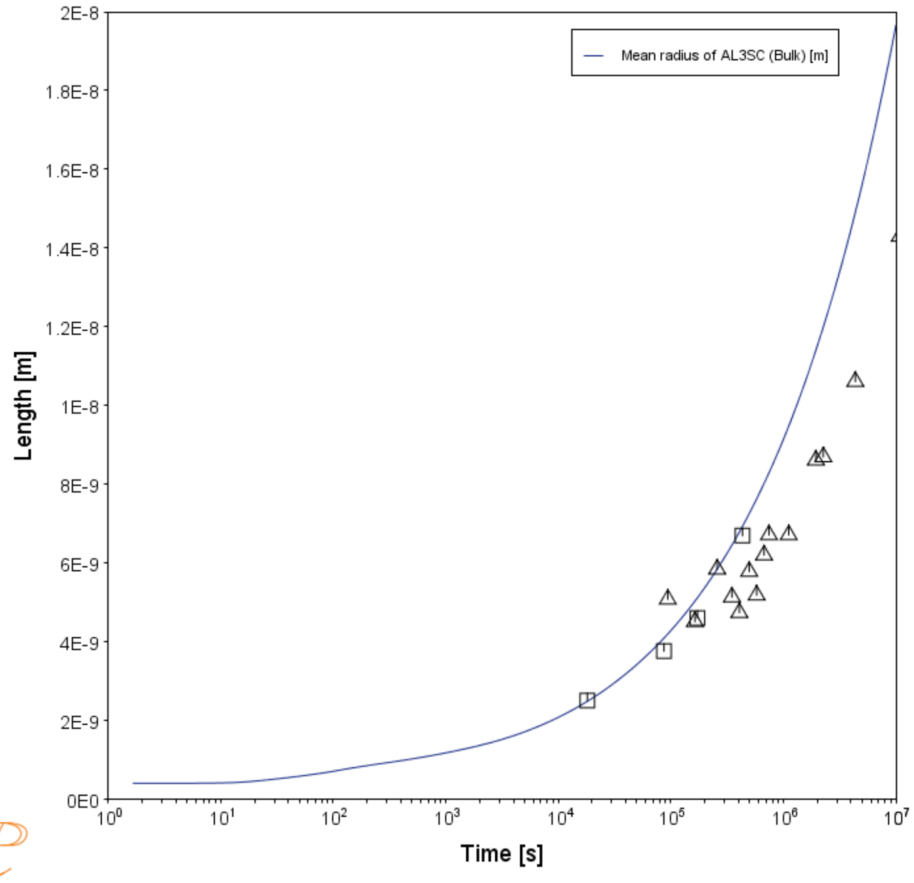


Figure 84: The mean radius of the AL3SC precipitate as a function of time.

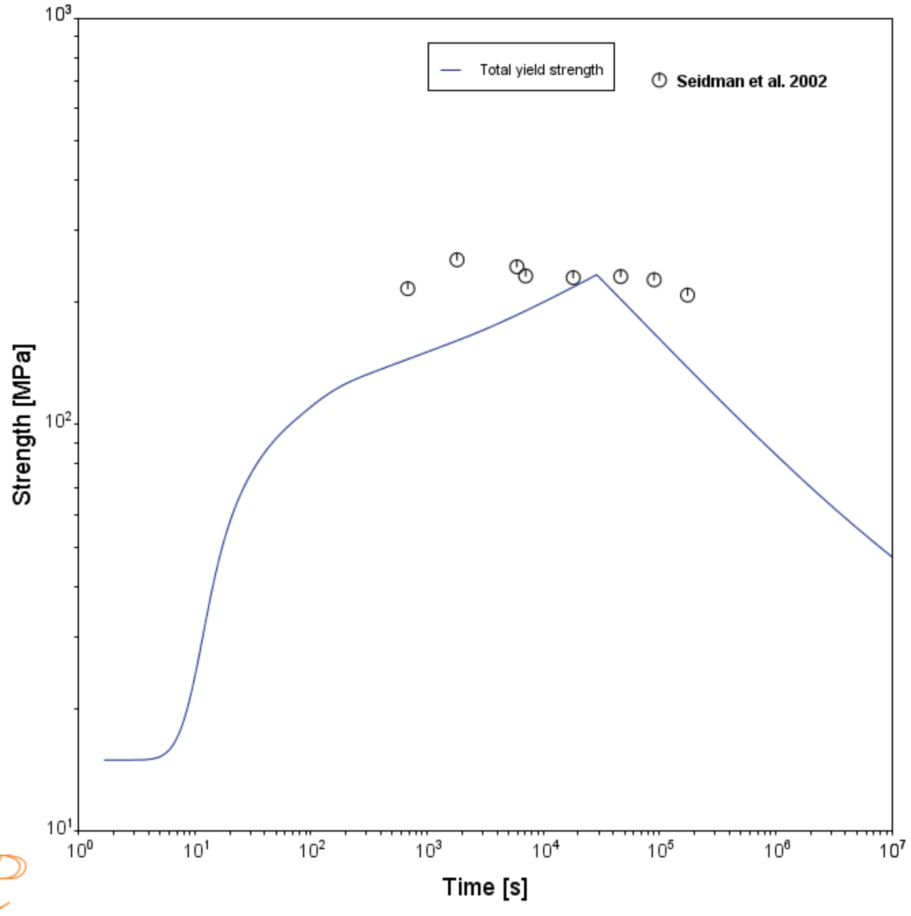


Figure 85: The total yield strength of the AL3SC precipitate as a function of time compared to experimental data from Sieldmen et al. [2002, Seidman].

Project File, Step-By Step Instructions and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_01_Precipitation_Al-Sc_AL3SC.tcu*

This example is available as a video tutorial on our website and YouTube channel.

You can also use the step-by-step instructions included in a PDF to follow the video or compare to the project file in Thermo-Calc. Note that at this time, the Yield Strength Model included with this example is not specified in the step-by-step instructions.

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent
Matrix phase	FCC_A1
Precipitate phase	AL3SC
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	Calculated
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	1.0E7 seconds
Experimental File Reader 1 and 2	
There are two Experimental File Reader nodes used. One for the mean radius plot and one to demonstrate the *Yield Strength Property Model*.	

References

[2001, Marquis] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

[2001, Novotny] G. M. Novotny, A. J. Ardell, Precipitation of Al3Sc in binary Al–Sc alloys. Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318, 144–154 (2001).

[2002, Seidman] D. N. Seidman, E. A. Marquis, D. C. Dunand, Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys. Acta Mater. 50, 4021–4035 (2002).

Isothermal Precipitation Calculation: Example P_01 – Precipitation Al-Sc AL3SC

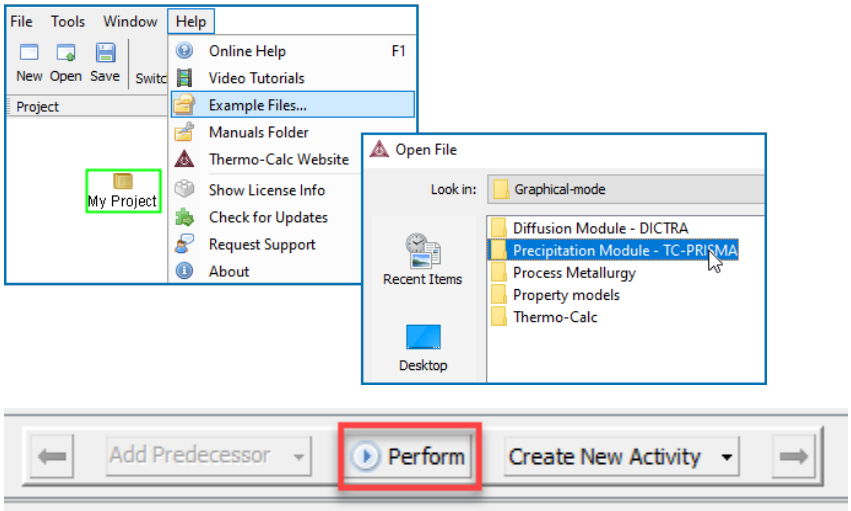
This example shows you how to set up an isothermal precipitation calculation for the formation of AL_3SC in an aluminium-scandium alloy at 350° using the Precipitation Module (TC-PRISMA).

The end of the example also shows how to use the results of the calculation to model Yield Strength.

This is one of the most basic calculations using the Precipitation Module (TC-PRISMA), so it is a good place to start if you are new to this simulation type.

HELPFUL INFORMATION

- **All users can run this calculation,** even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ
- This calculation is based on Precipitation Module example *P_01 – Precipitation Al-Sc AL3SC*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.

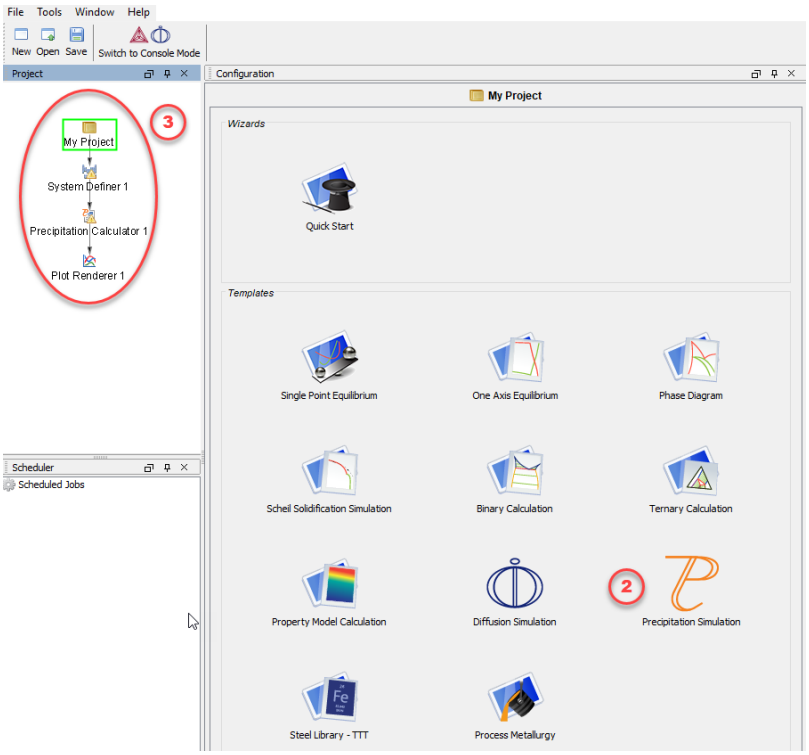


ABOUT THE EXAMPLE

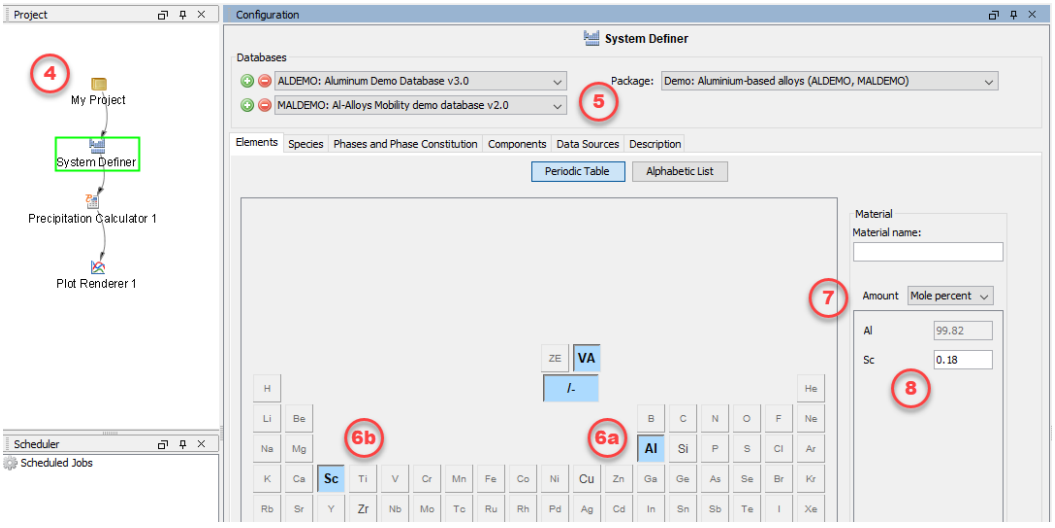
This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The results of the simulation are also used to model yield strength.

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under *Templates*, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Aluminium-based alloys (ALDEMO, MALDEMO)**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the **Periodic Table**, select the elements as follows. Select Al first so that it is the dependant element:
    a. **Al** (aluminium)
    b. **Sc** (scandium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter `0.18` for **Sc**. This automatically sets **Al** to 99.82.



The system is now defined. However, before starting the precipitation calculation, it is recommended to run a one axis calculation to find the phases present around 350° C.

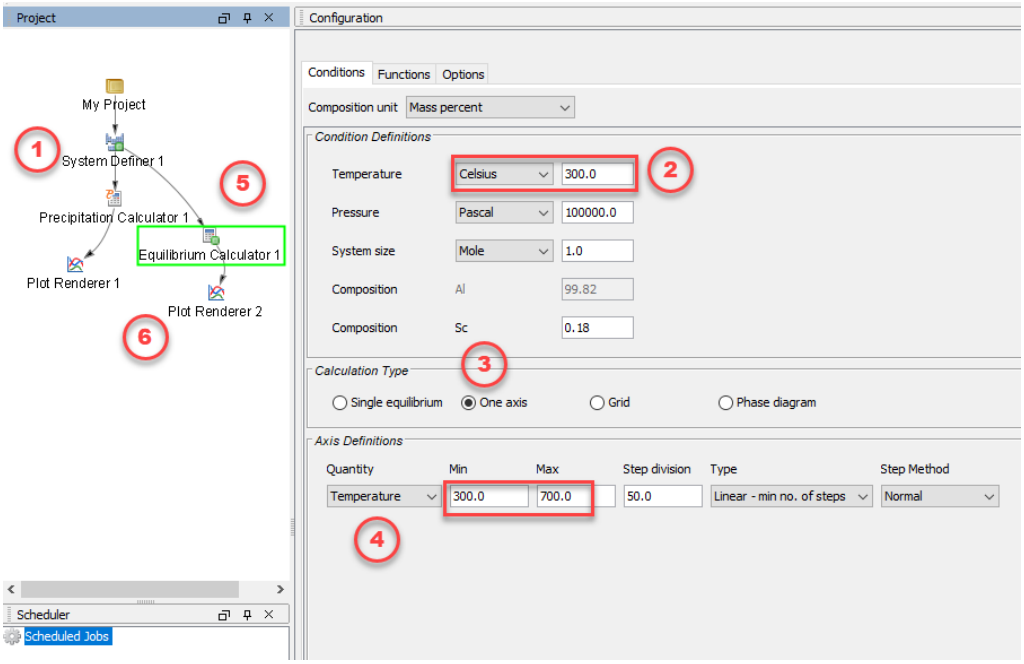
ONE AXIS CALCULATION

Why We Do This

In order to set up an isothermal precipitation calculation, you need to know which phases are present at 350 °C. A *one axis* calculation provides this information.

Setting up a One Axis Calculation

1. In the **Project** window, right-click the **System Definer 1** node, and select **Create New Successor** > **Equilibrium Calculator**.
2. In the **Configuration** window, set *Temperature* to **Celsius** and enter 300.
3. Under *Calculation Type*, select **One axis**.
   You now want to find the phases present around 350 °C.
4. Under *Axis Definitions,* enter the **Temperature** range from **Min** 300 to **Max** 700.
   Keep the default values for everything else. The system is now defined.
5. Right-click the **Equilibrium Calculator** node and select **Create New Successor > Plot Renderer**.
6. In the **Project** window, right-click the **Plot Renderer 2** node you just created and select **Perform Now**. Or click **Perform** at the bottom of the **Configuration** window.



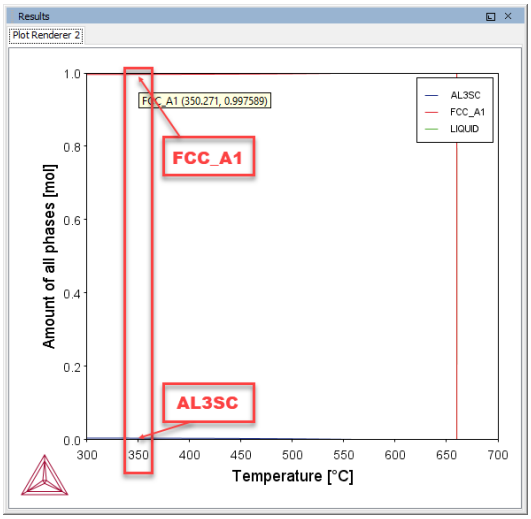
Interpreting the Results of the One Axis Calculation

Once the calculation is complete, a plot is displayed in the **Results** window. This plot shows you which phases are present at each temperature between 300° and 700° and the amount of that phase at each temperature.

If you hover your cursor over any of the lines on the plot, a label gives you the name of the phase, the temperature and the amount of the phase at that temperature.

We can see that there are two phases present at 350°. FCC_A1 is at the very top of the plot and makes up more than 99% of the system. The remainder of the system is made up of Al_3SC, which is near the very bottom of the plot and is the precipitate phase in the alloy we are considering.

Remember these two phases because these are used in the precipitation calculation.



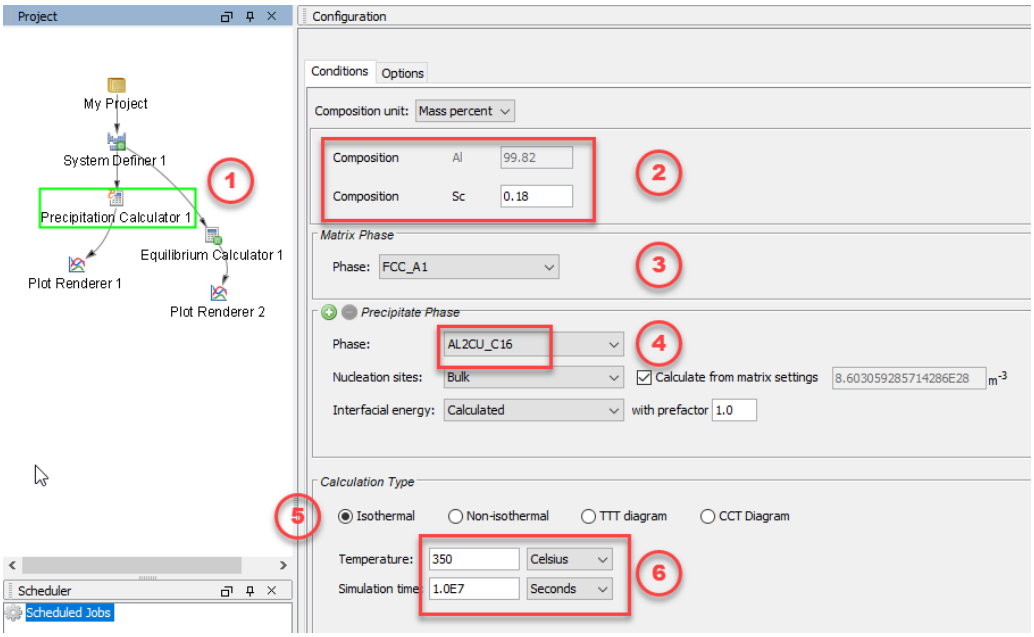
PRECIPITATION CALCULATION

Setting up the Precipitation Calculation

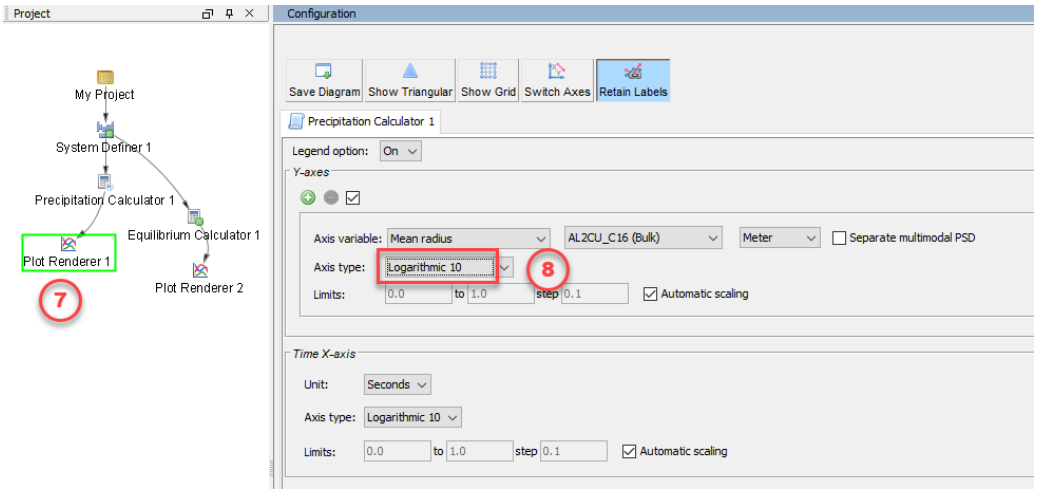
1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the *Composition* set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, the *Phase* defaults to **FCC_A1**, which is the primary phase present in the one axis calculation.

NOTE: If you do not see any phases listed here it is probably because you do not have a kinetic database selected. If so, go back to the *System Definer* and add a kinetic (mobility) database. In this example it should be the **MALDEMO** database.

4. Under *Precipitate Phase,* select **AL3SC** from the *Phase* list because that is the other phase present around 350 °C, as shown in the one axis calculation.
5. Accept the default settings in the *Precipitate Phase* section. You could choose to define your own interfacial energy settings if you have them.
6. Under *Calculation Type*, make sure **Isothermal** is selected.
7. Enter:
    a. `350` as the *Temperature* and select **Celsius**.
    b. `1.0E7` as the *Simulation time* and select **Seconds**, which is ten million seconds.

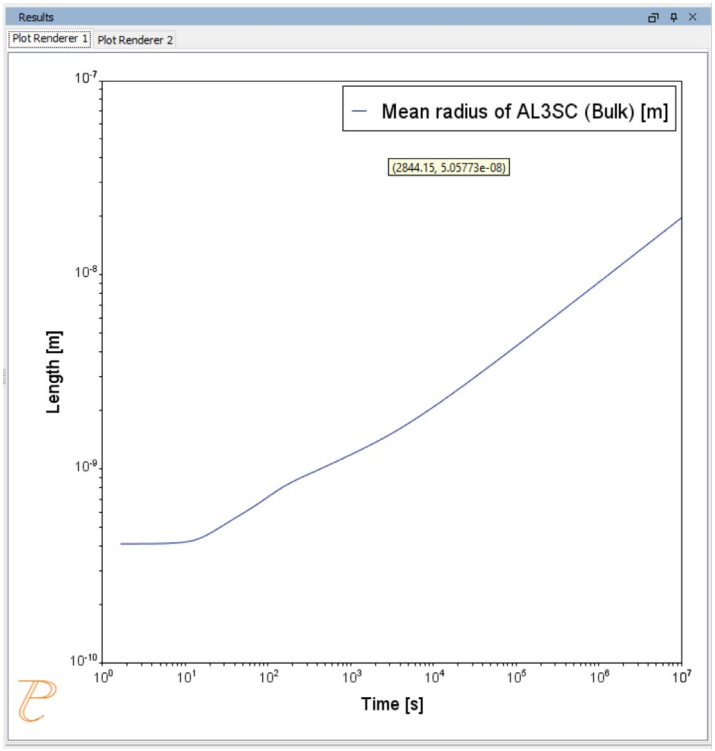


8. In the **Project** window, click the **Plot Renderer 1** node.
9. Under *Y-axes*, from the *Axis type* menu select **Logarithmic 10** for a better view of the plot.
10. Click **Perform** at the bottom, center of the **Configuration** window.



Interpreting the Results of the Precipitation Calculation

Once the calculation is complete, your plot is shown in the **Results** window.



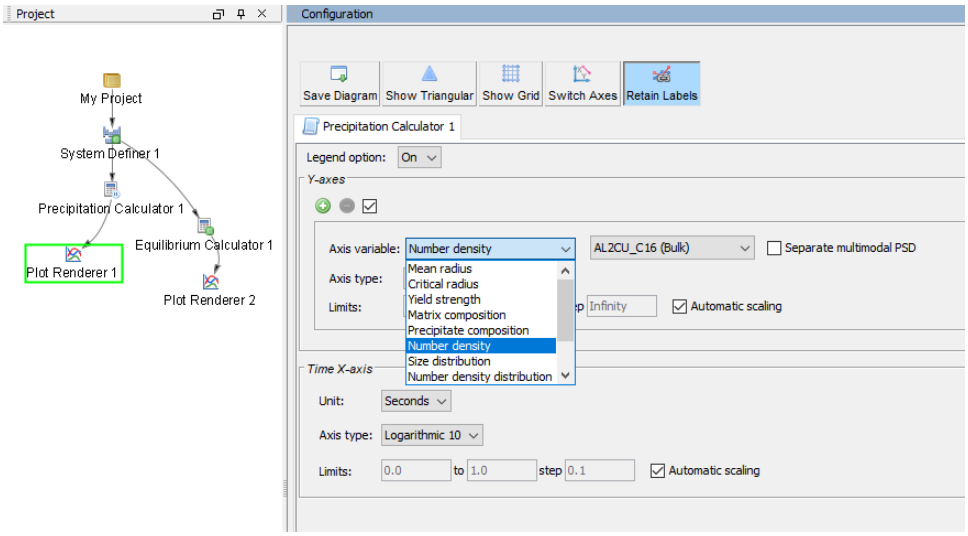
This plot shows the Mean radius of the AL3SC precipitate as a function of time.

At the beginning, which is the left-most side of the plot, the mean radius is quite small and then grows rapidly over time, which is represented by moving rightward on the plot.

Setting Other Variables in the Precipitation module (TC-PRISMA)

The Precipitation Module (TC-PRISMA) offers many variables that you can plot for the same calculation.

1. Click the **Plot Renderer 1** node.
2. Under *Y-axes*, click the Axis variable menu to see the other available options in the list.
3. Once you have made your selection, click **Perform** at the bottom, center of the **Configuration** window to create a new plot.

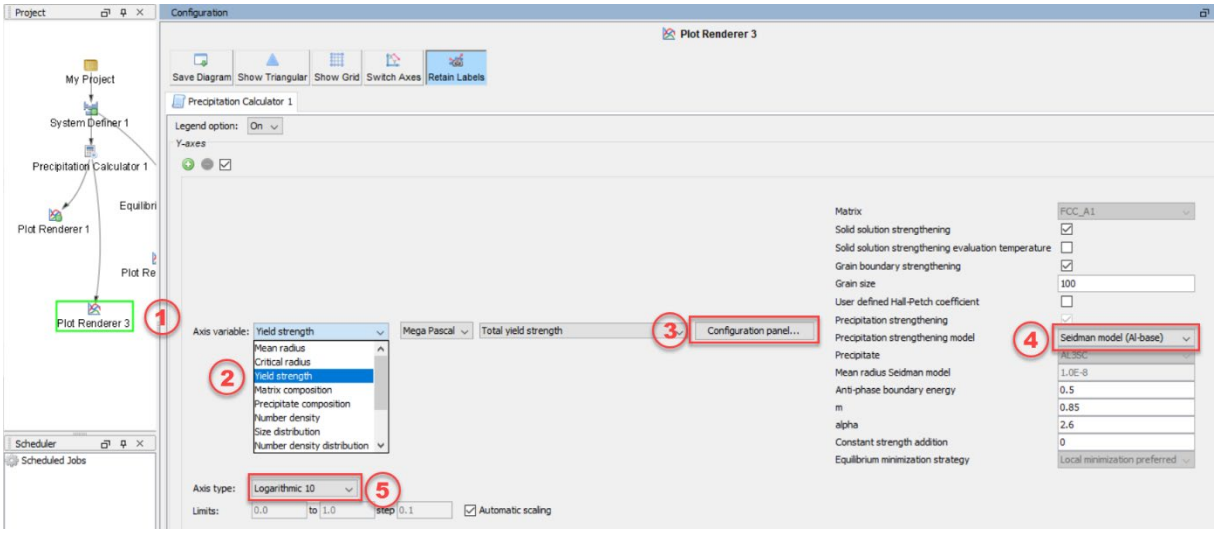


Model Yield Strength

Beginning with Thermo-Calc 2020b, results of a precipitation simulation can be used as input to model yield strength using the Yield Strength Property Model. The following simulation requires a license for Thermo-Calc 2020b or newer.

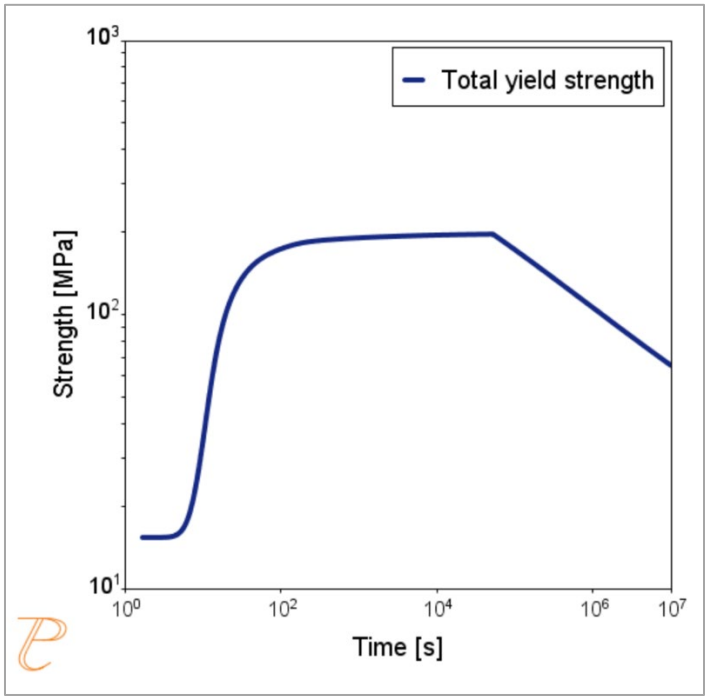
1. Right click the **Precipitation Calculator 1** node and select **Create New Successor > Plot Renderer**.
2. Under *Y-axes*, from the *Axis variable* menu, select **Yield strength**.
3. Click the *Configuration panel* button.
4. If required, expand the Plot Renderer Configuration window. Then from the *Precipitation strengthening model* menu select **Seidman model (Al-base)**.
5. Under *Y-axes*, from the *Axis type* menu, select **Logarithmic 10**.
6. Click **Perform** at the bottom, center of the program.

The program uses the results from the precipitation simulation as the input for the Yield Strength model.



Interpreting the Results of the Yield Strength Model

Once the calculation is complete, your plot is shown in the **Results** window.



This plot shows the yield strength of the AL3SC precipitate as a function of time.

P_02: Stable and Metastable Carbides - Isothermal

This example simulates the kinetics of precipitation of both stable and metastable carbides from ferrite phase. It demonstrates that metastable carbides (cementite, M7C3) may first emerge and then disappear and the stable phase (M23C6) prevails.

This example uses the Equilibrium Calculator and a one axis calculation to determine how the phases change with temperature. We are interested in the carbide precipitation at 1053K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

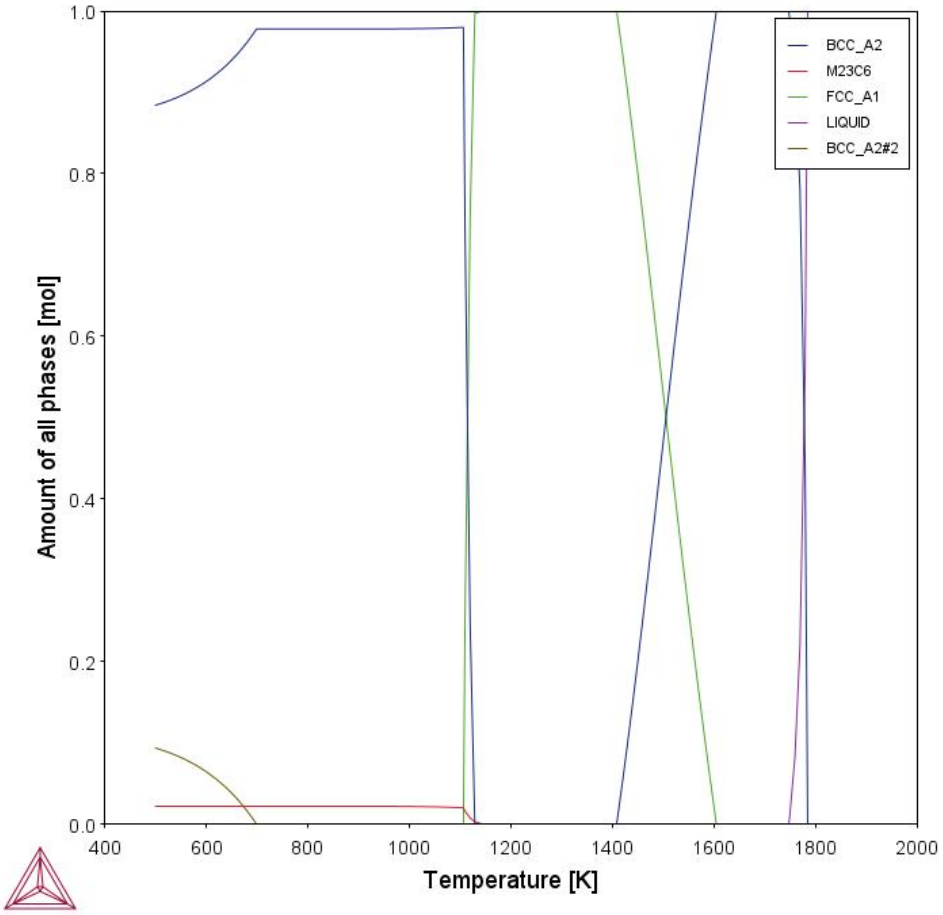


Figure 86: The Equilibrium Calculator and a One axis calculation is used to determine how the phases change with temperature.

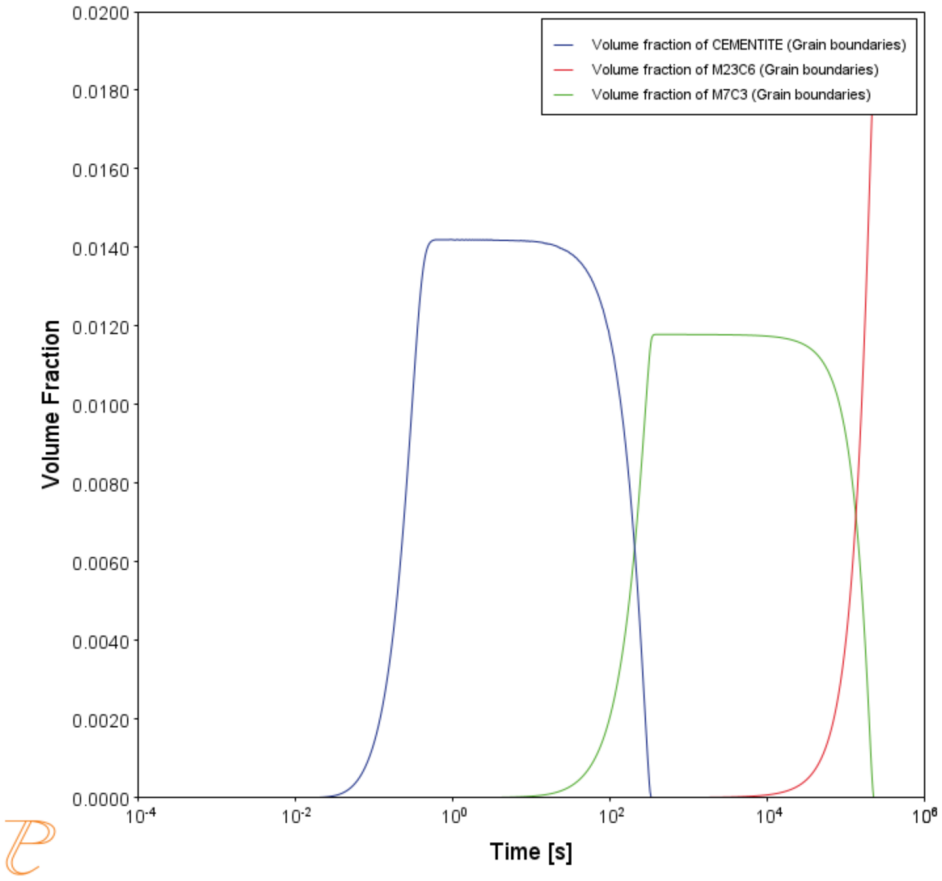


Figure 87: The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)

Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

P_03: Stable and Metastable Carbides - TTT Diagram

In this example, the kinetics of precipitation of both stable and metastable carbides is calculated from the ferrite phase. It demonstrates that metastable carbides may first emerge and then disappear and the stable phase prevails.

This example uses the Equilibrium Calculator and a one axis calculation type to determine how the phases change with temperature. Using this result, the Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

For a TTT diagram calculation, select **TTT diagram** in **Calculation Type**, then enter **Min**, **Max**, and **Step** of **Tempeature**, as well as **Max annealing time**. In **Stop criterion**, choose **Volume fraction of phase** and enter the value.

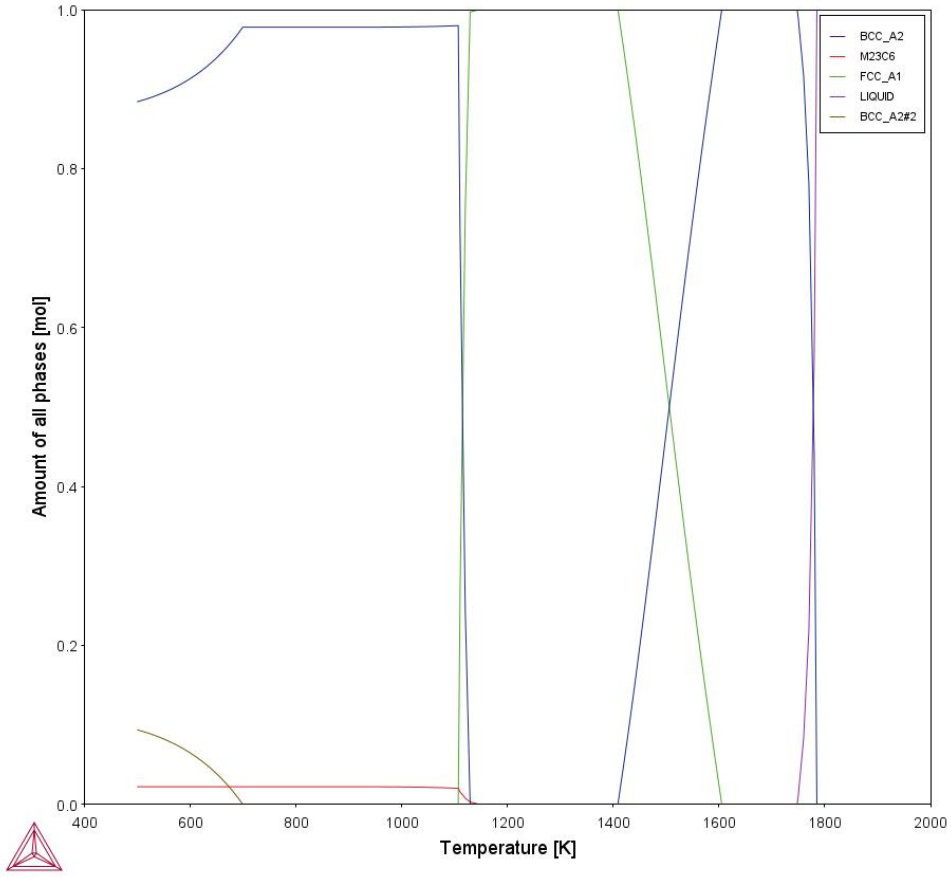


Figure 88: The Equilibrium Calculator is used to show how the phases change with temperature.

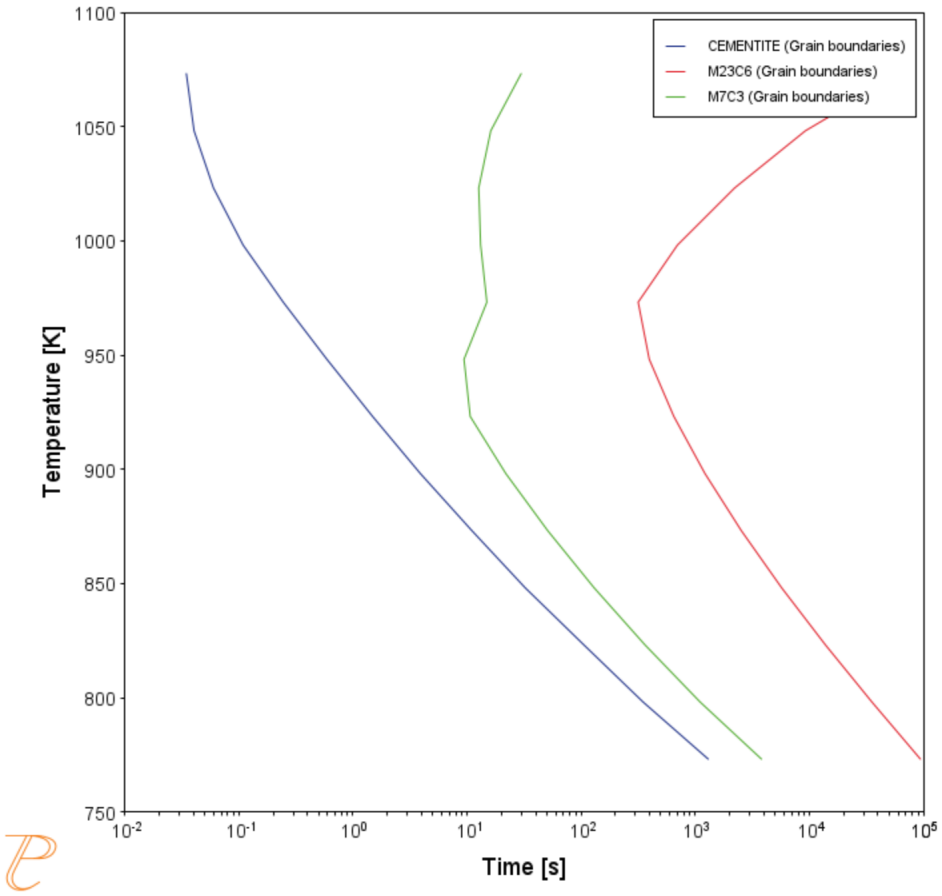


Figure 89: The Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

Project File and Video tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_03_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)

Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	TTT diagram
Temperature	500° to 800° C with 25° C steps
Max. annealing time	1.0E8 seconds
Stop criteria	Volume fraction of phase is set to 0.0001
Options > Numerical Parameters	
No. of grid points over one order of magnitude in radius	150
Max no. of grid points over one order of magnitude in radius	200
Min no. of grid points over one order of magnitude in radius	100

P_04: Precipitation of Iron Carbon Cementite

Simulate the kinetics of precipitation of carbides from a BCC Fe solution phase. This example is based on Wert [1949].

This example uses two Experimental File Reader activities with the Precipitation Calculator and an isothermal calculation, to plot the volume fraction of the cementite phase.

This example takes several minutes to run.

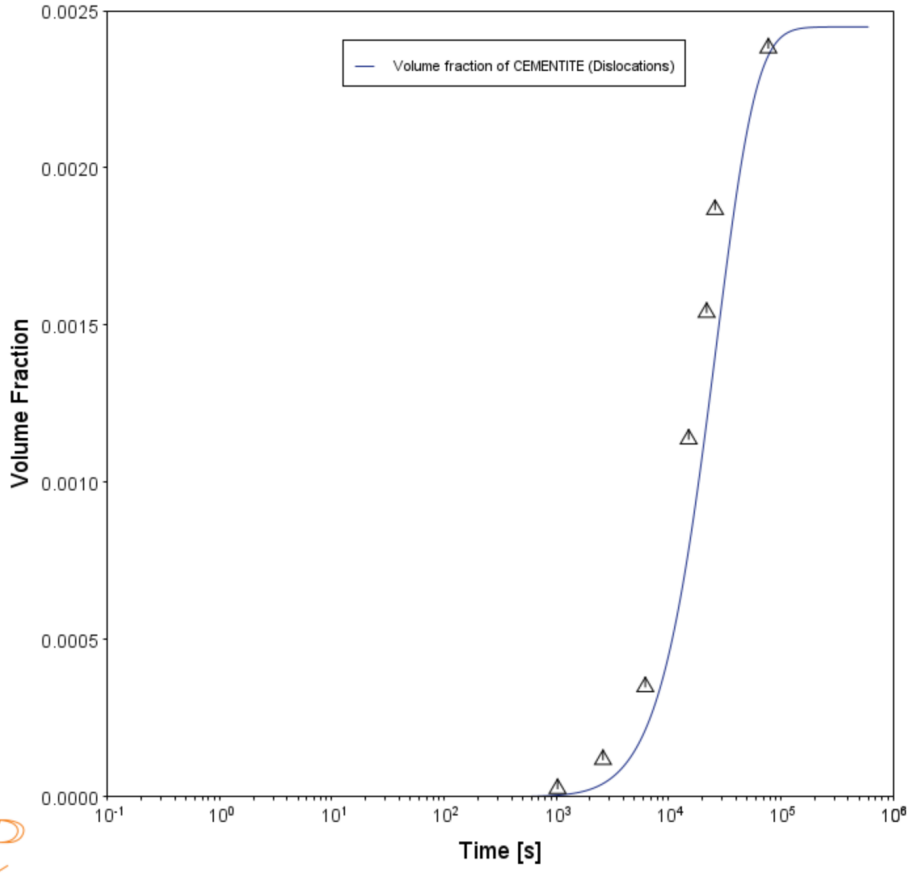


Figure 90: Volume fraction of the cementite phase.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_04_Precipitation_Fe-C_Cemetite.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.016C mass percent
Matrix phase	BCC_A2
Precipitate phase	Cementite
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain aspect ratio (click **Show details** to display this setting)	1.0
Dislocation density (click **Show details** to display this setting)	$1.5e11 m^{-3}$
Precipitate Phase Parameters (Precipitation Calculator)	
Nucleation sites	Dislocations
Interfacial energy	$0.24 J/m^2$
Growth rate model (click **Show details**)	Advanced
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	102° C
Simulation time	600 000 seconds

Reference

[1949,Wert] C. A. Wert, Precipitation from Solid Solutions of C and N in α-Iron. J. Appl. Phys. 20, 943 (1949).

P_05: Precipitation of γ' in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of γ' phase from γ phase. The simulation results can be compared with experimental data collected from Sudbrack et al. [2008].

This example uses three Experimental File Reader activities with the Precipitation Calculator. It does an isothermal calculation to plot the volume fraction, mean radius and number density of the cementite phase.

DIS_FCC_A1 needs to be selected on the System Definer.

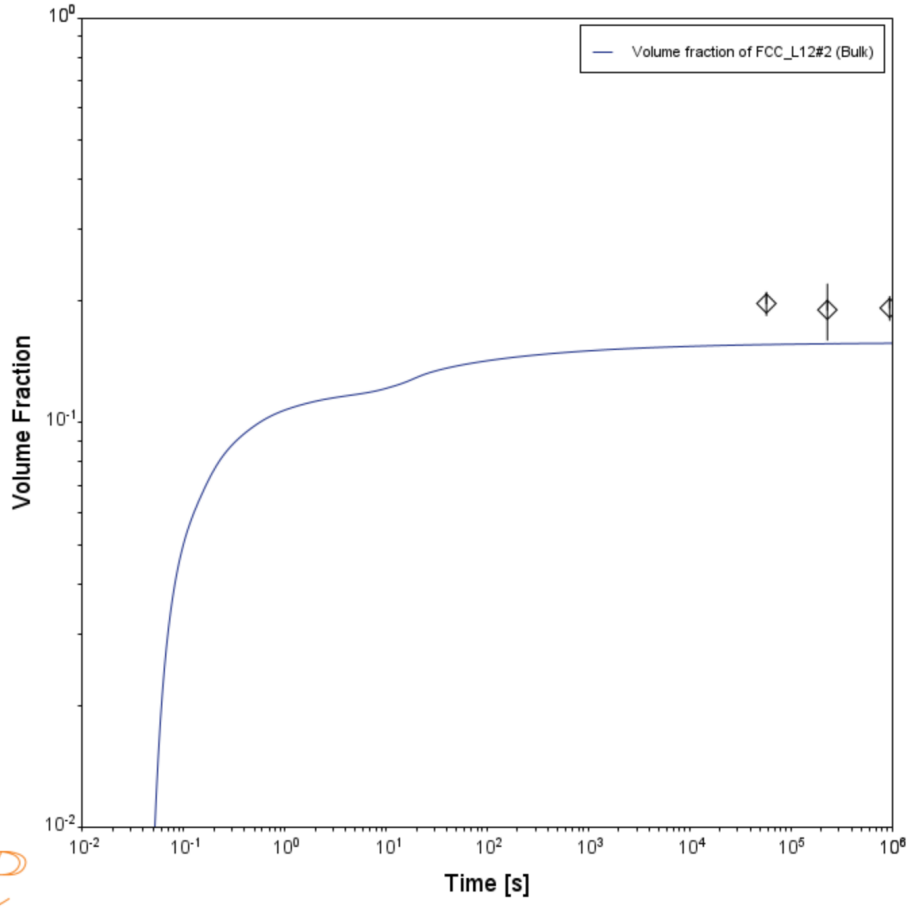


Figure 91: The results of an isothermal calculation to plot the volume fraction of the cementite phase.

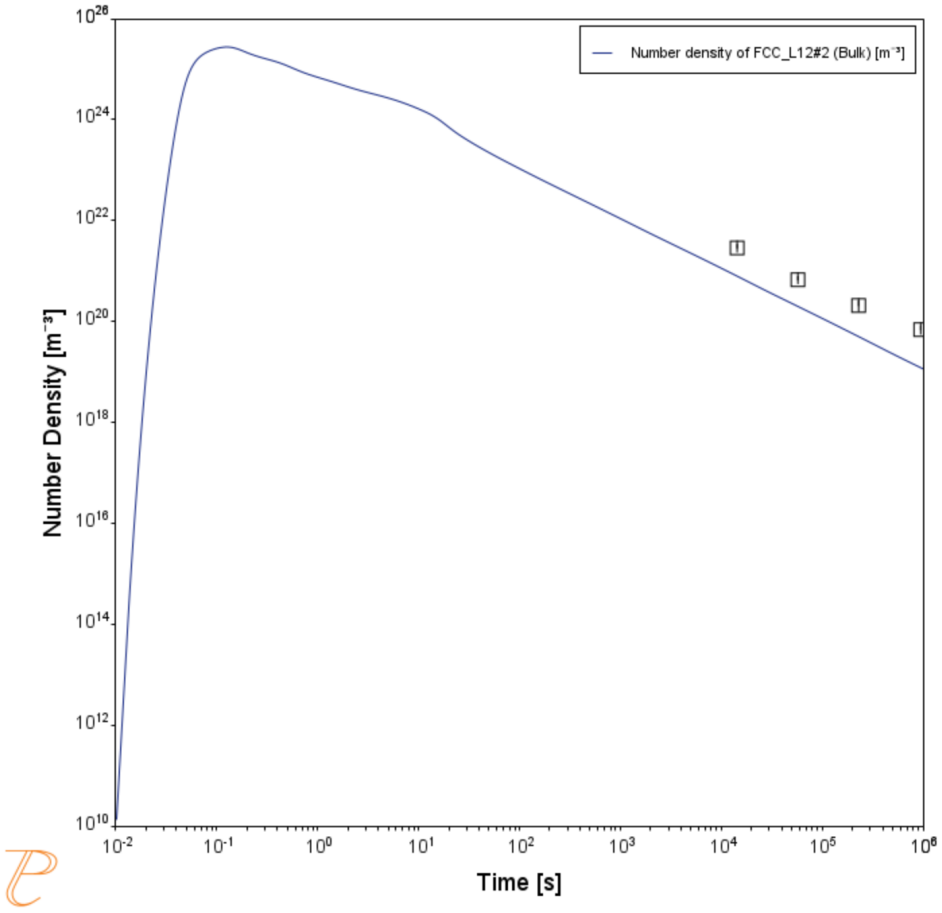


Figure 92: The results of an isothermal calculation to plot the number density of the cementite phase.

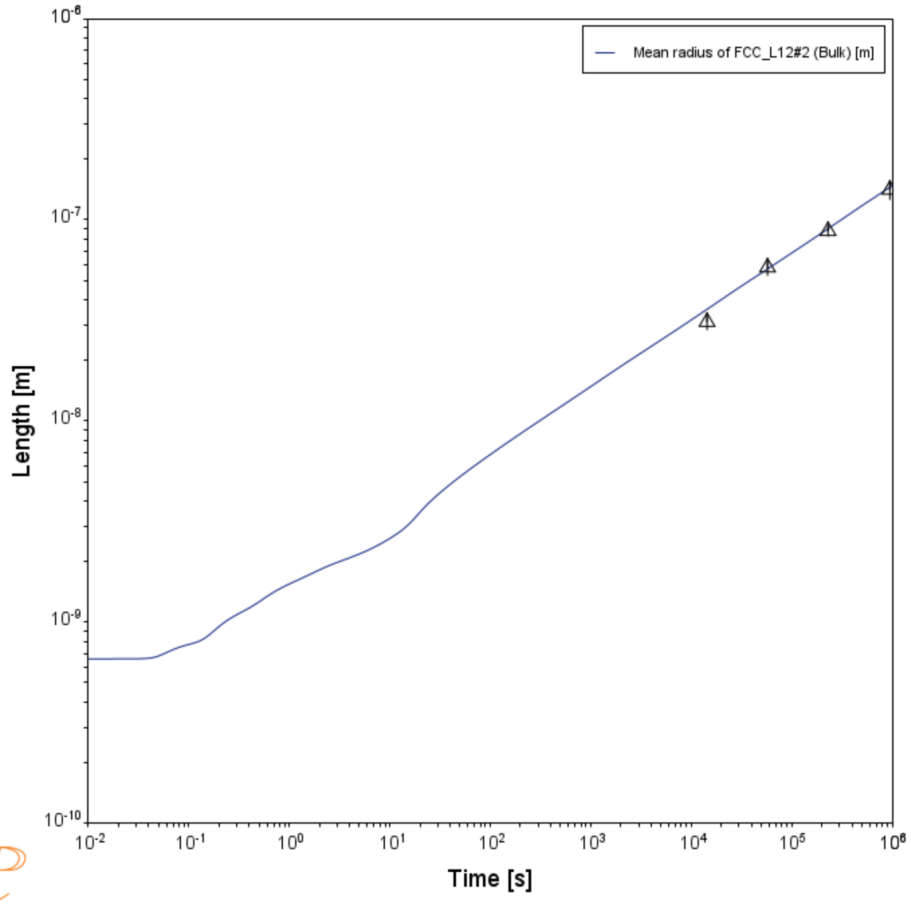


Figure 93: The results of an isothermal calculation to plot the mean radius of the cementite phase.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_05_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)

Elements	Ni, Al Cr
Conditions (Precipitation Calculator)	
Composition	Ni-9.8Al-8.3Cr Mole percent
Matrix phase	DIS-FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.012 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	800° C
Simulation time	1 000 000 seconds

Reference

[2008, Sudbrack] C. K. Sudbrack, T. D. Ziebell, R. D. Noebe, D. N. Seidman, Effects of a tungsten addition on the morphological evolution, spatial correlations and temporal evolution of a model Ni–Al–Cr superalloy. Acta Mater. 56, 448–463 (2008).

P_06: Precipitation of γ' in Ni Superalloys - Non-isothermal

This example simulates the kinetics of precipitation of γ' phase from γ phase in Ni-8Al-8Cr and Ni-10Al-10Cr at.% alloys during continuous cooling. The simulation results can be compared with experimental results from Rojhirunsakool et al. [2013].

When you run (Perform) this example, it takes about 10 minutes for the calculations to complete.

DIS_FCC_A1 needs to be selected on the System Definer.

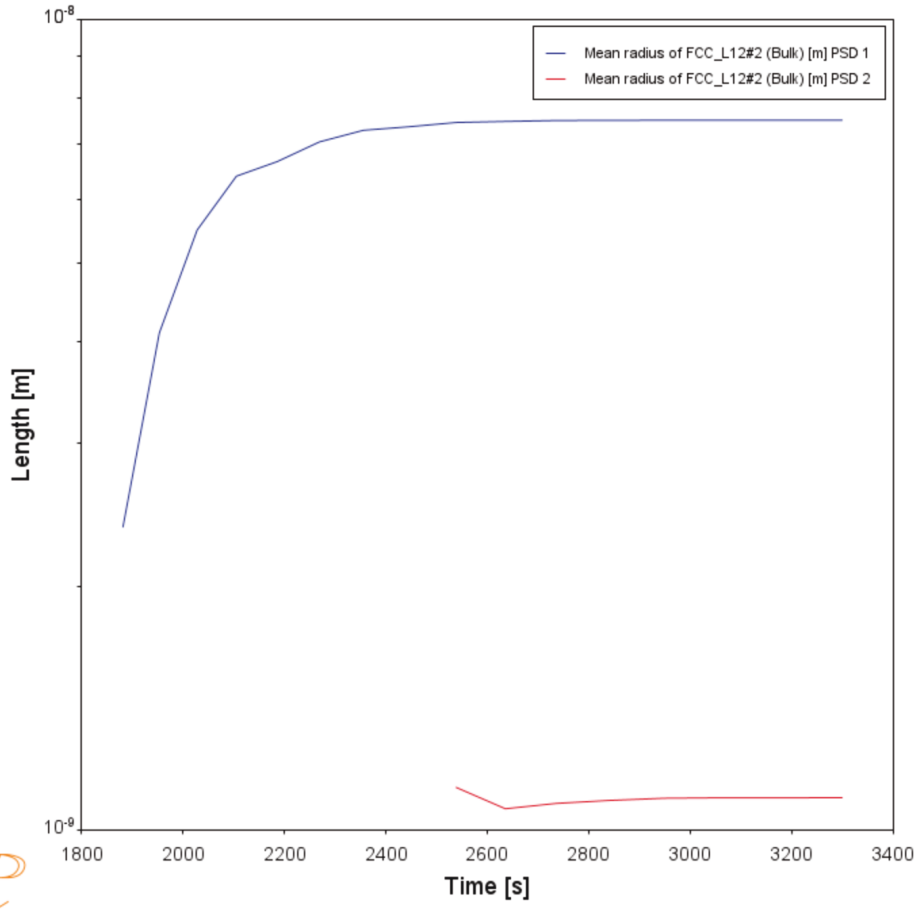


Figure 94: Mean Radius Ni-8Al-8Cr.

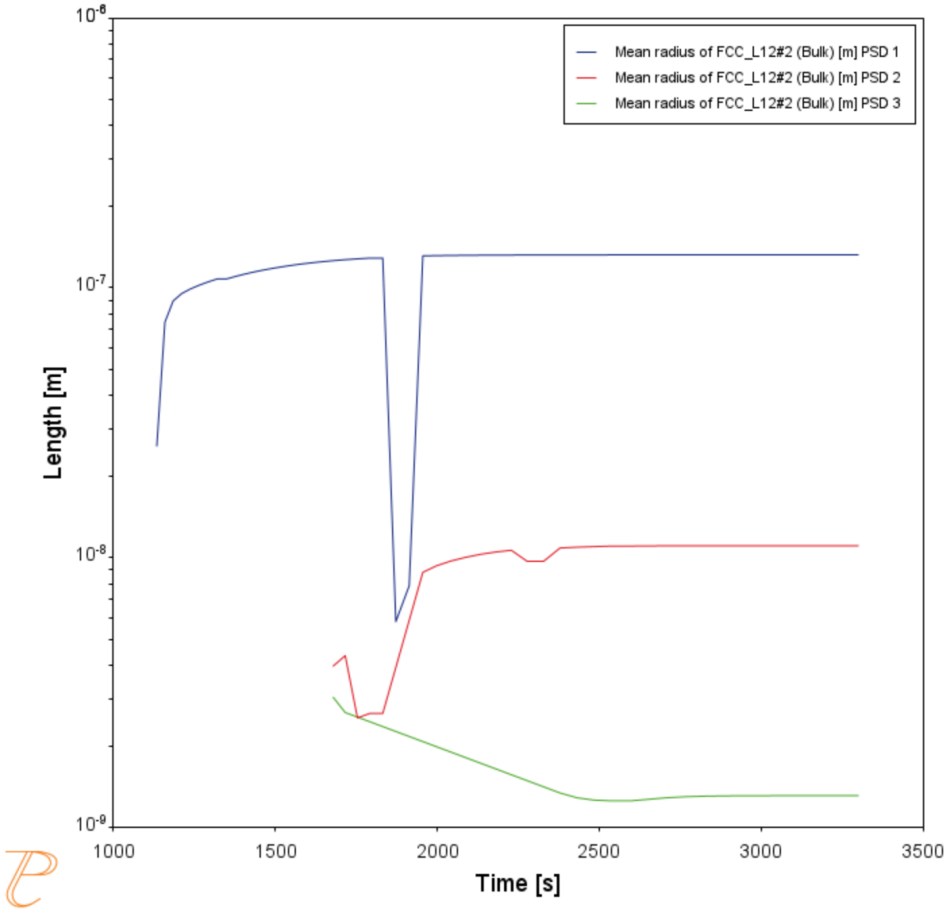


Figure 95: Mean Radius Ni-10Al-10CR.

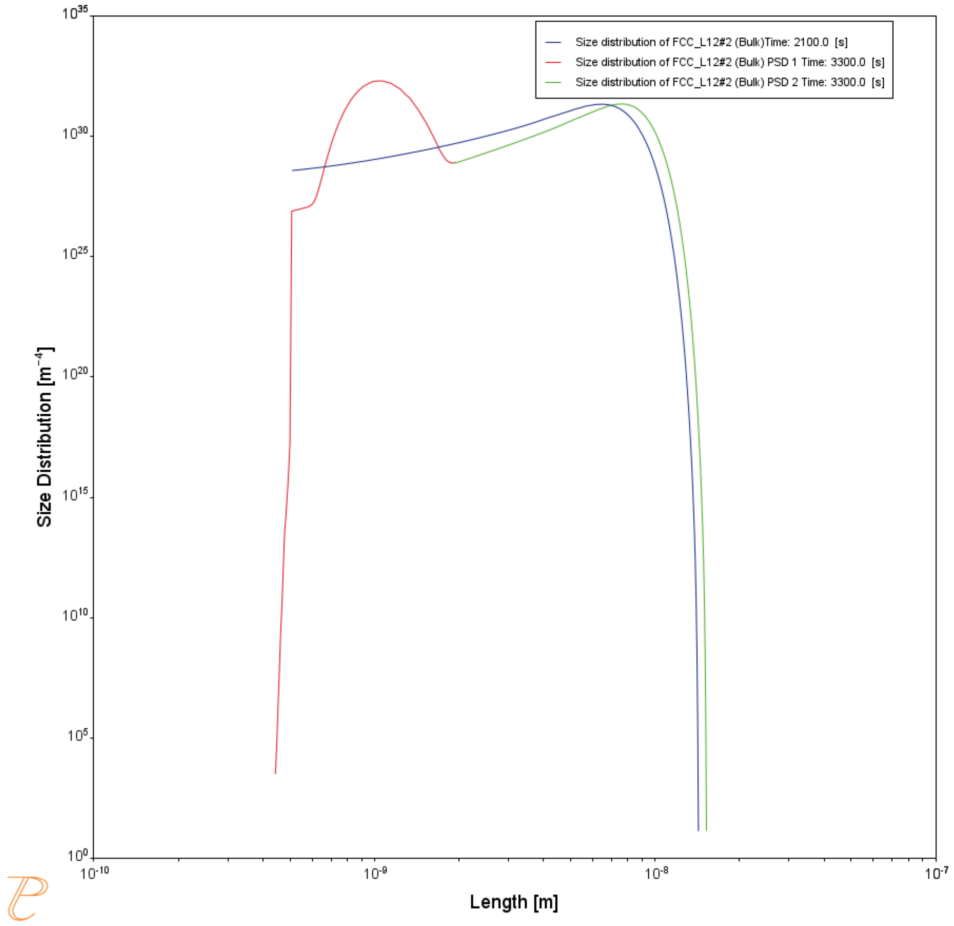


Figure 96: Size Distribution (PSD) Ni-8Al-8Cr.

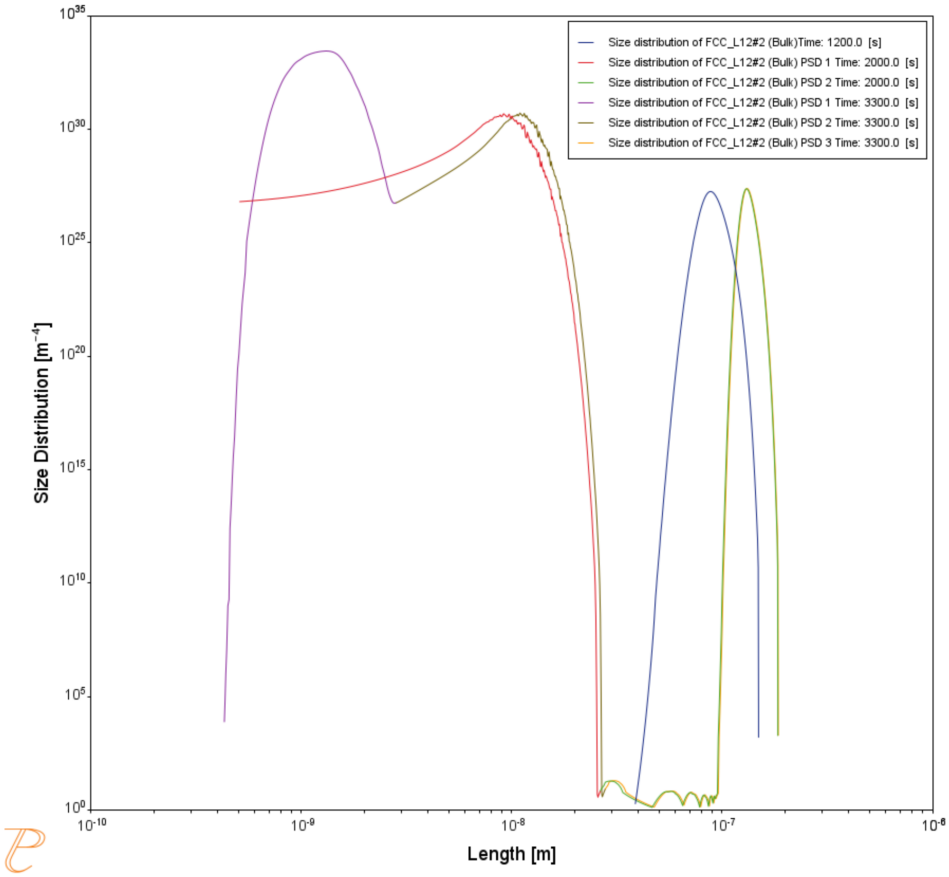


Figure 97: Size Distribution (PSD) Ni-10Al-10Cr.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)

Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility enhancement prefactor (click **Show details** to display this setting)	5.0
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.023 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Non-isothermal
Temperature unit	Celsius
Time unit	Seconds
Temperature	1150 - 380 °C Edit Thermal Profile Import... Time [s] / Temperature [°C] 0.0 / 1150.0 3300.0 / 380.0
Simulation time (Ni-8Al-8Cr)	3300 s

Simulation time (Ni-10Al-10Cr)	3300 s
Multimodal PSD (Plot Renderer)	
Separate multimodal PSD for 8Al-8Cr	The **Valley depth ratio** is set to 0.05 for both plots. The number of **Points** is increased to 200 for an average radius plot.
Separate multimodal PSD for 10Al-10Cr	The **Valley depth ratio** is set to 0.18 for both plots.

Reference

[2013, Rojhirunsakool] T. Rojhirunsakool, S. Meher, J. Y. Hwang, S. Nag, J. Tiley, R. Banerjee, Influence of composition on monomodal versus multimodal γ' precipitation in Ni–Al–Cr alloys. J. Mater. Sci. 48, 825–831 (2013).

P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ'

In this example, a Continuous Cooling Transformation (CCT) diagram for a Ni-10Al-10Cr γ-γ' alloy is calculated and plotted with superimposition of the cooling rate values.

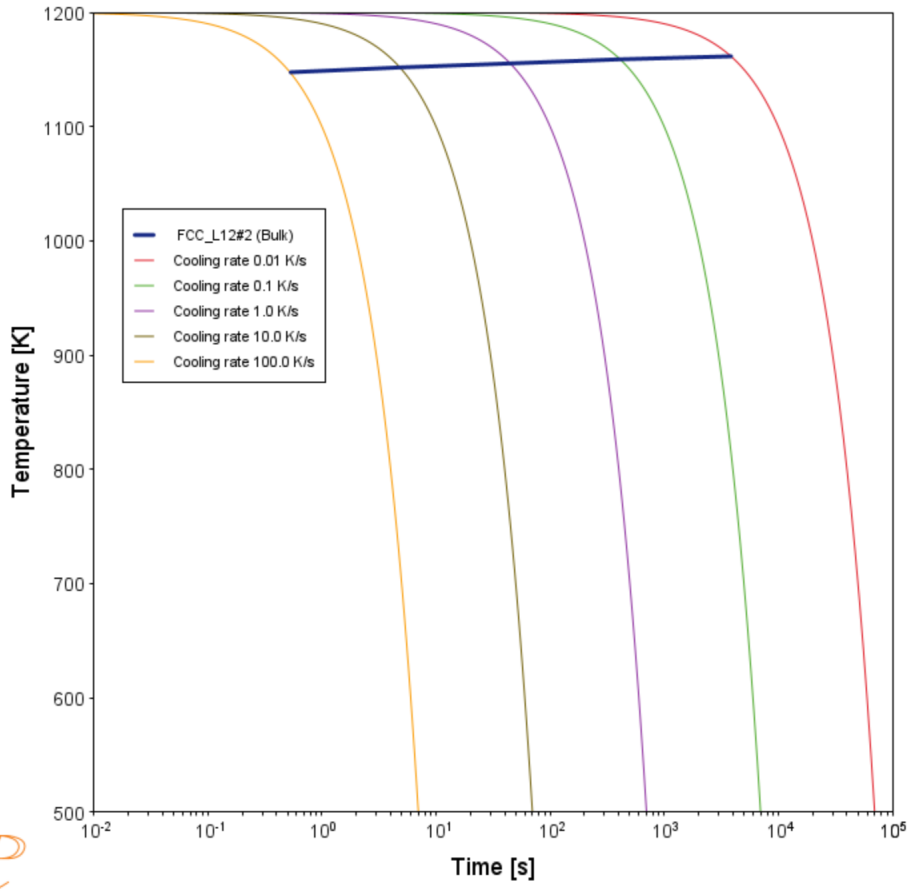


Figure 98: In this plot, the blue line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which we set as 1e-4 volume fraction. The cooling rates are represented by the multi-coloured curved lines.

Results

Plot Renderer 1 | Table Renderer 1

Temperature [K]	FCC_L12#2 (Bulk)
1147.52034	0.53291
1151.74192	4.83553
1155.24636	44.76534
1158.85368	411.49173
1161.48750	3851.47779

Figure 99: An example of the table shown in the Results window, which shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4.

Project File, Step-By Step Instructions and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_07_Precipitation_Ni-Al-Cr_CCT_Gamma-Gamma_prime.tcu*

This example is available as a video tutorial on our website and YouTube channel.

You can also use the step-by-step instructions included in a PDF to follow the video or compare to the project file in Thermo-Calc.

Example Settings

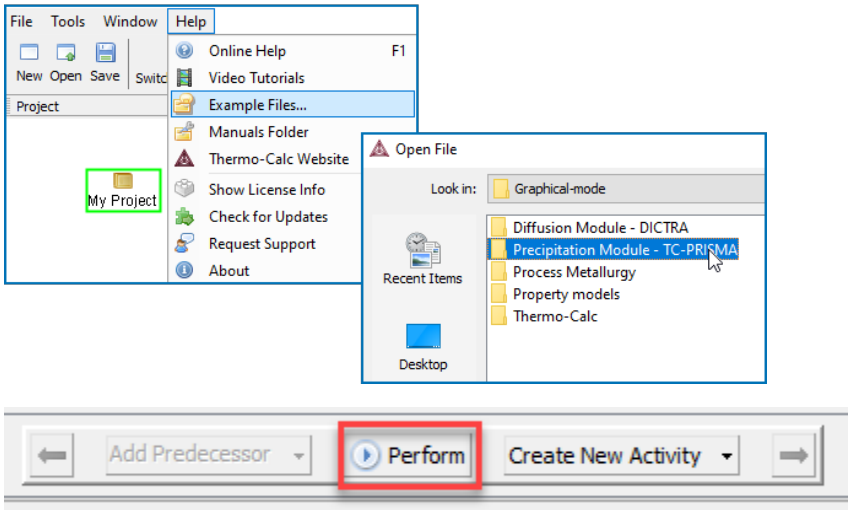
System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1

Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.023 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	CCT Diagram
Temperature Min to Max	500 to 1200 Kelvin
Cooling rate(s)	.01 .1 1 10 100 K/s
Stop criteria	Volume fraction of phase 1.0E-4

Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ': Precipitation Example P_07

HELPFUL INFORMATION

- **All users can run this calculation**, even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ
- This calculation is based on Precipitation Module example *P_07 – Precipitation NI-Al-Cr_CCT_Gamma-Gamma_prime*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.



ABOUT THE EXAMPLE

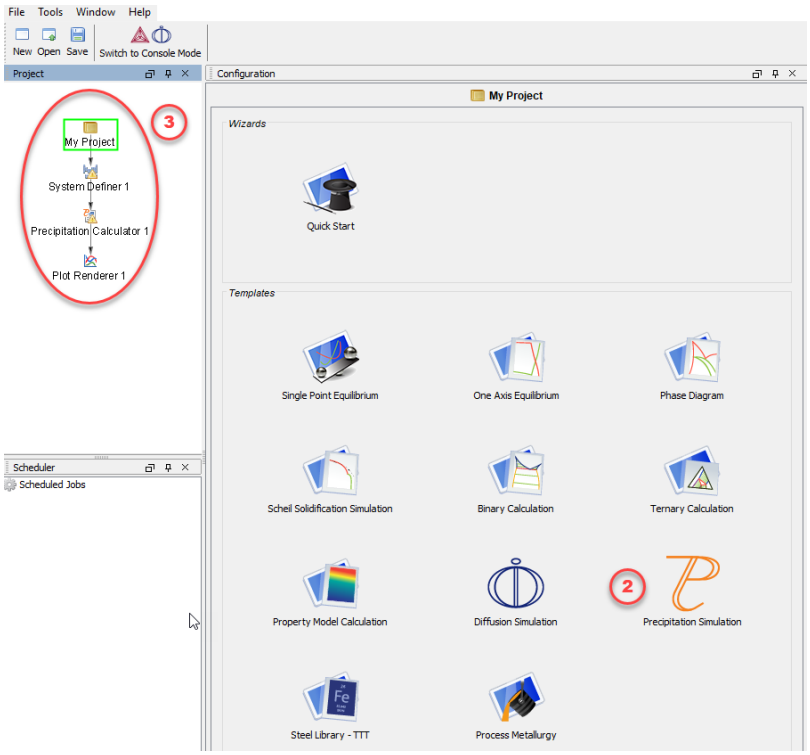
This example shows you how to simulate a CCT diagram for gamma prime (γ') precipitation in a Ni-Cr-Al alloy using the Precipitation Module known as TC-PRISMA.

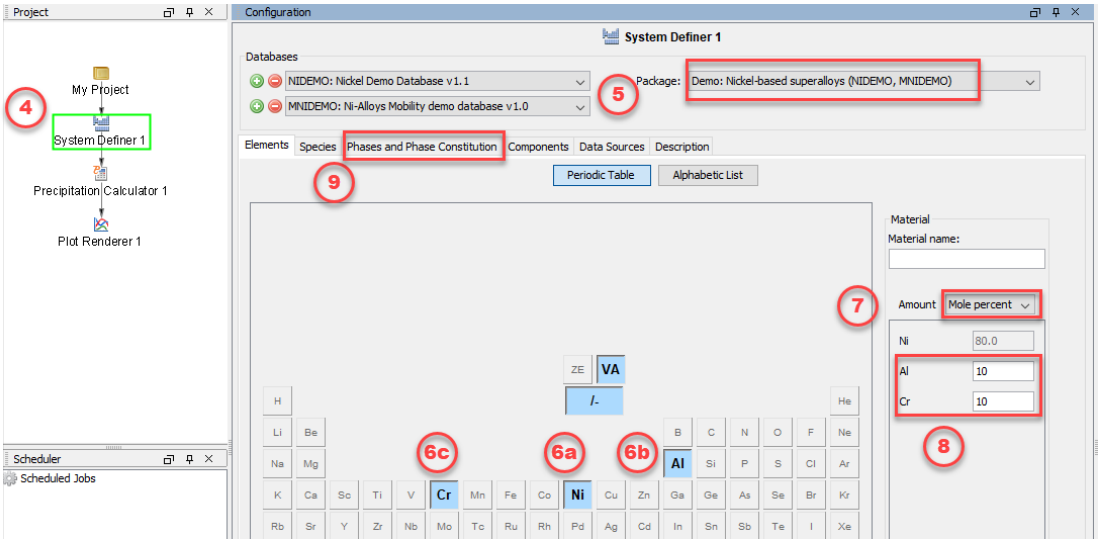
CCT stands for Continuous Cooling Transformation and is a calculation that maintains the same cooling rate the entire time.

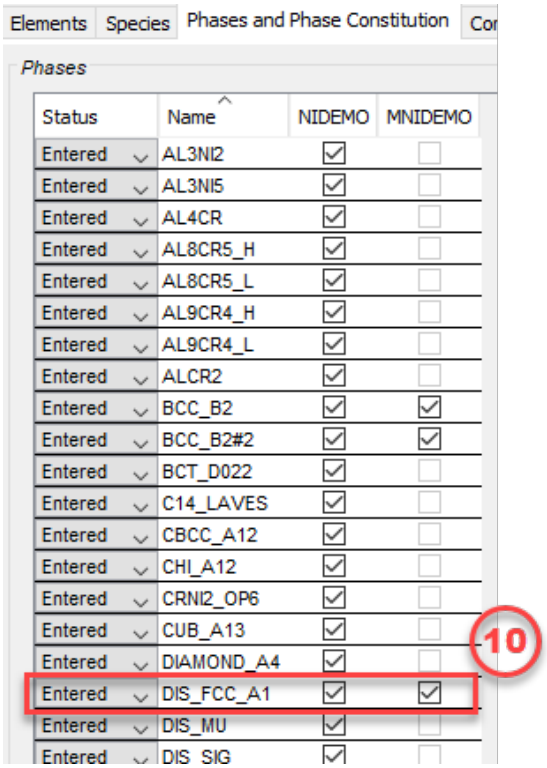
The system is a Ni-10Al-10Cr γ - γ' alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation Module (TC-PRISMA).

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under *Templates*, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



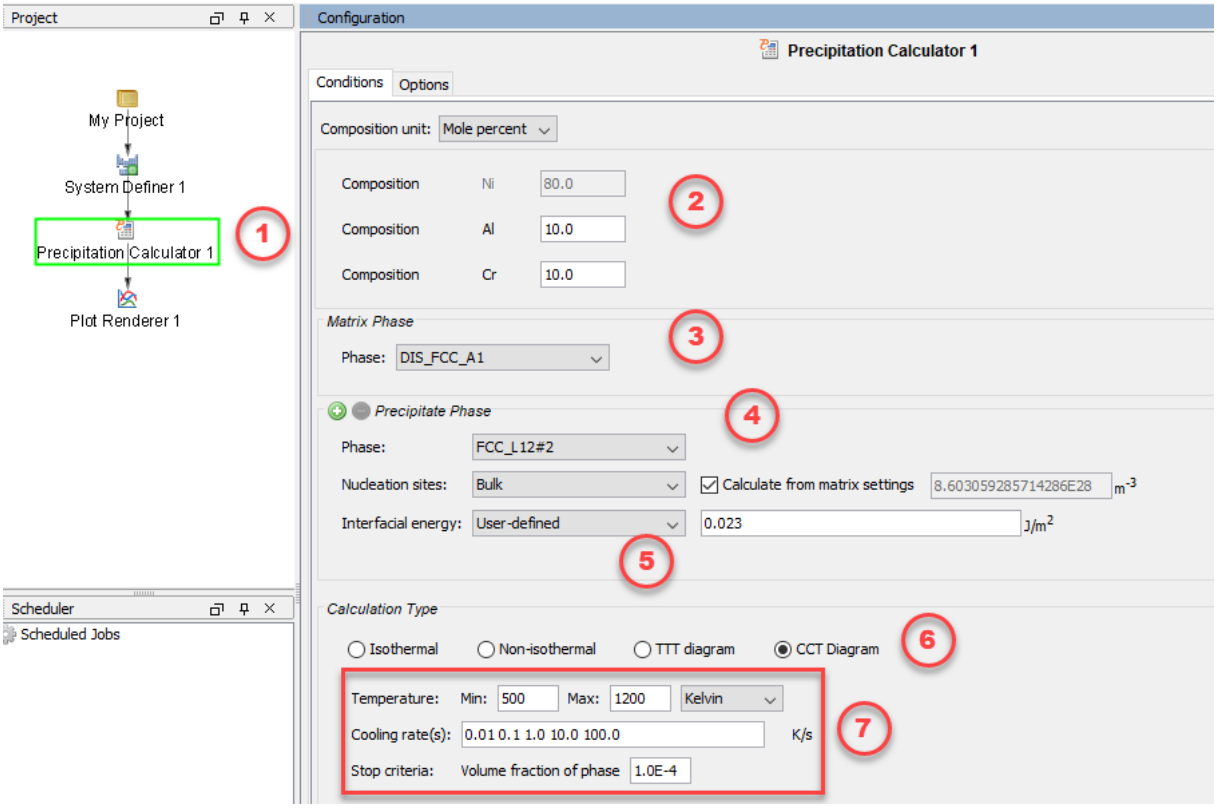
4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Nickel-based alloys (NIDEMO, MNIDEMO)**, which loads both thermodynamic and kinetic demonstration nickel databases.
6. From the **Periodic Table**, select the elements as follows. Select Ni first so that it is the dependant element.
    a. **Ni** (nickel)
    b. **Al** (aluminium) then
    c. **Cr** (chromium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter `10` for **Al** and `10` for **Cr**, which automatically sets **Ni** to 80 mole percent.
9. Click the **Phases and Phase Constitution** tab.
10. Click to select both check boxes next to the disordered FCC phase, **DIS_FCC_A1**.
11. 



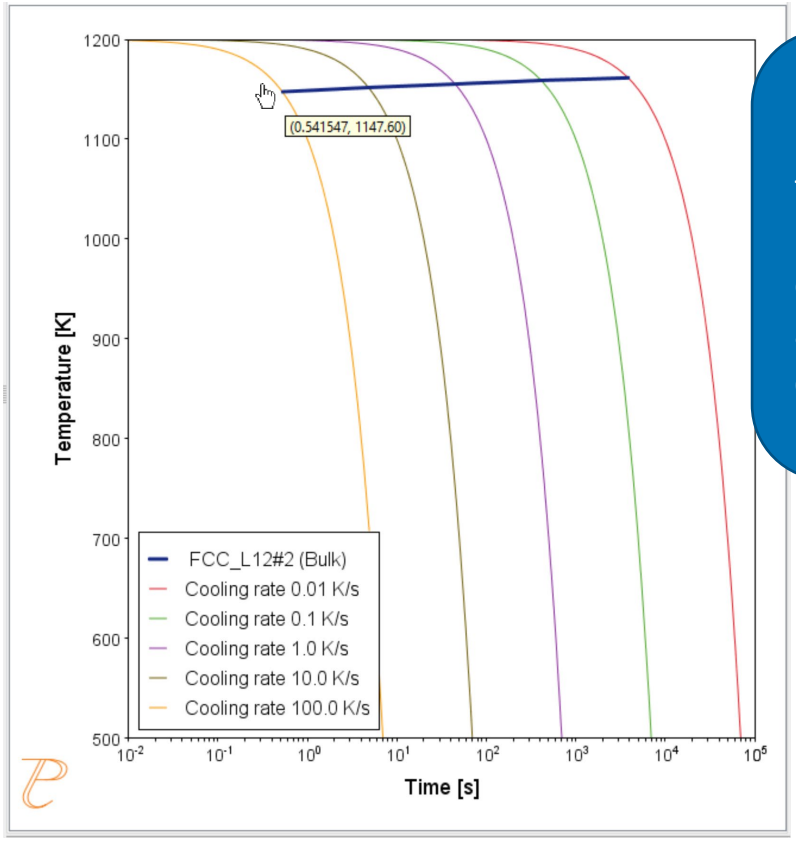
The system is now defined. Now set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATION

1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the composition set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, from the *Phase* list select **Dis_FCC_A1**, which is the disordered FCC phase.
4. Under *Precipitate Phase* from the *Phase* list select **FCC_L12#2**.
5. Change the *Interfacial energy* to **User-defined** then enter `0.023` in the field.
6. Under *Calculation Type*, click **CCT Diagram**, which stands for Continuous-Cooling-Transformation and means that the same cooling rate is maintained throughout the calculation.
7. In the fields set:
    a. *Min* (minimum) *Temperature* to `500`.
    b. *Max* (maximum) *Temperature* to `1200`.
    c. Choose **Kelvin** as the temperature unit.
    d. Enter several cooling rates for the calculation. The rates are separated by a space. Enter these values as shown: `.01 .1 1 10 100`.
    e. Keep the default **Stop criteria** of `1E-4` volume fraction of the γ' phase.
8. The calculation is now set. Click **Perform CCT Diagram Simulation** at the bottom, center of the **Configuration** window.



INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATION



In this plot, the blue, horizontal line shows the time it takes for gamma prime to transform at each of the cooling rates according to the stop criteria, which we set as 1e-4 volume fraction.

In this plot, the blue line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which is set as 1e-4 volume fraction. The cooling rates are represented by the multi-coloured curved lines.

If you hover your mouse over the intersection of the blue line and any of the vertical lines, a yellow box shows the approximate time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4, followed by the approximate temperature. In the image above, you can see a time of 0.54147 seconds and a temperature of 1147.60 Kelvin for the cooling rate of 100.0 K/s, which is represented by the yellow line.

SHOWING THE RESULTS AS A TABLE

You can also view these results in the form of a table, which gives you more precise results.

1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Create New Successor>Table Renderer**.
2. Right-click the **Table Renderer 1** node and select **Perform Now**.

Time [s]	FCC_L12#2 (Bulk)
0.53291	1147.52034
4.83553	1151.74192
44.76534	1155.24636
411.49174	1158.85368
3851.40881	1161.48822

The table is shown in the **Results** window and shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4.

P_08: Precipitation of Cu-Ti CU4TI with Assumptions of Sphere and Needle Morphologies

In this isothermal calculation example, the precipitation of Cu4Ti phase in a Cu-Ti binary alloy is calculated. To make a comparison, two separate simulations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming needle morphology whose shape, determined by competition between interfacial energy and elastic strain energy, is changed during the simulation. The transformation strain is obtained from Borchers [1999]. The results are compared with experiment results from Kampmann et al. [1987].

This example takes a few minutes to run.

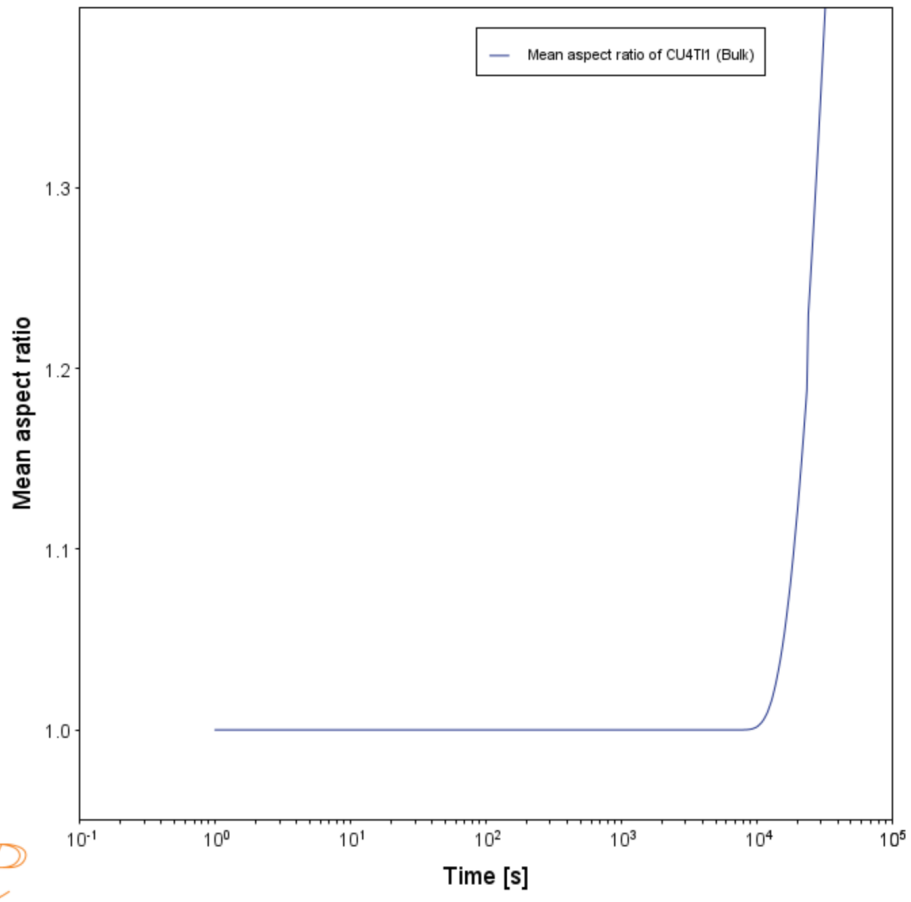


Figure 100: Mean Aspect Ratio.

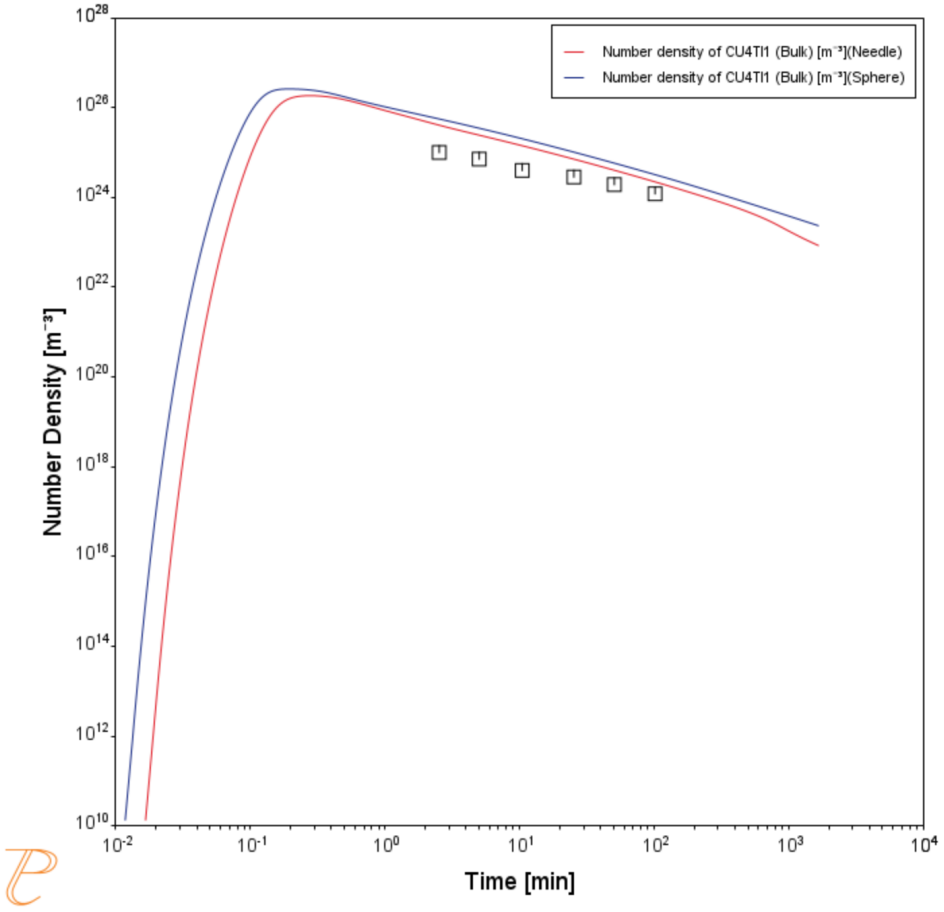


Figure 101: Number Density.

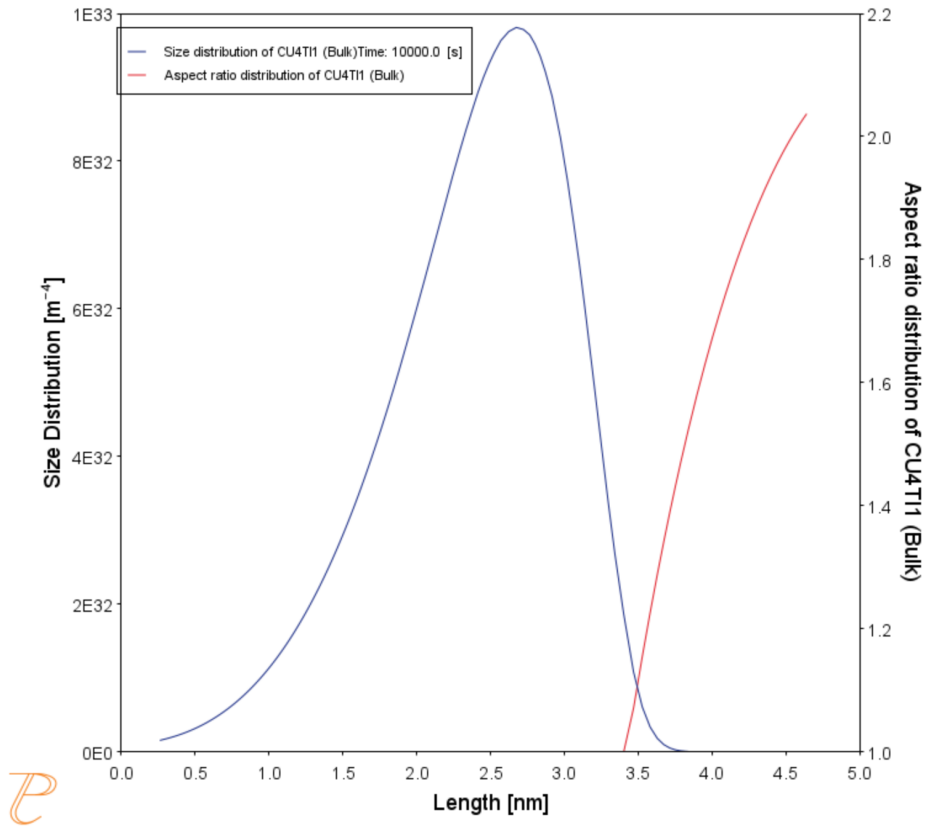


Figure 102: PSD and ASD.

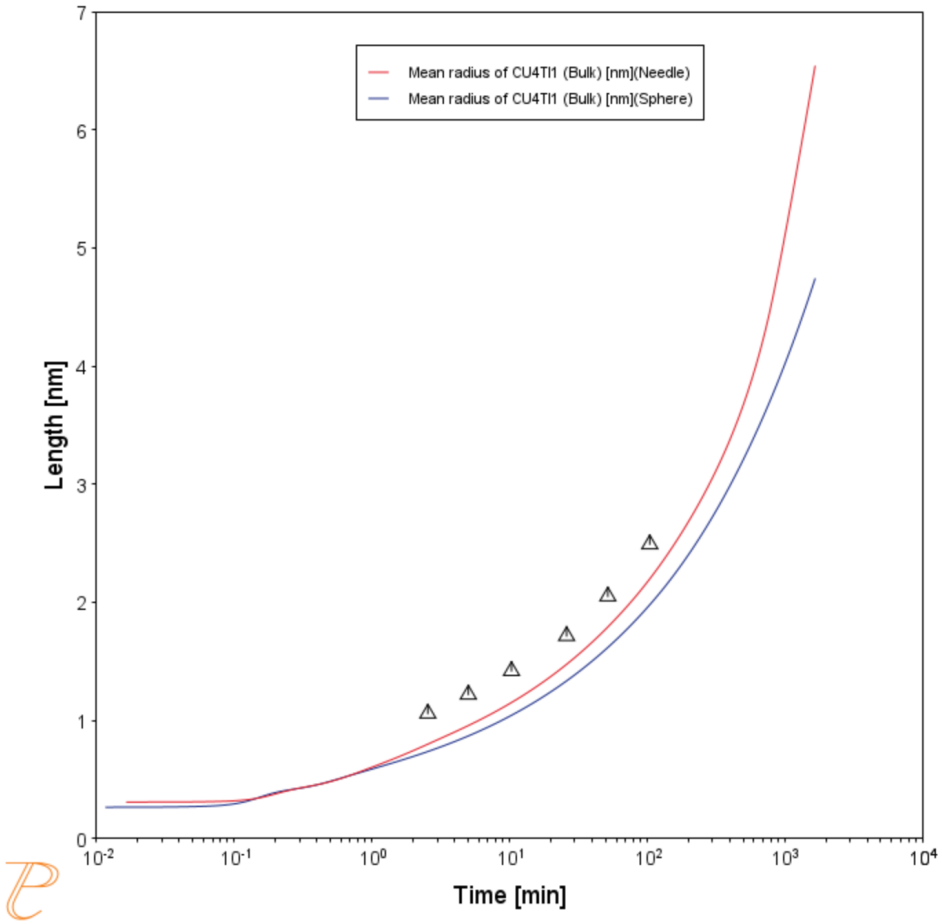


Figure 103: Mean Radius.

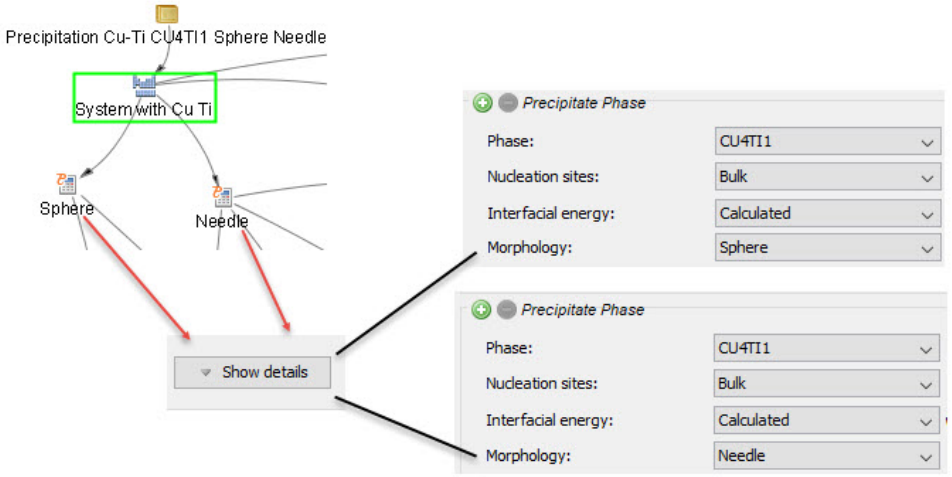
Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_08_Precipitation_Cu-Ti_CU4TI1_Sphere_Needle.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Needle** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**.



System (System Definer)	
Database package	Demo: Copper-based alloys (CUDEMO and MCUDEMO)
Elements	Cu, Ti
Sphere and Needle Conditions (Precipitation Calculator)	
Composition	Cu-1.9Ti Mole percent
Matrix phase	FCC_L12

Precipitate phase	CU4TI1
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility enhancement prefactor (click **Show details** to display this setting)	100
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Needle** node (renamed from Precipitation Calculator), **Needle** is selected.
Transformation strain (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Needle**node (renamed from Precipitation Calculator), **User defined** is selected. In this example, the following settings are defined: • ε11 and ε22 are set to **0.022** • ε33 is set to **0.003**
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	10,000 seconds
Datasets (Experimental File Reader)	
Borchers Mean radius vs Time and Borchers Number density vs Time	Data sets included with this example and imported to two Experimental File Readers. These data sets are used for the Mean Radius and Number Density plots, respectively.

References

[1987, Kampmann] R. Kampmann, H. Eckerlebe, R. Wagner, 1987. "Precipitation Kinetics in Metastab le Solid Solutions - Theoretical Considerations and Application to Cu-Ti Alloys." Mat. Res. Soc. Symp. Proc. 57: 525-542.

[1999, Borchers] C. Borchers, Catastrophic nucleation during decomposition of Cu-0.9at.% Ti. Philos. Mag. A. 79, 537–547 (1999).

P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies

In this isothermal calculation example, the precipitation of Al_3Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy is simulated. To make a comparison, two separate calculations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The simulation results are compared with experimental data collected from Marquis and Seidman [2001] and Novotny and Ardell [2001]. In addition, mean cubic factor and cubic factor distribution are also plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

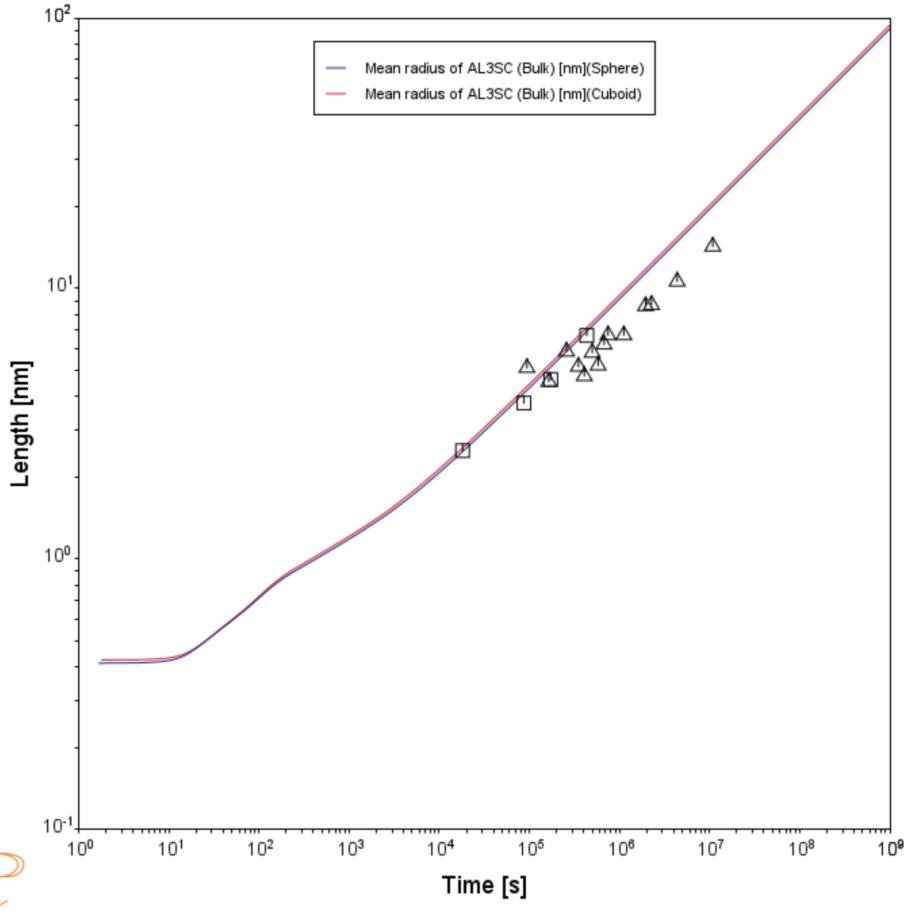


Figure 104: Mean Radius

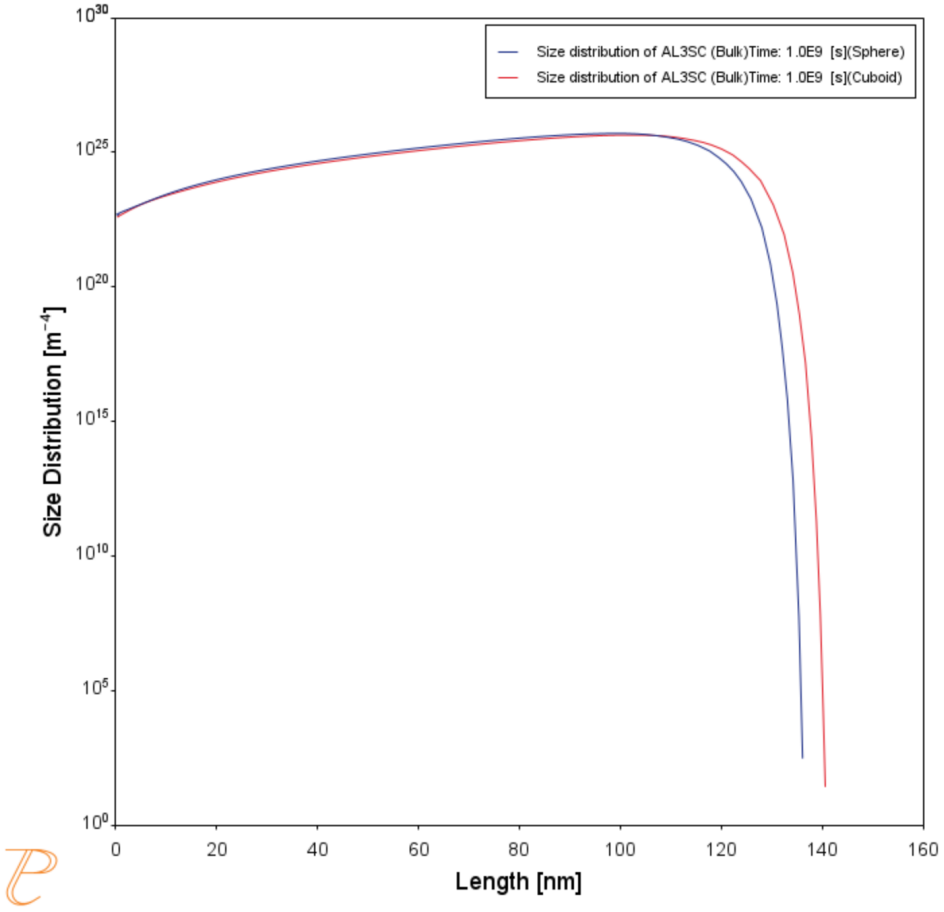


Figure 105: Particle size distribution (PSD).

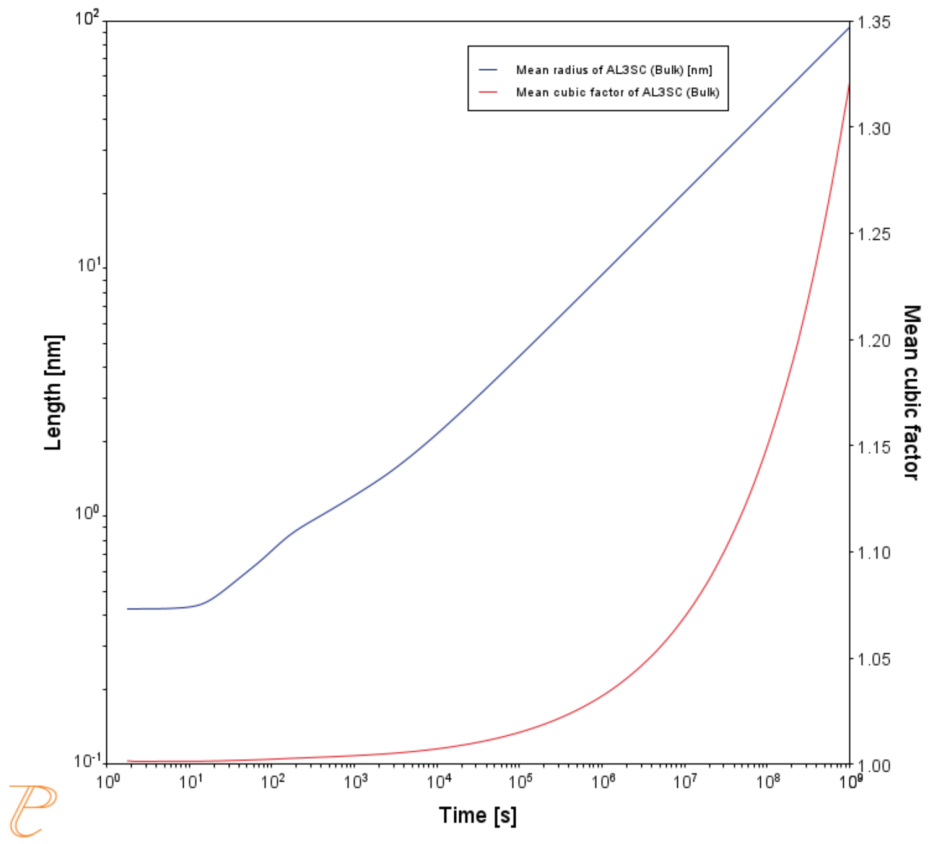


Figure 106: Mean Radius and Cubic Factor

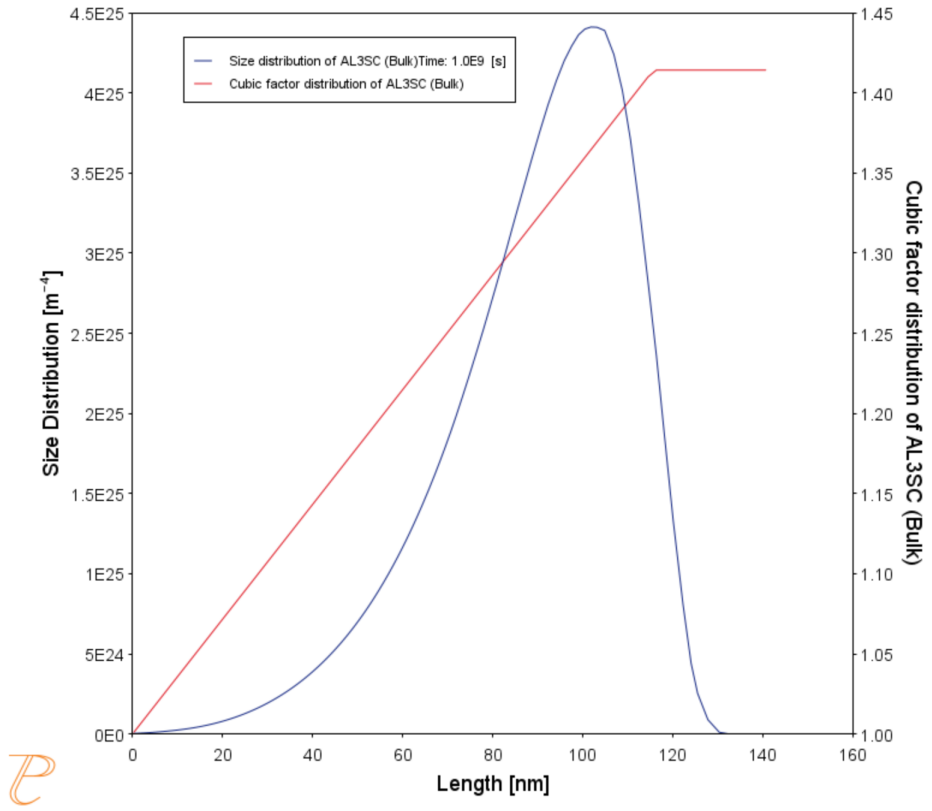


Figure 107: Particle size distribution (PSD) and cubic factor.

Project File, Step-By Step Instructions and Video tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_09_Precipitation_Al-Sc_AL3SC_Sphere_Cuboid.tcu*

This example is available as a video tutorial on our website and YouTube channel.

You can also use the step-by-step instructions included in a PDF to follow the video or compare to the project file in Thermo-Calc.

Example Settings

To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Cuboid** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**. See P_08 for an example of this.

System (System Definer)	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Sphere and Cuboid Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent
Matrix phase	FCC_A1
Precipitate phase	AL3SC
Matrix Phase Data Parameters (Precipitation Calculator)	
Elastic properties (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), the default, **Disregard** is kept. For the **Cuboid** node (renamed from Precipitation Calculator), choose **Cubic**. Then enter the elastic constants accordingly. Default elastic constants are given based on the major element of the alloy system. In this example that is • c11 is **108.2** GPa • c12 is **61.3** GPa

	• c44 is **28.5** GPa
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Cuboid** node (renamed from Precipitation Calculator), **Cuboid** is selected.
Transformation strain (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Cuboid** node (renamed from Precipitation Calculator), **Calculate from molar volume** is selected to obtain a purely dilatational strain.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	1.0E9 seconds
Datasets (Experimental File Reader)	
Dataset 1 and Dataset 2	Data sets included with this example and imported to one Experimental File Reader. It is used for the Mean Radius plot.

References

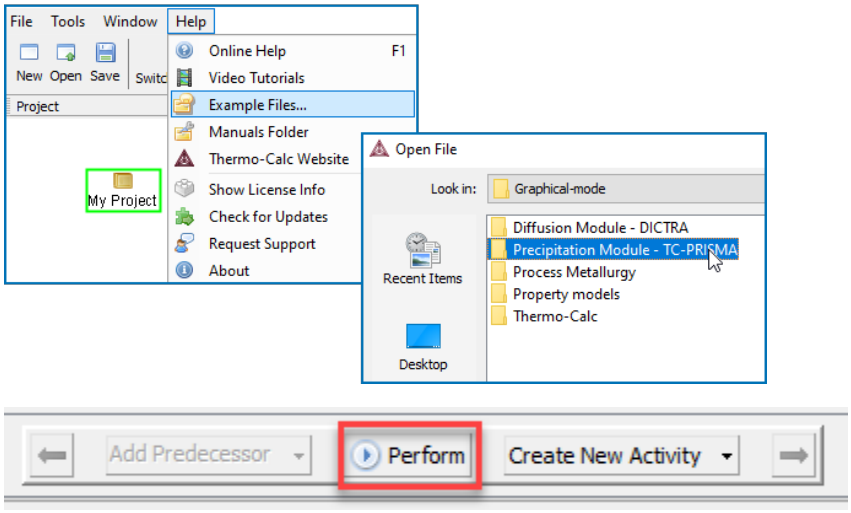
[2001, Marquis] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

[2001, Novotny] G. M. Novotny, A. J. Ardell, Precipitation of Al3Sc in binary Al–Sc alloys. Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318, 144–154 (2001).

Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies: Precipitation Example P_09

HELPFUL INFORMATION

- **All users can run this calculation**, even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ
- This calculation is based on Precipitation Module example *P_09 – Precipitation_Al-Sc_AL3SC_Sphere_Cuboid*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.



ABOUT THE EXAMPLE

This example shows you how to calculate the precipitation of Al_3Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy using the Precipitation Module (TC-PRISMA).

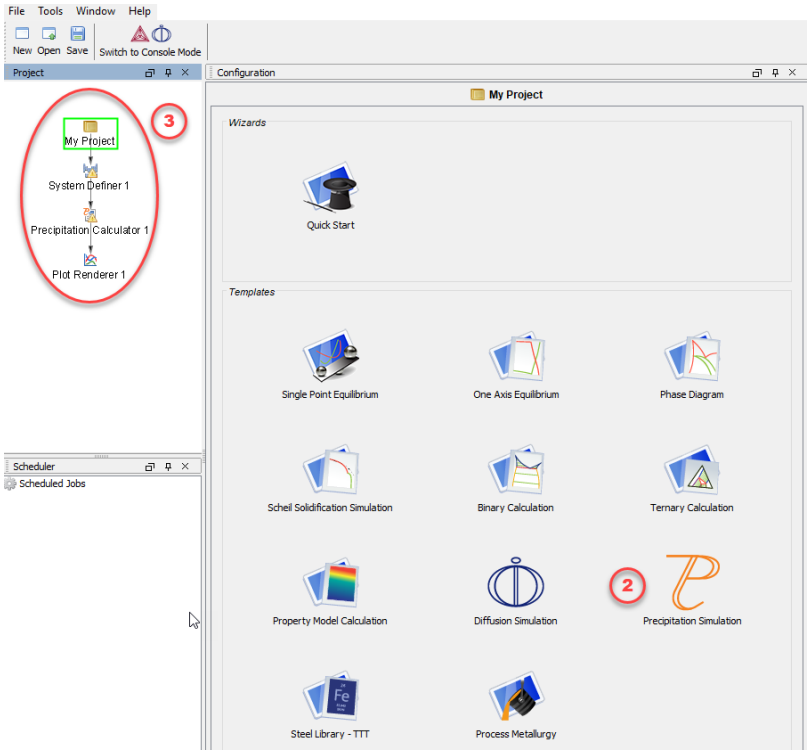
Two separate calculations are performed so you can make a comparison of the results, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy.

In addition, mean cubic factor and cubic factor distribution are plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

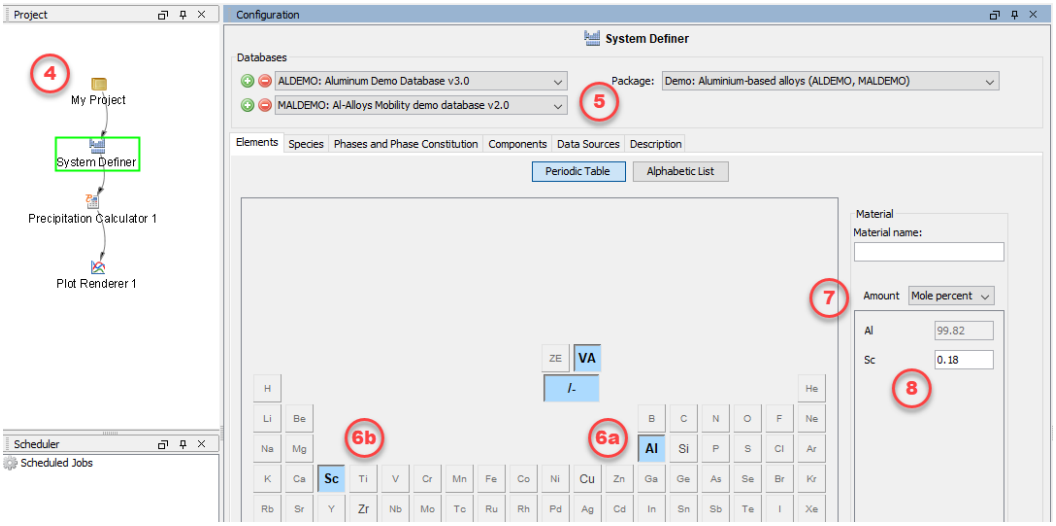
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under *Templates*, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Aluminium-based alloys (ALDEMO, MALDEMO)**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the **Periodic Table**, select the elements as follows. Select Al first so that it is the dependant element:
    a. **Al** (aluminium)
    b. **Sc** (scandium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter `0.18` for **Sc**. This automatically sets **Al** to 99.82.



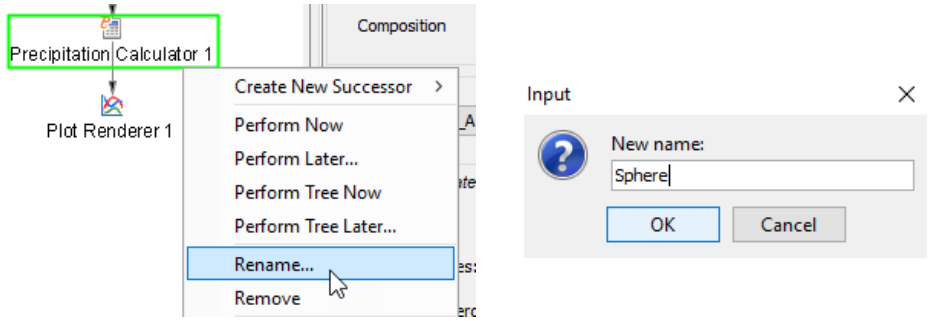
Our system is now defined. Now set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATIONS

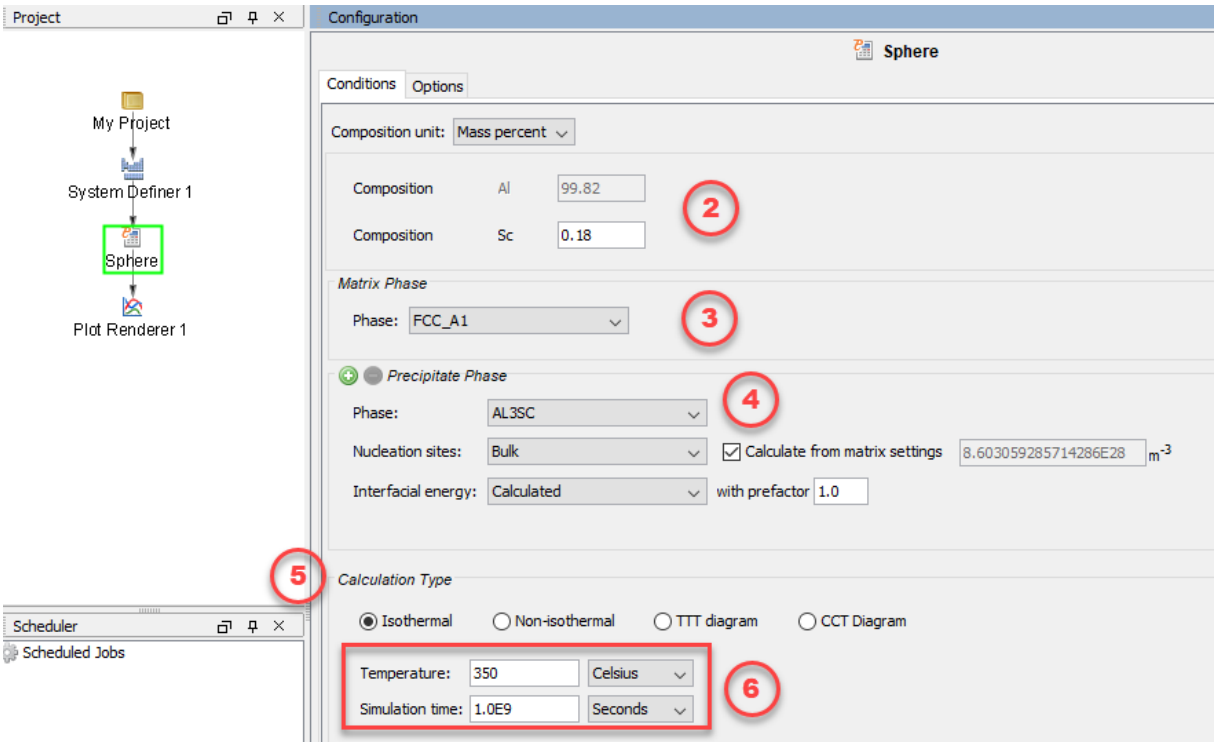
There are two precipitation calculations in this example, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The results are then compared for both calculations.

Setting up the Precipitation Calculation with Spherical Morphology

1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Rename.** Enter `Sphere`, then press Enter or click **OK**.



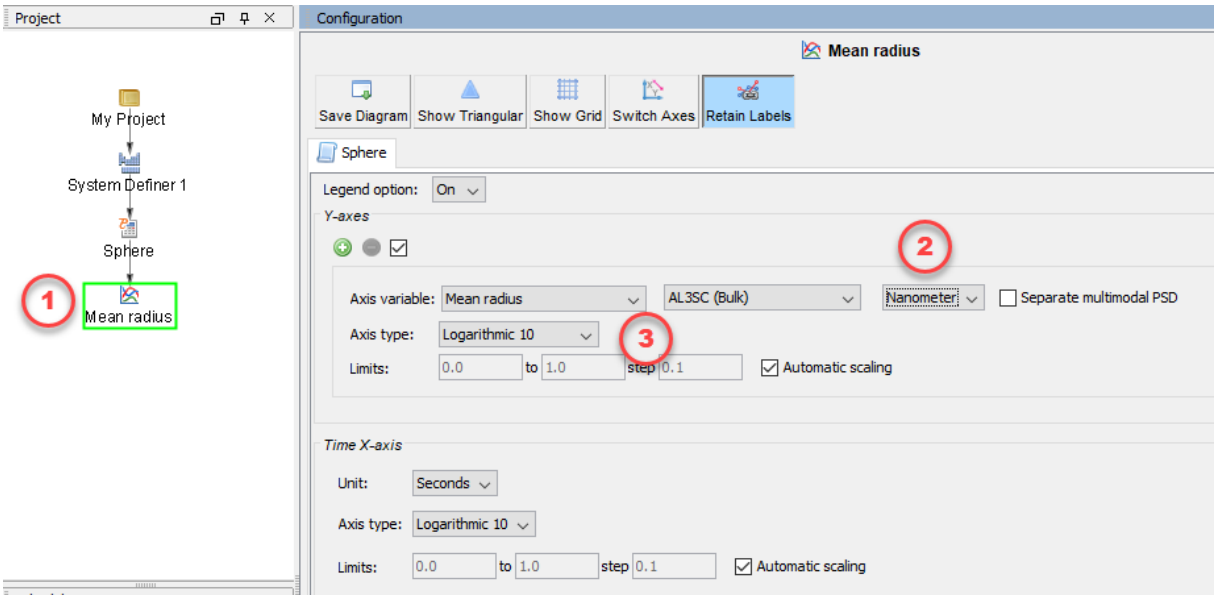
2. Notice that the composition set in the *System Definer* auto-populated on the Precipitation Calculator.
3. Under *Matrix Phase* from the *Phase* list it defaults to **FCC_A1**.
4. Under *Precipitate Phase* from the *Phase* list select **AL3SC**.
5. Under *Calculation Type*, make sure **Isothermal** is selected, which means that the same temperature is maintained throughout the calculation.
6. Enter
    a. `350` as the *Temperature* and select **Celsius**.
    b. `1.0E9` as the *Simulation time* and select **Seconds**.



Our first calculation is set, so next configure the plot.

Configuring the Plot

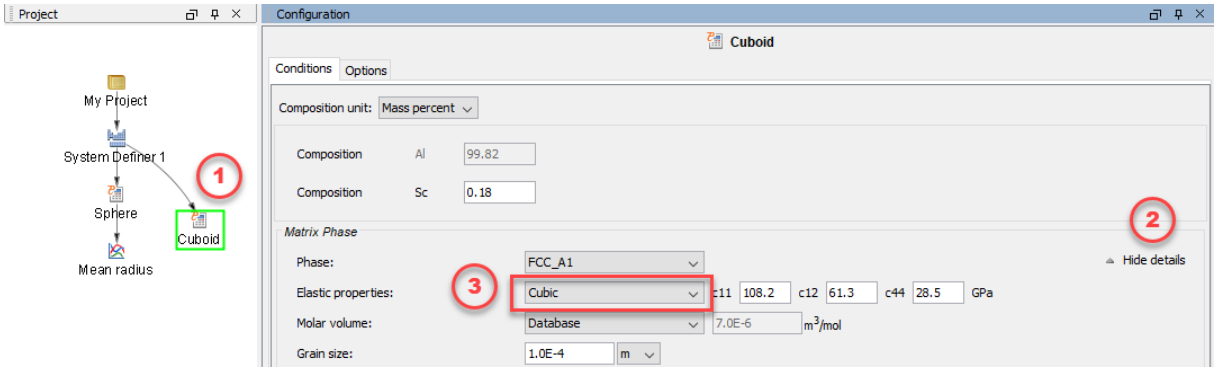
1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot `Mean radius` then press Enter or click **OK**.
2. Under *Y-axes* change the units to **Nanometer** (nm).
3. From the *Axis type* list select **Logarithmic 10**.



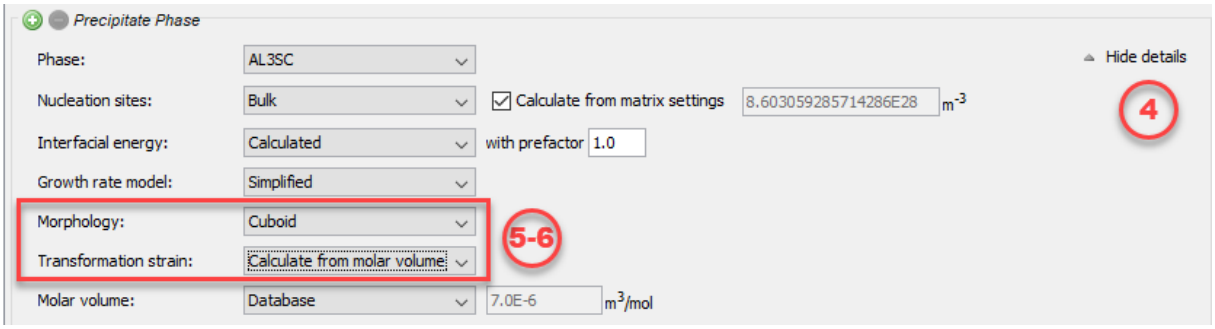
The plot is now set, but before running the simulation you set up another calculation and link it to the same Plot Renderer.

Setting up the Precipitation Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Sphere** node and select **Clone**.
   a. Right-click the **Sphere 1** node and select **Rename**.
   b. Name the node `Cuboid` and press Enter or click **OK**.
2. On the **Configuration** window to the right of *Matrix Phase* click **Show Details**.
3. From the *Elastic Properties* list select **Cubic**. Keep the suggested default values. Click **Hide details**.



4. To the right of *Precipitate Phase*, click **Show details**.
5. From the *Morphology* list select **Cuboid**.
6. From the *Transformation strain* list select **Calculate from molar volume**.

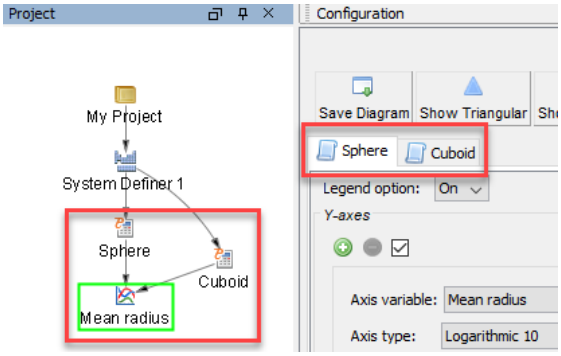


The second calculation is now set up, so now link it to the Plot Renderer node.

Linking the Plot to the Calculation with Cuboid Morphology

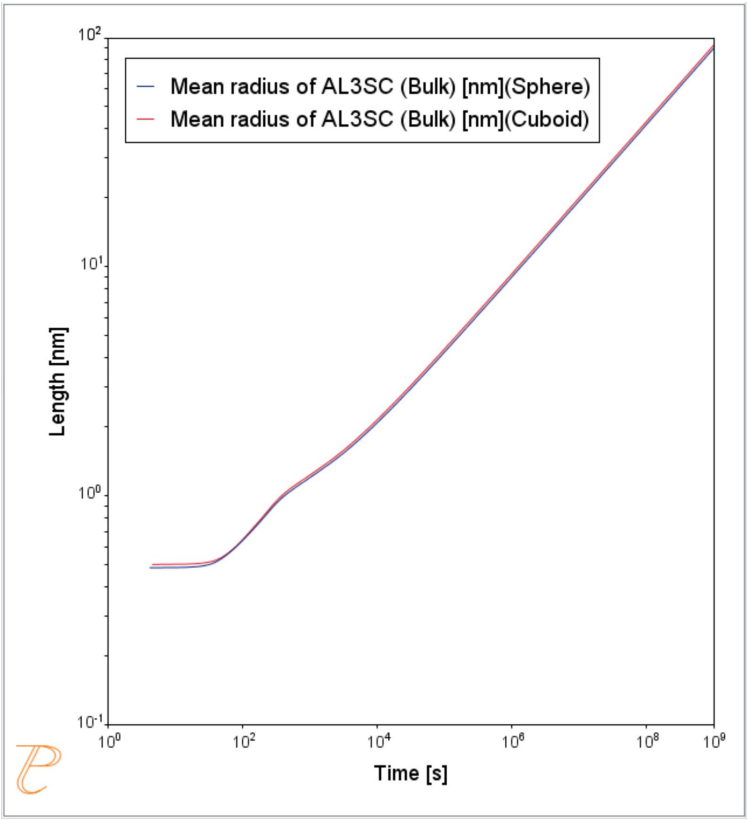
1. In the **Project** window, right-click the **Mean radius** node and select **Add Predecessor >Cuboid**.
2. Notice that in the **Configuration** window there are two tabs associated with this plot, one for **Sphere** and one for **Cuboid**. The Sphere settings are already configured, so you just need to

set up the Cuboid tab.



3. Click the **Cuboid** tab.
4. Under *Y-axes* change the units to **Nanometer** (nm).
5. From the *Axis type* list select **Logarithmic 10**.
6. The calculation is now ready to run. Right-click the **Mean radius** node and select **Perform Now** or click **Perform** on the **Configuration** window.

INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATIONS



In this plot, the blue line represents the sphere calculation and the red line represents the cuboid calculation. You can see that, in this instance, they are almost identical.

In this plot, the blue line represents the sphere calculation and the red line represents the cuboid calculation. You can see that, in this instance, these are almost identical.

By ‘radius for non-spherical particles’ it means the radius of equivalent spheres with the same volume.

If you run the example file that is included in your software, the plot also contains an experimental file, which you can see closely matches the calculations.

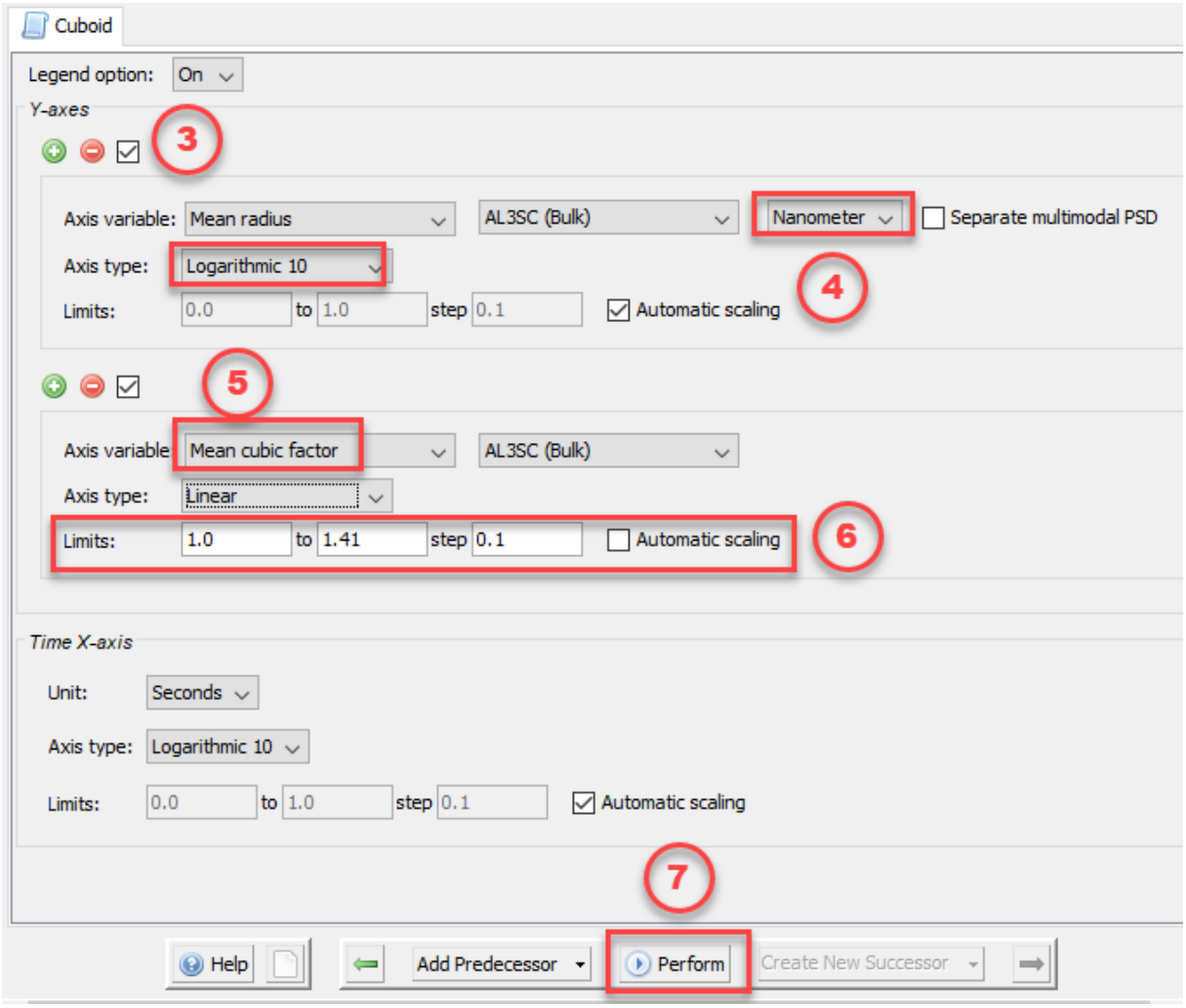
PLOTTING ADDITIONAL VARIABLES

Now you use the same calculation to set up additional plots using the many available variables. The examples below include two Y-axes each.

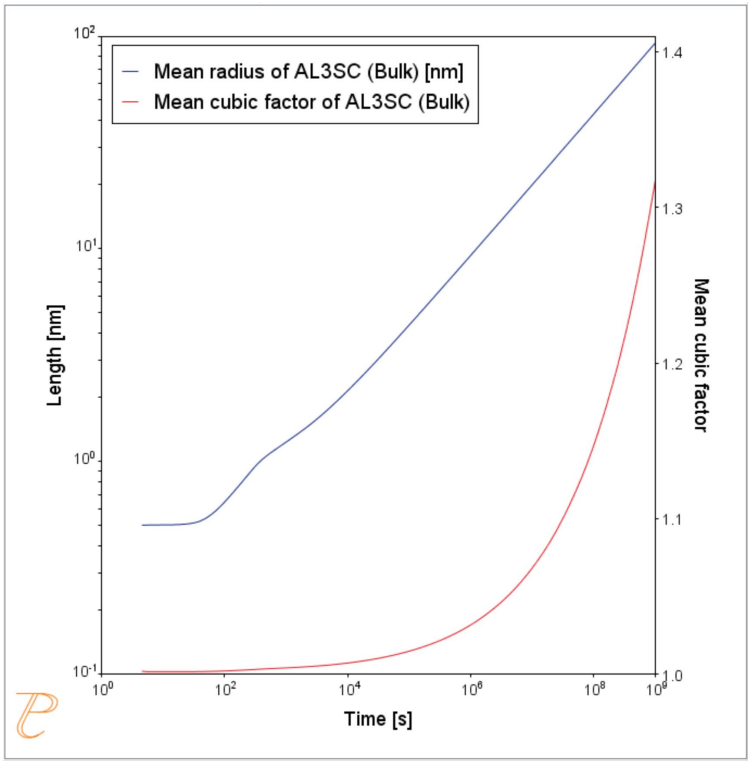
Plotting Mean Radius and Cuboid Factor

This plot has two Y-axes: *Mean radius* and *Cuboid factor*.

1. Right-click the **Cuboid** node and add a **Plot Renderer**.
2. Right-click the new node and rename it `Mean radius and Cuboid factor`.
3. Under *Y-axes* click the green plus sign to add another axis.
4. Keep *Mean radius* as the first axis variablebut change the units to **Nanometers** (nm) and set the axis type to **Logarithmic 10**.
5. Set the second *Axis variable* to **Mean cubic factor**.
6. Click to clear the *Automatic scaling* check box. In the fields, enter the *Limits* from `1` to `1.41` and the *step* to `0.1`.
7. The plot is now set. Click **Perform**.



Interpreting the Results of Mean Radius and Cuboid Factor



In this plot, the blue line represents the evolution of the average radius of the cubic particles as a function of time. The red line shows the average cubic factor as a function of time.

The blue line represents the evolution of the average radius of the cubic particles as a function of time. Again, for non-spherical precipitates this means the radius of equivalent spheres with the same volume.

The red line shows the average cubic factor as a function of time. A value of one represents a spherical shape. A square root of two represents a cubic shape.

The evolution of the shape when the particles grows is determined by competition between interfacial energy and elastic strain energy. In general, the shape is close to spherical at small particle sizes because the interfacial energy term dominates.

At large sizes the elastic energy dominates and it is therefore more favourable with a non-spherical shape. You can see that the particles get a more cubic form at later times when they grow to larger sizes.

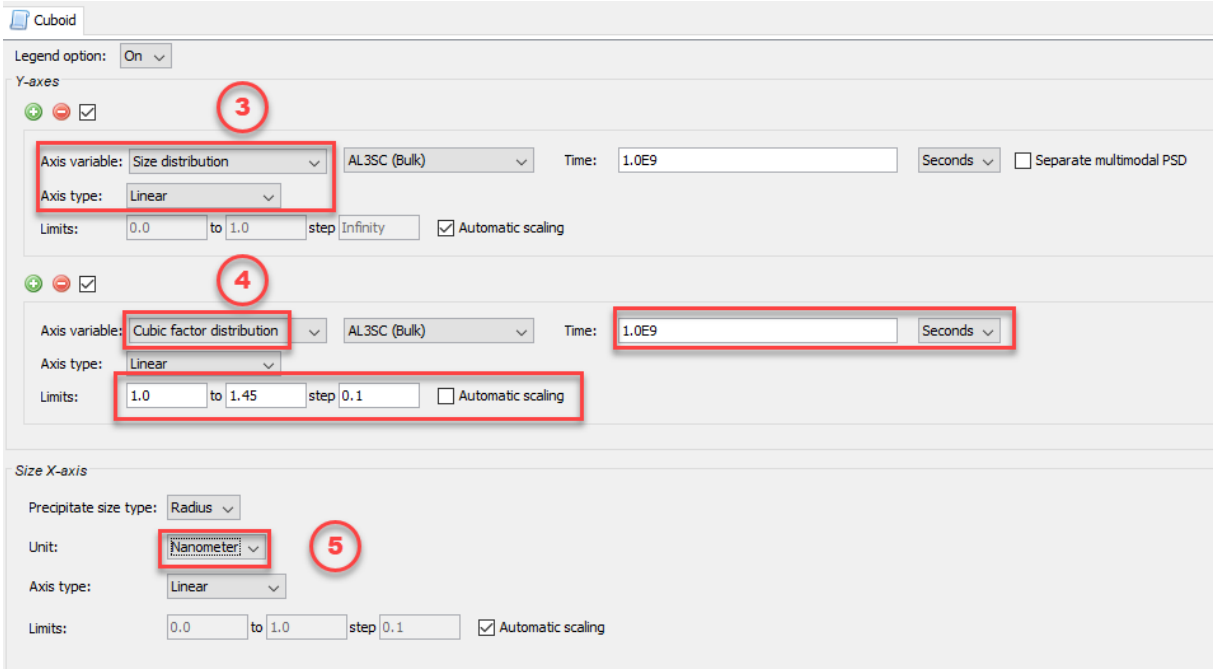
Plotting Particle Size and Cubic Factor Distribution

This final plot shows the particle size distribution (PSD) and cubic factor distribution at the end of the simulation.

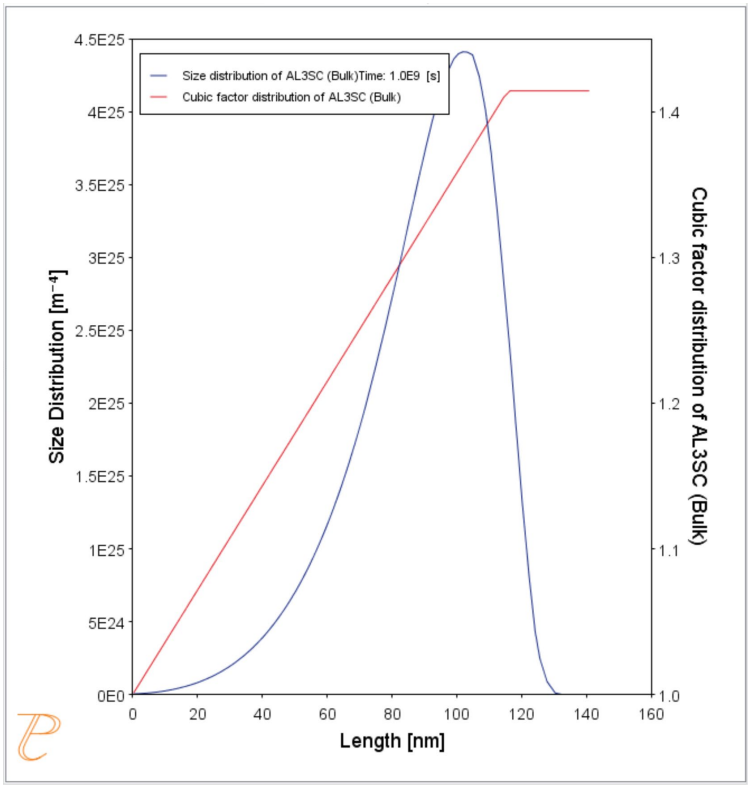
This plot also has two Y-axes, so you can clone the previous plot.

1. Right-click the **Mean radius and Cuboid factor** node and select **Clone**.
2. Right-click the new node and rename it `PSD and Cuboid factor`.
3. Under the *Y-axes*
    a. Select **Size distribution** as the first *Axis variable*.
    b. Change the *Axis type* to **Linear**.
4. Set the second Y-axis to **Cubic factor distribution** and enter a *Time* of `1e9` **Seconds**.

5. Keep the *Automatic Scaling* check box cleared. Enter the *Limits* from `1` to `1.45` and the *step* to `0.1`.
6. Under *Size X-axis*, change the unit to **Nanometer** (nm).
7. Click **Perform** at the bottom center of the **Configuration** window.



Interpreting the Results of Particle Size Distribution and Cuboid Factor



In this plot, the blue curve shows the particle size distribution and the red line shows the cubic factor distribution.

The blue curve, which shows the particle size distribution, is close to the regular LSW size distribution that is expected for spherical particles.

The cubic factor distribution shows that the smallest particles are closer to spherical and that the larger ones get more and more cubic.

References

1. Marquis, E.A, and D.N Seidman. 2001. “Nanoscale Structural Evolution of Al3Sc Precipitates in Al(Sc) Alloys.” *Acta Materialia* 49 (11): 1909–19.
2. Novotny, Gabriel M., and Alan J. Ardell. 2001. “Precipitation of Al3Sc in Binary Al–Sc Alloys.” *Materials Science & Engineering, A*: Structural Materials: Properties, Microstructure and Processing 318 (1–2): 144–54.

P_10: Initial Particle Size Distribution of Fe-Cr-C

This example demonstrates the effect of initial particle size distribution of the precipitate phases on the overall precipitation kinetics. It uses two Precipitation Calculators to simulate and compare carbide precipitations from a ferritic BCC_A2 matrix in a Fe-0.1C-12Cr alloy. Three carbides, CEMENTITE, M23C6 and M7C3, are included in the calculations for competitive precipitations, and the precipitation kinetics are compared with or without initial particle size distribution.

The example illustrates the use of the particle size distribution setting. You can import data from a spreadsheet or text file (.xls, .xlsx, .csv or .txt formats are acceptable). The Preexisting Particle Size Distribution window shown below, provides a graphical representation of the radius versus corresponding frequencies.

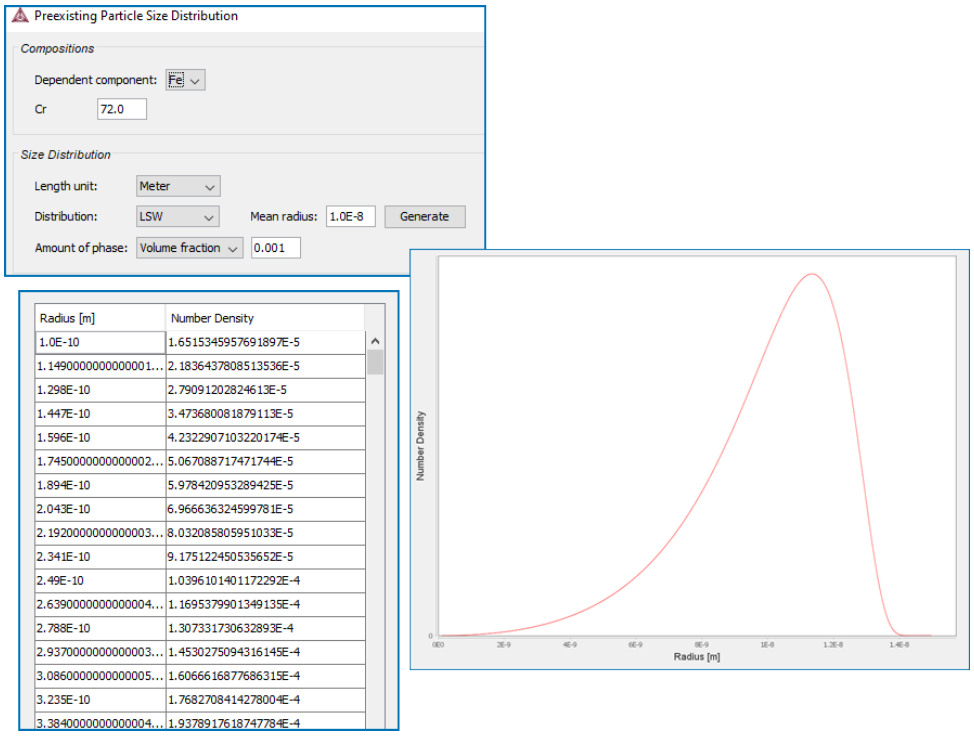


Figure 108: The Preexisting Particle Size Distribution (PSD) settings window for example P_10.

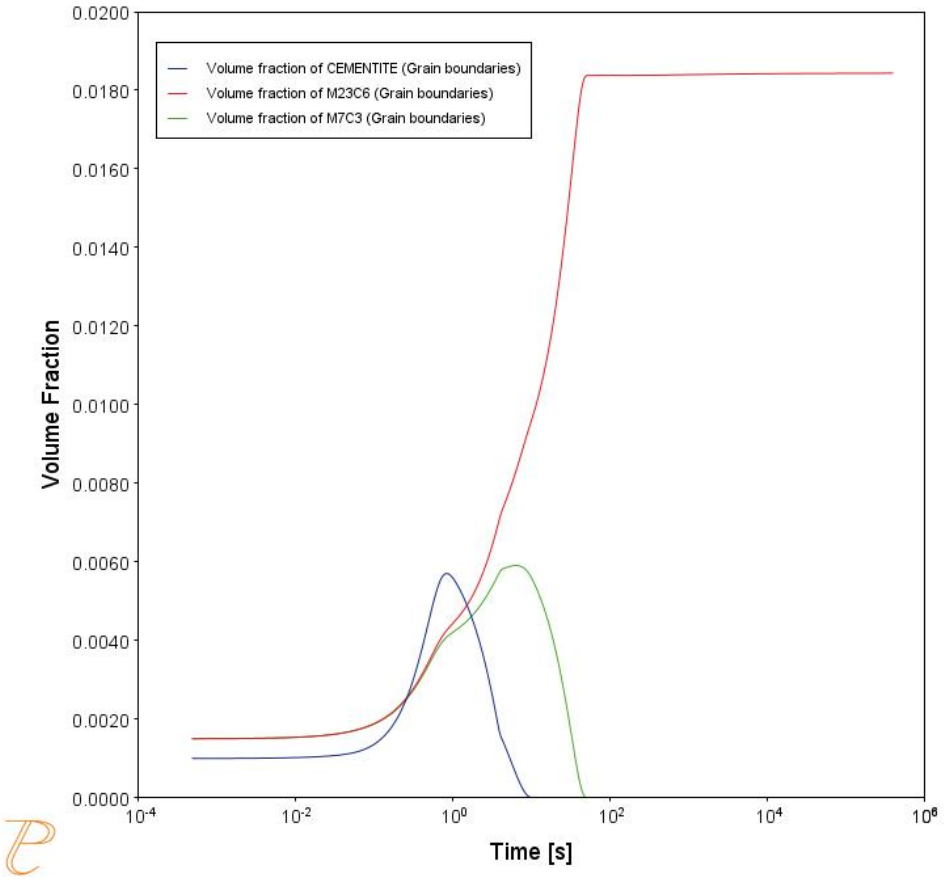


Figure 109: Volume fraction with initial particle size distribution (PSD).

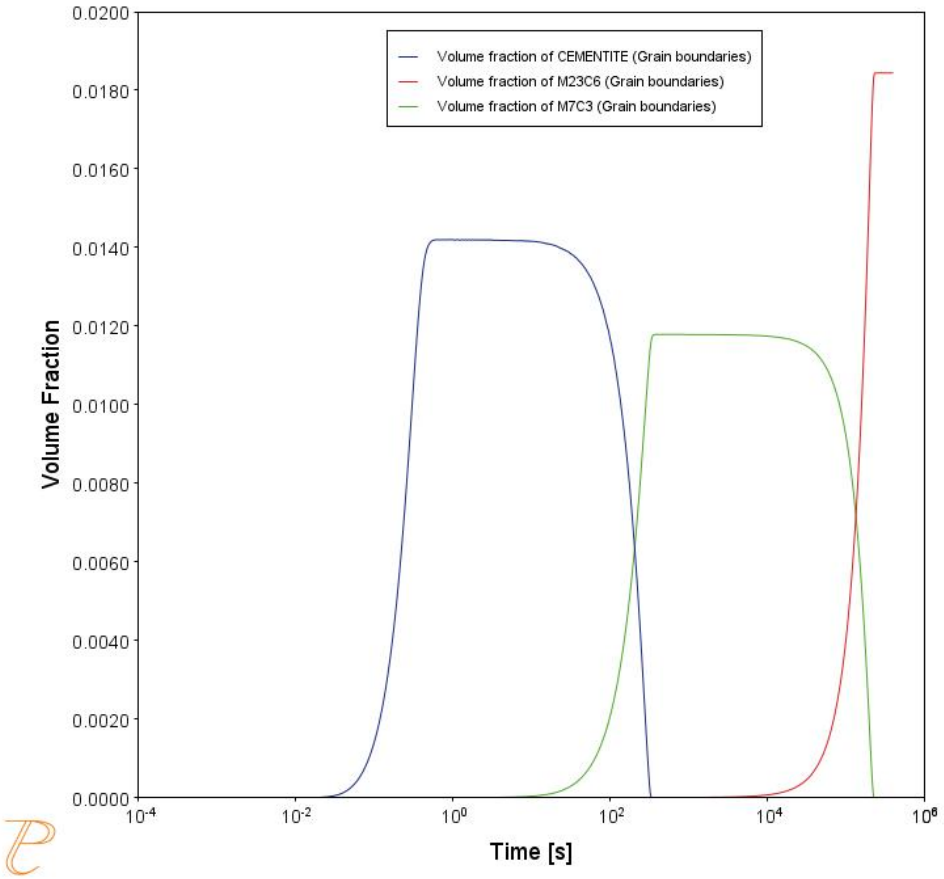


Figure 110: Volume fraction with no initial particle size distribution (PSD).

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_10_Precipitation_Initial_PSD_FeCrC.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)

Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2 All other defaults are kept.
Precipitate phases	CEMENTITE, M23C6 and M7C3
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries (all calculations): Calculated from the matrix settings with a wetting angle of 90°
Interfacial energy	User-defined function f(r,T) (all calculations): • CEMENTITE: 0.167 J/m^2 • M23C6 0.252 J/m^2 • M7C3 0.282 J/m^2
Preexisting size distribution (click **Show details** to display this setting)	For the Precipitation Calculator including particle size distribution, and for all precipitate phases, this check box is selected. For each precipitate phase (CEMENTITE, M23C6 and M7C3), click **Edit particle size distribution** to make changes to the parameters. A window opens with a graphical representation of the radius vs number density.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

P_11: Interfacial Energy Function

In some cases, interfacial energy may be a function of temperature and/or particle radius. This example uses four Precipitation Calculators at four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K. It is an isothermal calculation to examine the mean radius of an Al-0.12Sc system. It uses an FCC_A1 matrix phase and AL3SC precipitate phase with bulk nucleation sites and user-defined interfacial energy function. The user defined interfacial energy function uses an error function to set a smooth transition of the interfacial energy from 0.065 J/m^2 to 0.085 J/m^2 for particle radii below and above 1e^{-8}m and 5e^{-8}m, respectively.

A dataset based on Iwamura and Miura (2004) data is compared with the calculated results.

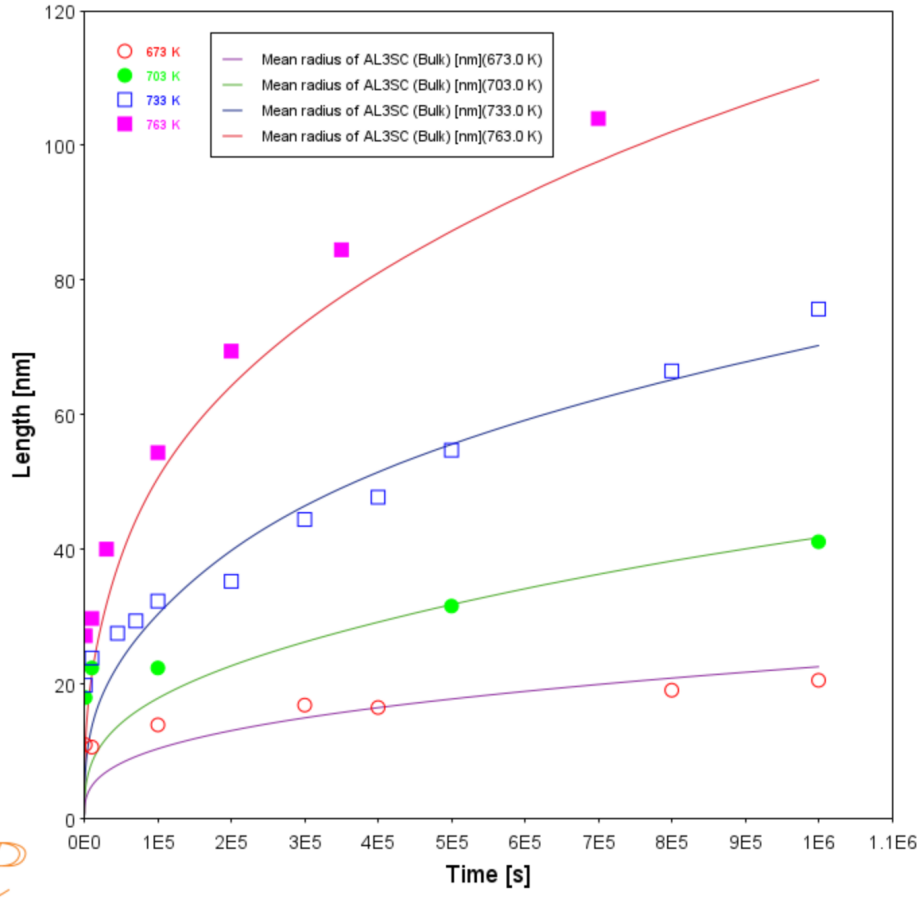


Figure 111: The results of an isothermal calculation to examine the mean radius of an Al-0.12Sc system.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_11_Interfacial_energy_function.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.12Sc Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3SC Nucleation sites (all calculations): Bulk (6.025E28 m^{-3}) Interfacial energy (all calculations): User-defined function f(r,T): 0.075+0.011*erf ((r-3e-8)/1e-8 J/m^2)
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal (all calculations)
Temperature	Four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K.
Simulation time	1 000 000 seconds (all calculations)
Datasets (Experimental File Reader)	
Wamura 2004 (Dataset 1)	Data set included with this example and imported to one Experimental File Reader.

Reference

[2004, Iwarmura] Iwamura, S, and Y Miura. 2004. “Loss in Coherency and Coarsening Behavior of Al3Sc Precipitates.” *Acta Materialia* 52 (3): 591–600.

P_12: Comparing Growth Rate Models for an Al-Zr System

This example compares the **Simplified**, **General** and **Advanced** growth rate models for an Al-Zr system. The resulting plot compares the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.



The example takes several minutes to run.

All models treat a spherical particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Local equilibrium at the precipitate-matrix interface is assumed.

When you use the *Advanced* model, the velocity of a moving phase interface and the operating tie-line are solved together from flux-balance equations. This model can treat both high supersaturation and cross diffusion rigorously. It can also capture the transition between NPLE (non-partitioning local equilibrium) and PLE (partitioning local equilibrium) without any *ad hoc* treatment.

The *Simplified* model is based on the quasi-steady state diffusion approximation, and estimates solute partitioning with matrix composition and nuclei composition instead of time-consuming stepwise tie-line calculations. It also neglects cross diffusion for simplicity.

The *General* model can be considered the same theoretical approximation as, but an improvement over, the *Simplified* model, with cross-diffusion terms taken into account, as well as adjustment of Gibbs-Thomson effect and effective diffusivity implemented.

A dataset based on Knipling et al. [2008] data is compared with the calculated results.

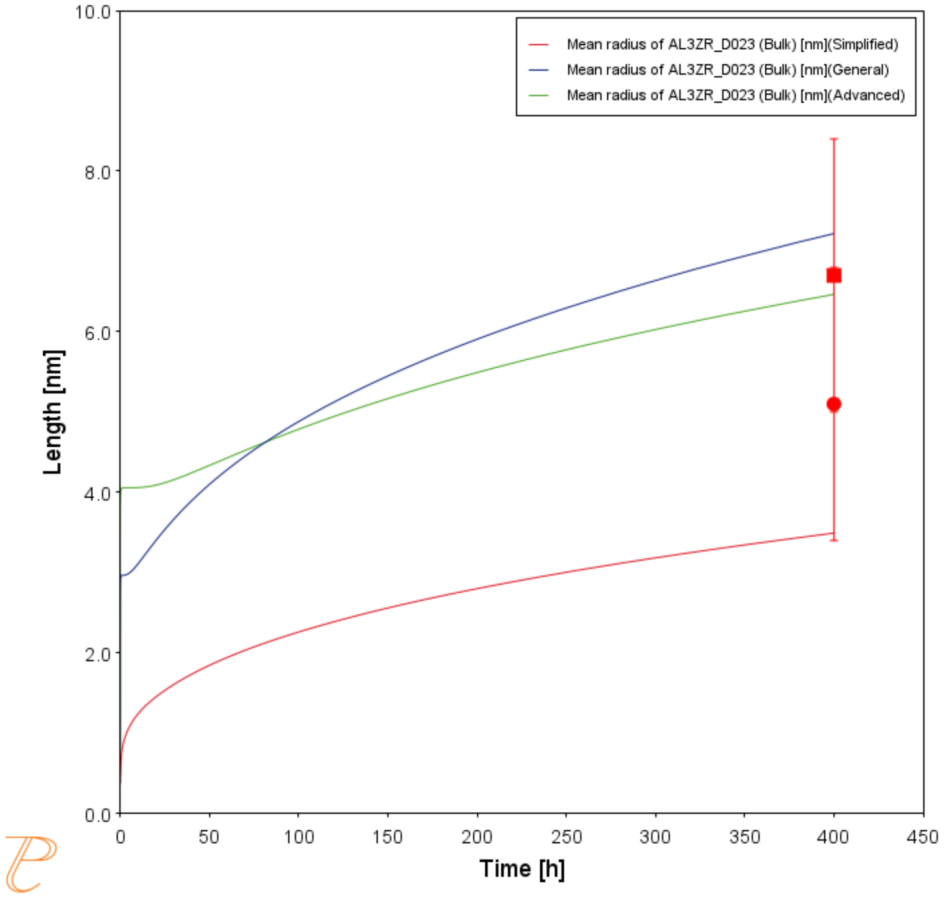


Figure 112: Result comparing the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_12_Precipitation_Al-Zr_GrowthRateModel_comparison.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)

package	
Elements	Al, Zr
Conditions (Precipitation Calculator)	
Composition	Al-0.2Zr Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3ZR_D023 Click **Show details** to select the **Growth rate model** (**Simplified**, **Advanced** and **General**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	425 Celsius
Simulation time	400 hours
Datasets (Experimental File Reader)	
2008 Knipling	Data set included with this example and imported to one Experimental File Reader.

Reference

[2008, Knipling] K. E. Knipling, D. C. Dunand, D. N. Seidman, Precipitation evolution in Al–Zr and Al–Zr–Ti alloys during isothermal aging at 375–425°C. Acta Mater. 56, 114–127 (2008).

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr

In this example, the precipitation of cementite during tempering of a Fe-Cr-C steel is simulated considering two interface conditions: one is the usual ortho-equilibrium condition; the other is the para-equilibrium condition. The simulation results are compared with the experimental data from Sakuma et al. [1980].



The example may take over two hours to run.

This example demonstrates that the early stage of the cementite precipitation can only be accounted for by a simulation applying the para-equilibrium condition, under which the precipitation kinetics are controlled by the diffusion of C. The comparison also shows a later stage gradual transition from the para-equilibrium condition to the ortho-equilibrium condition, and if the tempering time is long enough the diffusion of Cr has a dominating effect on the coarsening of cementite.

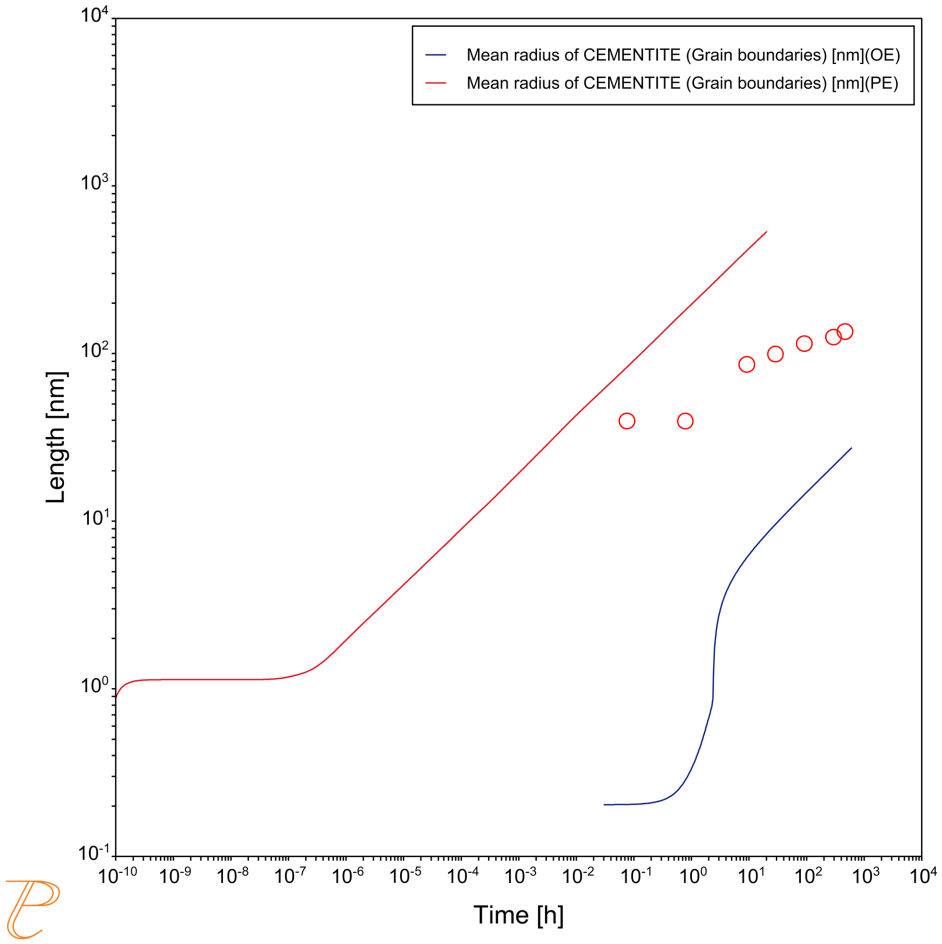


Figure 113: Comparing results from Para-eq (PE) and Simplified (OE) growth models.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_13_Precipitation_Fe-C-Cr_Paraequilibrium_Precipitation_of_Cementite.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)
Elements	Fe, Cr, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.95Cr-1.065C Mass percent
Matrix phase	BCC_A2 All other defaults are kept.
Precipitate phase	CEMENTITE Click **Show details** to select the **Growth rate model** (**Simplified** and **Para-eq**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	773 Kelvin
Simulation time	20 hours for the paraequilibrium model and 600 hours for the simplified model.
Datasets (Experimental File Reader)	
1980 Sakuma	Data set included with this example and imported to one Experimental File Reader.

Reference

[1980, Sakuma] T. Sakuma, N. Watanabe, T. Nishizawa, The Effect of Alloying Element on the Coarsening Behavior of Cementite Particles in Ferrite. Trans. Japan Inst. Met. 21, 159–168 (1980).

Thermo-Calc User Guide: Console Mode

Thermo-Calc Version 2021b



Working in Console Mode

In this section:

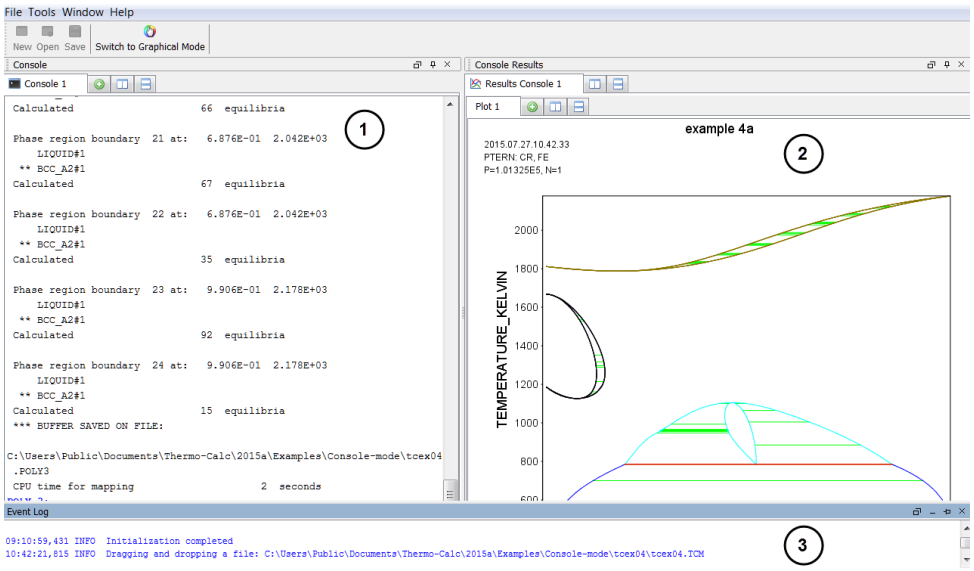
The Console Mode Layout 2
Console Window 4
Console Mode Results Window 5
Event Log Window 6
Keyboard Shortcuts to Navigate Between Tabs 7

The Console Mode Layout

By default the first time you launch Thermo-Calc it opens in Graphical Mode. After this, the mode defaults to the most recent one. You can switch back and forth between modes. To open the Console Mode interface, click **Switch to Console Mode** on the toolbar.

Keyboard Shortcuts to Navigate Between Tabs

The Console Mode User Interface

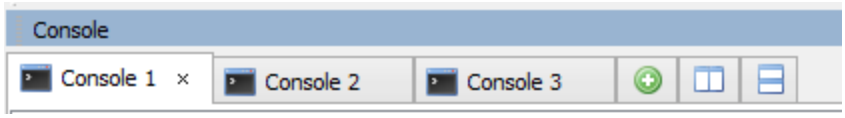


The currently selected window is called the *active* window. This has a darker title bar than the other windows. The windows are:

1. **Console**, with a **Console 1** tab.
2. **Console Results**, with a **Results Console 1** tab as well as a sub-tab (**Plot 1**), which is what is displayed in the window in the figure.
3. **Event Log**, which is the active window in this example.

Console Tabs

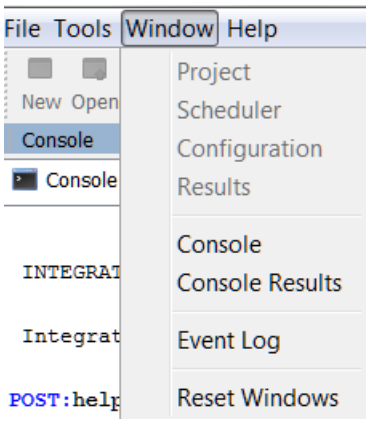
By default, the tabs are side-by-side:



You can toggle to view the tabs top-to-bottom/stacked (click the button) and back to side-by-side (click the button) or the button.

How to Open Console Windows

Open a specific window from the **Window** main menu, or select **Reset Windows** to return to the default window layout.



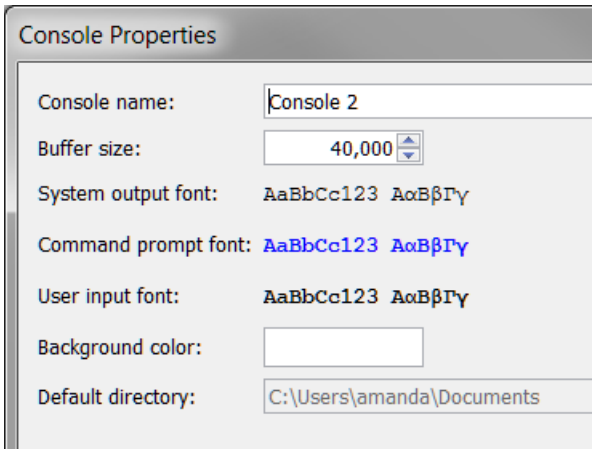
Console Window

By default the Console window is on the left-hand side of the console. This is where you enter commands. The window can have several Console tabs.

To open and close Console tabs:

- To open (or add), click the button, press <Ctrl+T> when the Console window is active, or right-click a tab header and select **New Console**.
- To close, click the button, press <Ctrl+W> or <Ctrl+F4>, or right-click the tab header and select **Close**.
- To close all tabs except one, right-click the header of the tab you want to keep and select **Close Other**.
- To close all tabs and open a new one, right-click the header of any tab and select **Close All**.

You can change the tab name, font and colors for an individual Console tab by right-clicking its header and selecting **Properties**.



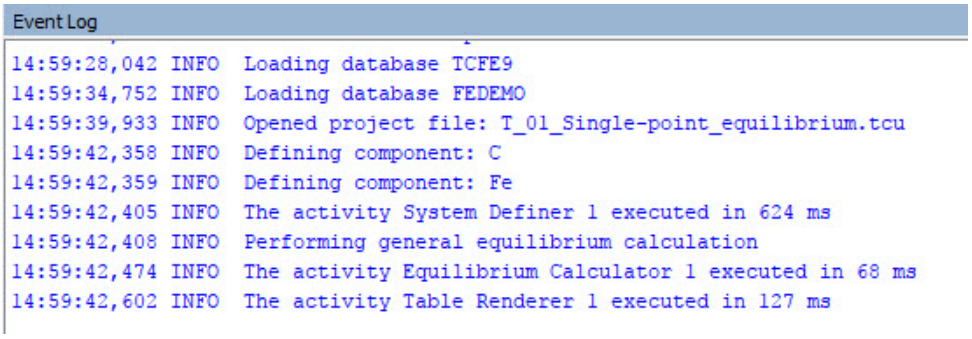
Console Mode Results Window

By default, the Console Results window is on the right-hand side of the screen. This is where plotted diagrams display. Each Console has its own Results tab in the Results window. All the plots and tables generated are presented in the Results tab.

- To open new **Plot** tabs press <Ctrl+Shift+T> or click the add button.
- To open a new Plot tab for the currently active Console tab, press <Ctrl+Shift+T>. To close the Plot tab, press <Ctrl+Shift+W> or <Ctrl+Shift+F4>.

Event Log Window

By default the Event Log window is collapsed (closed). It includes important information about the commands that run and are completed, including error messages. Click once to toggle it open and closed.

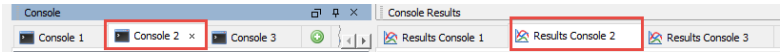


Keyboard Shortcuts to Navigate Between Tabs

Use keyboard shortcuts to move between the tabs available in the Console and Results windows.

Windows

- Press CTRL + TAB to move forward sequentially through each open tab. When you are focused on the Console window, you move forward simultaneously through the Console Results tabs, e.g. If you are on Console 1 and press CTRL + TAB, you move forward to Console 2 and Results Console 2 and so forth.

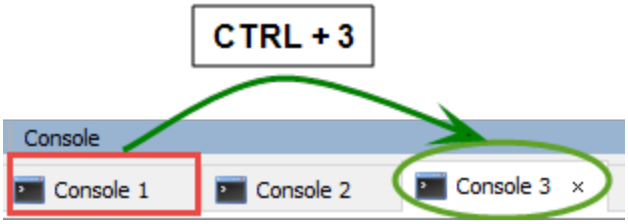


- Press CTRL + SHIFT + TAB to move back through the open tabs. This is useful if you have multiple tabs open, otherwise you can use the CTRL + TAB to cycle through the windows.

- Press CTRL + [tab number 1 to 9] to move directly to the numbered tab. For example, if you are focused on Console 1 and want to move to Console 3, press CTRL+3 and the focus jumps to that tab.

  The tab number corresponds to the order of the tabs, not necessarily the name. That is, if Console 4 is first, then it is what is highlighted when CTRL + 1 is used.

  For **EXAMPLE**, press CTRL + 3 on the keyboard to move focus from Console 1 to Console 3.



When you are focused on the **Console Results** window and use any of the shortcuts this only moves you through the open tabs on this window.

Linux and macOS

The same **Windows** keyboard shortcuts are used but must be pressed twice to move forward and backward.

Modules and Commands

In this section:

Console Mode Workflow 10

Defining a System in Console Mode 12

Console Mode Modules 14

Moving Between Modules and Submodules 21

Entering Command Names or Abbreviations 22

Using the Command Line Prompt 24

Main Menu Commands 25

Command History 26

Wild Card Characters 27

Console Mode Workflow

Working with Thermo-Calc involves moving between different modules. The workflow differs depending on the type of calculation:

- If you want to perform a calculation using the POLY module, you typically first retrieve thermodynamic data in the DATA module, perform the calculation in POLY, and visualize the results in the POST module. It is possible to define a system directly in POLY using the DEFINE_MATERIAL and DEFINE_DIAGRAM commands.
- If you want to calculate and plot a diagram using a response-driven module, such as POTENTIAL or SCHEIL, then you can go directly to that module. Response-driven modules prompt you to go through the steps to do the calculation and the required post-processing. These modules include BIN, TERN, POTENTIAL, POURBAIX, and SCHEIL. You typically end up in the POST module after having used a response-driven module. In the POST module you can modify the plots and save the diagram.
- If you want to tabulate a chemical substance, phase, or reaction, go directly to the TAB module.

The basic workflow is:

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module define the system. Before performing a calculation, you must define the system and retrieve thermodynamic data. The data is retrieved from a database file (*.TDB or *.TDC).
3. The data needed to describe a system is then sent to the **GIBBS** module. This data is accessed by the **POLY** module when you instruct it to perform calculations.
4. In the **POLY** module, perform the calculations.
    - In POLY, the conditions are set for an equilibrium calculation (temperature, pressure, system composition, etc.), then an equilibrium calculation is done.
    - If you want to make a property or phase diagram, you set the conditions for a stepping or mapping operation and perform that operation.
    - This generates data that can be used to plot a property diagram (if a stepping operation is performed) or a phase diagram (if a mapping operation is performed).

5. In the **POST** module plot and visualize your data.
    - If a stepping or mapping operation is performed, then you can go to the POST module and plot a property or phase diagram.
    - The diagram can be plotted quickly using default settings, but you can also modify which variables to plot of the diagram axes and change the appearance of the diagram.
    - You can save the diagram either as a plain text file with data about all the coordinates or as an image file.

Defining a System in Console Mode

Defining a system means to select the chemical components and to retrieve thermodynamic data about those components from an appropriate database in order to do the calculations. You use database(s) with thermodynamic data and then define what system elements as components. Once the system is defined, you retrieve the system's thermodynamic data from the database(s).

- If you use a *response-driven module* to perform your calculation, such as BIN or POURBAIX, then the module prompts you to select database(s) and define the system.
- When doing calculations in the POLY module, you typically have to manually select databases and define the system in the DATA module. However, it is also possible to define the system directly in POLY using the DEFINE_MATERIAL and DEFINE_DIAGRAM commands.

Database (TDB) Module Commands

How to Define a System in Console Mode

1. Go to the DATA (TDB) module. At the `SYS` prompt, use GOTO_MODULE and enter `Data`.

2. Change the default database unless you directly specify the name of the database as a parameter to the command. Type `SWITCH_DATABASE` and follow the prompts.

   The second part of the command prompt indicates the current default database. For example, if the prompt is `TDB_TCFE10`, then the current database is TCFE10.

3. Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`). For example, if you want to have Fe and C in your system, type:

   ```
   DEFINE_ELEMENTS Fe C
   ```

4. Use REJECT and choose `Phases` if you want to avoid retrieving any phases from the database. (To list the phases that are available in your current database, use LIST_DATABASE and choose `Phases`. To list the phases that can form in the defined system, use LIST_SYSTEM and choose `Constituent`.) For example, if you do not want the graphite phase to be retrieved, you type:

   ```
   REJECT PHASES GRAPHITE
   ```

If the number of phases to include is much lower than the total number of phases, then it can be convenient to first `Reject Phases *` and then restore the phases to include using `Restore Phases`.

5. Use GET_DATA to search the database and send the thermodynamic data about your system to the GIBBS workspace.

   At this point you can proceed to the POLY module (with GOTO_MODULE POLY). However, you may want to add elements, phases and species to the GIBBS workspace from other databases. If so, then proceed to the next step.

6. Use APPEND_DATABASE to select the (additional) database from which you want to retrieve data. This command works exactly in the same way as the SWITCH_DATABASE command, with the exception that it does not reinitialize the DATA module and the GIBBS workspace, but instead appends or replaces the data that has already been retrieved with new data from the additional database.
7. Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way when using the SWITCH_DATABASE command (see steps 2 and 3).
8. Use GET_DATA to search the database and add the thermodynamic data to the data that already exists in the GIBBS workspace.
9. Use APPEND_DATABASE again if you want to add data from yet another database. When you have retrieved all the data you need, you can proceed to the POLY module.

Console Mode Modules

- Graphical Mode Activities vs Console Mode Modules

Below are each of the available modules you access in Console Mode. Most of the modules have commands, some are the same no matter what module you are in (e.g. general commands like BACK. GO TO MODULE, EXIT, HELP and so forth). Other commands have different prompts based on the module you are in how you define the system and so forth.



Most modules have several commands available. The exceptions are the BINARY, TERNARY, SCHEIL, POURBAIX and POTENTIAL modules which do not have any additional commands once you access the modules. These are response-driven modules that prompt you with a series of questions and then build the diagram automatically based on your responses.

System Utilities (SYS)

This is the module where you start. It also has several commands. Throughout the other modules there are some general commands, both of which are listed together.

- System Utilities (SYS) Commands

Gibbs Energy System (GES)

The Gibbs Energy System (GES) module is an important Thermo-Calc Console Mode module and consists of a comprehensive subroutine package for various thermochemical calculations. The module is interactively connected with all basic and advanced modules in Thermo-Calc and the add-on Diffusion Module (DICTRA). Most users will not directly use the GES module and commands unless you perform assessments.



The GES module is in essence the Thermo-Calc calculation engine, sometimes referred to as the *calculation core*. When working in Graphical Mode you are using the GES calculation engine behind the scenes, whereas in Console Mode, and if you are performing assessments, you are directly interacting with the module. This is also applicable if you are working with any of the software development kits (SDKs).

- About the Gibbs Energy System (GES) Module

- Gibbs Energy System (GES) Commands

POLY3 (POLY) (Equilibrium)

With the equilibrium calculation module, POLY3, it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams.

- The Equilibrium Calculation Module (POLY3)
- POLY Module Commands

Database (TDB)

The Database module (full name is Database Retrieval) is where you select and retrieve various types of thermodynamic and kinetic information from the selected databases you are going to use for your system. Once you enter the module the short name is `TDB`.

- Database (TDB) Module Commands
- Defining a System in Console Mode
- Also see the Database Manager User Guide and the available information for the specific databases.

POST - A POLY3 Submodule

The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

- Using the POST Module
- POST Module Commands

Scheil (SCHEIL) Simulations

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

- Scheil in Graphical Mode vs Console Mode



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase

About the Scheil-Gulliver Solidification Simulations

SCHEIL Module Commands

Pourbaix Diagram (POURBAIX)

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases. Once you have calculated the Pourbaix diagram, you can also use the saved results of the calculation (the POLY3-file), and make a property diagram based on stepping calculation. You can also plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

- About Aqueous Solutions and the Pourbaix Diagram

Potential Diagram (POT)

The POTENTIAL_DIAGRAM module (short name, the POTENTIAL module) is a potential phase diagram calculation module. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables.

- About Potential Diagrams

Binary Diagram (BIN)

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Binary phase diagrams are by far the most common found in the literature and calculated by computers. However, most real systems have more than two components and thus binary diagrams are more a kind of exercise in order to calculate more realistic phase diagrams.

- About Binary Phase Diagrams

Ternary Diagram (TERN)

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram. There are many types of ternary phase diagrams but perhaps the most common is the isothermal section. In this case, the temperature is constant, which means that the tie-lines are in the plane of the calculation.

- About Ternary Phase Diagrams

PARROT (Optimization)

The PARROT module makes use of the GES module to handle the models of the various phases that might form in a multicomponent system, as well as of the POLY module to store and calculate complex heterogeneous equilibria.

- PARROT Module Commands
- Also see the Data Optimization User Guide

Tabulation Reaction (TAB)

The TABULATION_REACTION (TAB) module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

- About the Tabulation Reaction Module
- Tabulation Reaction (TAB) Commands

Reactor Simulator (REACTOR)

Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.

- REACTOR (REACTOR_SIMULATOR) Commands

DICTRA Monitor (DICTRA)

DICTRA Monitor (DICTRA) and DIC Parrot (optimization for DICTRA): These are available with the add-on Diffusion Module.

Moving Between Modules and Submodules

To go to a specific module, you typically use GOTO_MODULE (or just GOTO) followed by the name of the module. For example, to go to the DATA module, type `GOTO DATA`.

The exceptions are the submodules POST and ED-EXP:

- To go to the POST module, you must enter the POST command from within the POLY module or DICTRA module (if you have the add-on license).
- To go to the Edit Experiments module you must enter the ED-EXP command from within the PARROT module.

To go back to the previous module type `Back`. For example, if you are in the DATA module and entered it from the SYS module, when you type `Back`, you return to the SYS prompt. This command is also available to exit from the submodules POST and ED-EXP.



Without a valid Thermo-Calc license, you cannot leave the SYS module. To enter the DICTRA and DIC_PARROT modules, you also need a valid Diffusion Module (DICTRA) license key.

Entering Command Names or Abbreviations

The name of a command typically consists of terms linked with underscores, for example, LIST_EQUILIBRIUM. Note the following:

- UPPER or lower case letters are OK.
- Hyphens (-) instead of underscores (_) are OK, e.g. LIST-EQUILIBRIUM.
- You can abbreviate commands as long as it is unambiguous, e.g. when more than one command begins with LIST_, you need to type the next letter or word to distinguish between the commands.
- Each word can be abbreviated e.g., L_E for LIST_EQUILIBRIUM.

Examples

Examples of how to abbreviate commands at the command line prompt in Console Mode.

Command Name	Abbreviation
CALCULATE_EQUILIBRIUM	C-E
CALCULATE_ALL_EQUILIBRIA	C-A
LIST_EQUILIBRIUM	L-E
LIST_INITIAL_EQUILBRIUM	LI-I-E
LOAD_INITIAL_EQUILBRIUM	LO-I-E
LIST_PHASE_DATA CBCC	L-P-D CBC
LIST_PHASE_DATA CEMENTITE	L-P-D CEM
SET_ALL_START_VALUES	S-A-SS-AL
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025	S-A-V 1 X(F,FE) 0 .89 .025
SET_START_CONSTITUENT	S-S-C
SET_START_VALUE	S-S-V
SET_AXIS_PLOT_STATUS	S-A-P
SET_AXIS_TEXT_STATUS	S-A-T-SS-A-TE

Command Name	Abbreviation
SET_AXIS_TYPE	S-A-TY
SET_OPTIMIZING_CONDITION	S-O-C
SET_OPTIMIZING_VARIABLE	S-O-V
SET_OUTPUT_LEVEL	S-O-LS-OU

Using the Command Line Prompt

The command line prompt in the Console window tells you which module you are currently in. When Thermo-Calc is first opened in Console Mode, you are in the SYS module, which is indicated with the command line prompt `SYS`.

To use Console Mode, you type in commands at the command line prompt. The available commands depend on which module you are in. You can list the commands by typing `?` at the prompt and then press <Enter>.

- Moving Between Modules and Submodules
- Entering Command Names or Abbreviations
- Specifying Parameters
- Wild Card Characters
- Command History
- Keyboard Shortcuts to Navigate Between Tabs
- Working with the Console Mode Output

Main Menu Commands



In Console Mode you use commands to access these menu options. If there is an equivalent command, it is listed below.



The **File** menu and toolbar are reserved for Graphical Mode. The **Tools**, **Window** and **Help** menus are described in Menu, Toolbar and Keyboard Shortcuts.

How to Open Files

- In the SYS module: MACRO_FILE_OPEN
- In the SYS module: OPEN_FILE

Opening Console Mode Macro Files



Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Save (Workspace)

This command depends on the module you are in. Type ? at the prompt to look for a command such as SAVE_GES_WORKSPACE (GIBBS module).

Exit

In any module: EXIT

Close

In the SYS module: CLOSE_FILE

Display License Info

In the SYS module: DISPLAY_LICENSE_INFO

Command History

- To scroll through the last twenty commands used, type two exclamation marks (`!!`) and press <Enter>.
- To repeat the last n commands, type `!` followed by the number of previous commands to be executed again.
- To scroll through previous performed commands, use the Up (↑) or Down arrow (↓) keys.
- To read more information about the command history functionality in Thermo-Calc, type `! ?` at the command line prompt.

Wild Card Characters

You can sometimes use the asterisk (*) as a wild card character to, for example, refer to all components, phases, or species, when showing calculated properties in the POLY module, or when you set axis variables for plotting diagrams in the POST module.

When showing calculated properties in the POLY module, you can also use the dollar sign ($) to refer to all stable phases.



For activity and/or chemical potential properties, the *and $ normally do not work properly as wild card characters.

Examples

These are examples of the wild card characters you can use to search commands at the command line prompt.

Command	Action
SHOW_VALUE B(*)	Lists mass (gram) of all components in the system.
SET_AXIS_VAR Y B(*) *	Sets mass (gram) of all components in the system as Y-axis variable.
SHOW_VALUE MUR(*)	Lists chemical potentials of all components in the system.
SET_AXIS_VAR Y ACR(*) *	Sets activities of all components in the system as Y-axis variable.
SHOW_VALUE HM(*).T	Lists heat capacities of all phases.
SET_AXIS_VAR Y GM(*) *	Sets molar Gibbs free energies of all phases as Y-axis variable.
SHOW_VALUE TC($)	Lists curie temperature of all stable phases.
SHOW_VALUE W(*,*)	Lists mass fractions of all components in all phases.
SHOW_VALUE W($,*)	Lists mass fractions of all components in all stable phases.
SHOW_VALUE W(FCC,*)	Lists mass fractions of all components in the FCC phase.
SHOW_VALUE W(*,FE)	Lists mass fractions of the Fe component in all phases.

Command	Action
SHOW_VALUE W($,FE)	Lists mass fractions of the Fe component in all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.
SHOW_VALUE Y($,*)	Lists site fractions of all species in all sublattices of all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.

File Types

In this section:

Working with the Console Mode File Types 30
Opening Console Mode Macro Files 31
Log Files 34
Macro Files 35
Workspace Files 38
Editing the Default Console Directory 43
Experimental Data Files (*.POP, *.DOP) 46

Working with the Console Mode File Types

For DICTRA Console Mode see *File Formats* in the *Diffusion Module (DICTRA) User Guide*

In Console Mode, Thermo-Calc uses different types of files, including:

- Macro Files and Log Files both with the file extension *.TCM. Log files are created using the SET_LOG_FILE command.
- Workspace Files in POLY (*.POLY3), GIBBS module (*.GES5), and the PARROT module (*.PAR). (For the GIBBS module, this cannot currently be done with GES6).
- Experimental Data Files (*.POP, *.DOP) are a type of workspace file available with the PARROT module and have the file extension of *.POP. In the Diffusion Module (DICTRA), you work with .DOP files instead of .POP. These .POP and .DOP files are referred to as experimental data files.

Another type of experimental data file with the *.EXP file extension are also generated when working with DATAPLOT. See About the DATAPLOT Graphical Language.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Opening Console Mode Macro Files

The macro files (with the extension *.TCM) include comments, which you can either run in Thermo-Calc or open and read in a text editor.

You can open the macro files (*.TCM or *.DCM files) in different ways.

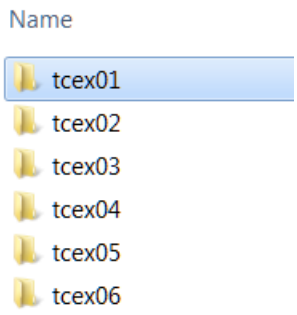
- From the main menu,
- Using a command,
- By dragging and dropping the file into the Console window, or
- Navigate to the file location on your computer and double-click to open it. If you already have Thermo-Calc open, this opens a new instance of the software.
- You can also read the commands listed in the macro file using a text editor.

If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Opening a Macro from the Main Menu

To open a Thermo-Calc example macro file:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.



For the Diffusion Module (DICTRA) examples (*.DCM macro files), open the **Diffusion Module - DICTRA** folder.

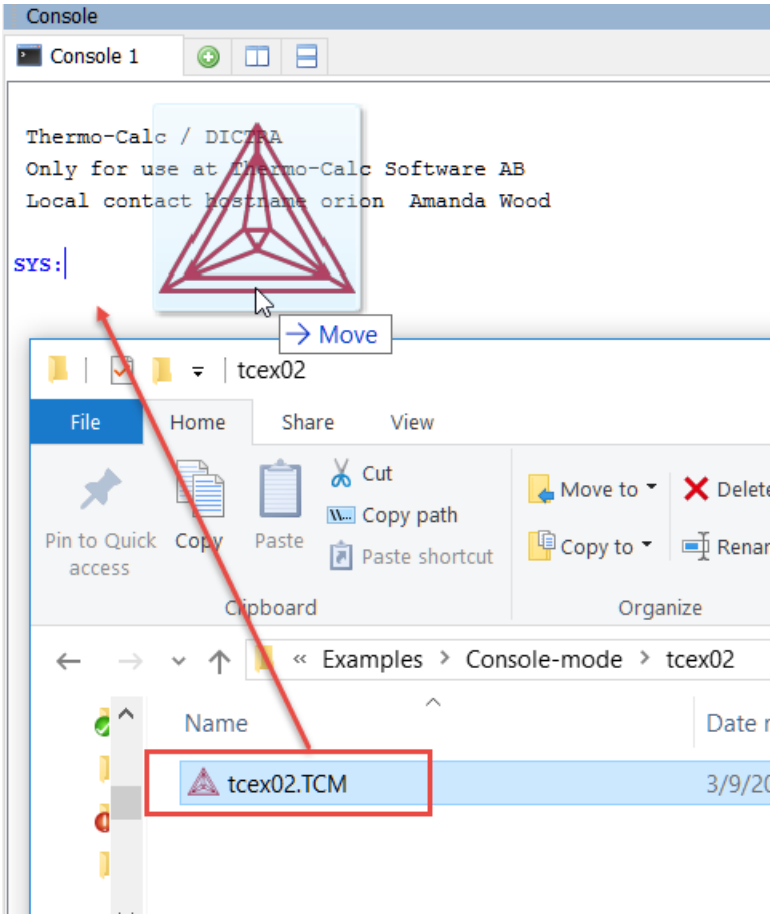
5. In the folder, double-click the *.TCM file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

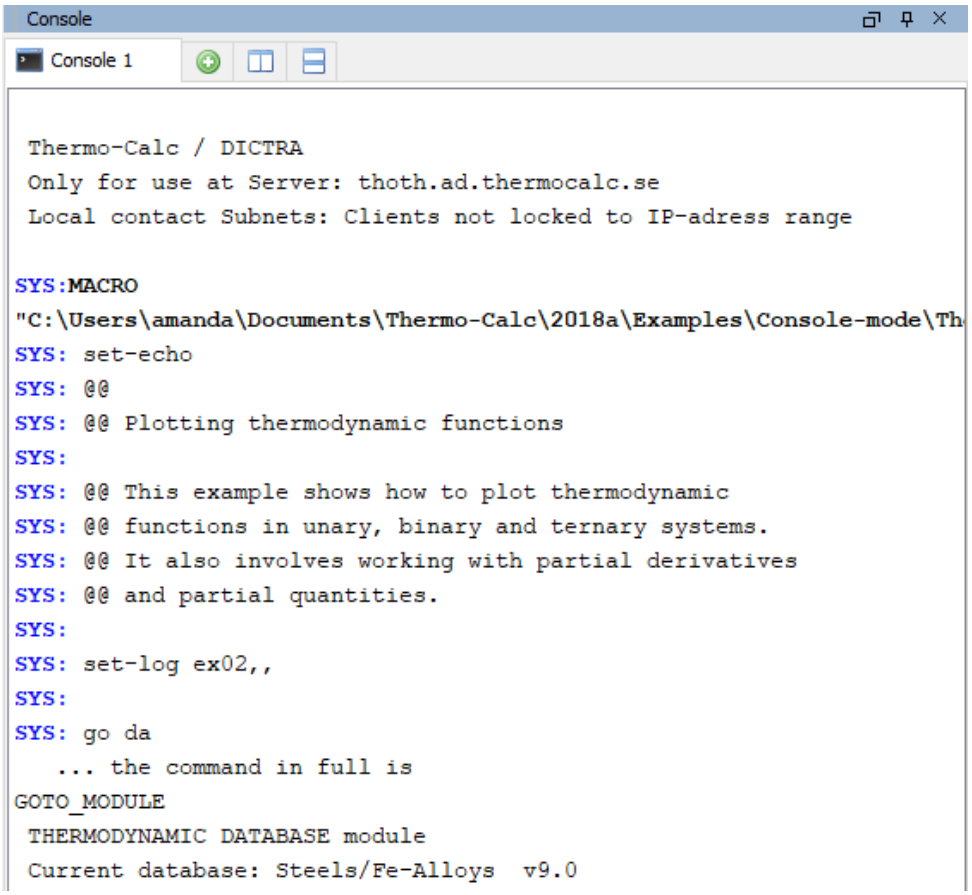
Opening a Macro Using a Command

At the SYS prompt, type MACRO_FILE_OPEN and press <Enter>. In the file dialogue window that opens, navigate to and select the macro file to open.

Drag and Drop a Macro File into the Console Window

For example, on your computer, navigate to the examples folder. Drag the file from its location into the Thermo-Calc Console window. When you release (drop) the file, the macro starts running. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.





Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Log Files

Log files with the file extension *.TCM are plain text files used to save a sequence of commands. Log files can be edited in a text editor.

- To start saving your input into such a file, use SET_LOG_FILE in the SYS module, followed by the name of the file that you want to save your command sequence to.
- If you want to save the output in the log file as well, use SET_ECHO before the SET_ LOG_FILE command. Doing this is useful if you want use the log file later as a macro file.

Macro Files

Macro files (with the file extension of either *.TCM or *.LOG) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

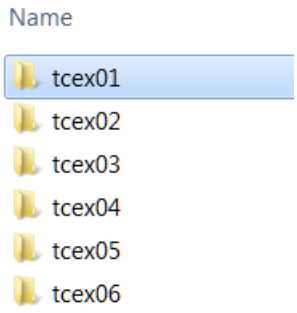
Macro files include comments, which you can either run in Thermo-Calc or open and read in a text editor.

If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file. It is recommended you run the macro to view all the details.

How to Open a Console Mode Example Macro File

To open a Thermo-Calc example macro file:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.



For the Diffusion Module (DICTRA) examples (*.DCM macro files), open the **Diffusion Module - DICTRA** folder.

5. In the folder, double-click the *.TCM file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

Macro File Commands

Action	Command	Description and Comments
To load a macro file	In the SYS module, MACRO_FILE_OPEN followed by the name of the macro file.	Thermo-Calc starts the command sequence that the file contains.
Regain control of the console	SET_INTERACTIVE	End a macro file with this command to have control of the Console returned to you.
Add comments to a macro file	Start a line with @@, or enclose it between an @ (-line and a @)-line.	When lines are enclosed the software ignores them when running the macro.
Open a macro file	MACRO_FILE_OPEN	When creating the log file, you can make a macro file load up to five other macro files.
Nest macro files inside of each other	MACRO_FILE_OPEN SET_INTERACTIVE	If a nested macro file ends with SET_INTERACTIVE, then Thermo-Calc resumes with the higher-level macro file at the command immediately following the MACRO_FILE_OPEN command that loaded and executed macro file that has just been terminated. If a nested macro file doesn't end with SET_INTERACTIVE (but with an end-of-file character), then the console shuts down and the macro is stopped.

Macro File Control Characters

The @? character allows you to make a macro interactive by allowing input. At the @? character, which is placed where a parameter value or argument is normally put, Thermo-Calc prompts to input the value of a parameter or argument. You can enter a string immediately following the @? character. This string is presented to the user when prompted to enter the parameter value or argument. The entered value is used by Thermo-Calc as input to the command in question. For example, you can request the user to specify the temperature range of a stepping calculation by entering the following in a macro file:

```
SET_AXIS_VARIABLE 1 T @?Low-temperature-limit: @?High-temperature-
limit:
```

You can also use up to nine variables in your macro file and prompt the user to enter values that can be assigned to these variables. Use the `@#n` character when you want to prompt the user to provide a value to the variable, where the n is a digit between `1` and `9`. You can then use this value by with the `##n` character. For example, you can request the user to provide the first element of a system by entering the following in the macro file:

```
@#3First-element?
```

You can then use this variable with the entering the character ##3 later in the macro file. For example, you can write:

```
SET_AXIS_VARIABLE 1 x(##3) 0 1,,,
```

Finally, there is the `@&` pause character. Thermo-Calc pauses and waits for input from the user when this pause character is read from a macro file. Inserting pause characters is useful if you want to allow the user to monitor what is happening when Thermo-Calc is running the macro.

Response-Driven Modules and Macros

Macro files that are created while you use a *response-driven module* begin with the module-entering command (for example, `Goto_Module Scheil)` followed by a number of lines with responses to the module's questions and requests. The file terminates with the commands POST or SET_INTERACTIVE (this command gives you back control of the Console). An empty line cannot be edited with any input rather than the default answer (to a specific question). Comment lines, commands to open other macro files, pause characters or input-controlling characters cannot be inserted between these empty lines (otherwise the response-driven module cannot be executed properly).

Workspace Files



For DICTRA Console Mode see *File Formats* in the *Diffusion Module (DICTRA) User Guide*

Workspaces files allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations. You use the command SAVE_WORKSPACES to create this file type, which is available in the POLY, GIBBS and PARROT modules.

When in Thermo-Calc Console Mode these are the workspace file extensions:

- POLY module (*.POLY3)
- GIBBS (GES) module (*.GES5)
- PARROT module (*.PAR and *.POP)



For DICTRA in Console Mode, the PARROT module file extension is *.DOP.

The workspace has all the settings specified and the result of any stepping or mapping operations performed after using SAVE_WORKSPACES. Consequently, the command opens a workspace in which all data is saved which is generated after the SAVE_WORKSPACE command is executed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and calculation results.

To load the data and calculation results of a workspace file, use the READ_WORKSPACES command available in the POLY module. The file can be used for calculation in POLY, visualization in POST, or data manipulation in GES. You are also given the option in the POURBAIX and SCHEIL modules to open a previously saved workspace file. This allows you to make new POURBAIX or SCHEIL calculations on the same chemical system as before but with different temperature, pressure, and composition conditions, or to plot new property diagrams based on the previous calculations.



A reminder that Linux and macOS are case sensitive; when applicable ensure you enter file extensions with capital letters.



Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Links to Workspace Commands

POLY module

- READ_WORKSPACES
- SAVE_WORKSPACES

Gibbs (GES) module

- READ_GES_WORKSPACE
- READ_WORKSPACES
- SAVE_GES_WORKSPACE
- SAVE_WORKSPACES

PARROT module

- READ_PARROT_WORKSPACES
- SAVE_PARROT_WORKSPACES

ED-EXP module (submodule to PARROT)

- READ_WORKSPACES
- SAVE_WORKSPACES

Reactor module

- READ_WORKSPACE
- SAVE_WORKSPACES

Important Information About Map and Step Commands and the Save_ Workspaces Command



A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Editing the Default Console Directory

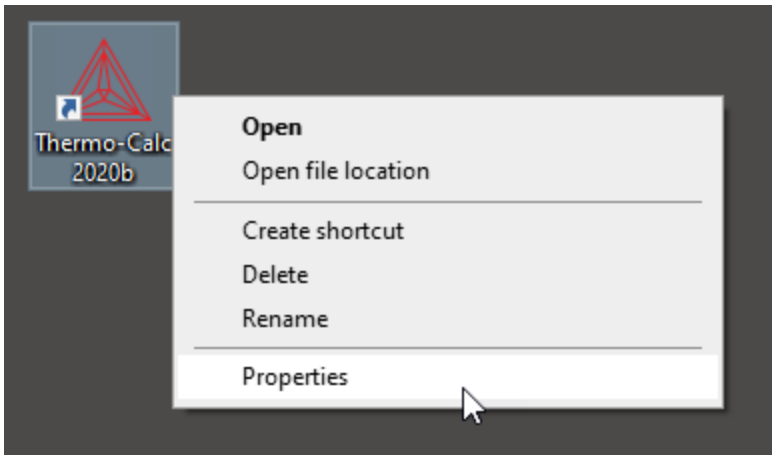
You can add a startup parameter to a shortcut when launching Thermo-Calc on any of the platforms. When you launch the revised shortcut, the file path is set to a user-defined default directory. An example of why you might want to have a custom directory path is if you use batch projects or if you have macro files for batch jobs. The custom directory file path can also be viewed from within Console Mode.

The shortcut is only valid throughout the existing session; it is not saved as a default. Each time you want to use this file path you must launch Thermo-Calc from the customized shortcut.

The following uses Windows for the example.

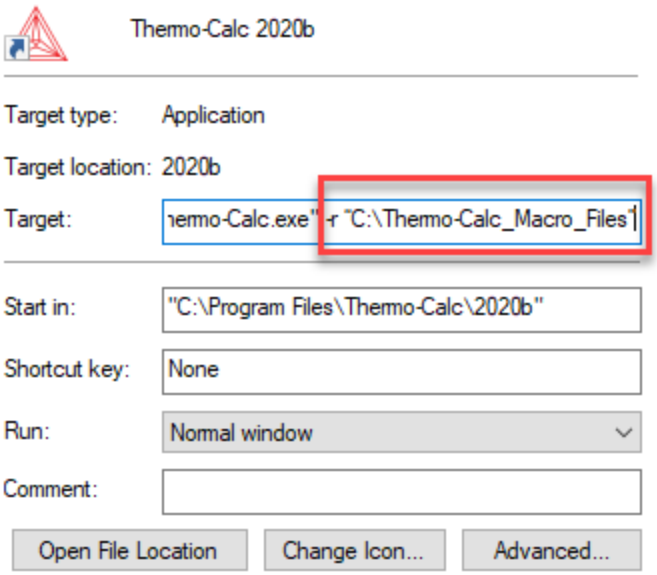
How to Set up the Default Console Directory

1. Right-click a shortcut to Thermo-Calc and click **Properties**.



2. In the **Thermo-Calc 2021b Properties** dialog, **Target** field, add the following to the end of the string: **–r** plus the *"path to the default directory"*. Include a space between the –r and path, and use quotation marks around the full file path. A simple example:

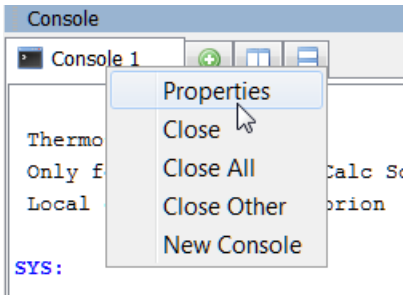
   -r "C:\Thermo-Calc_Macro_Files"



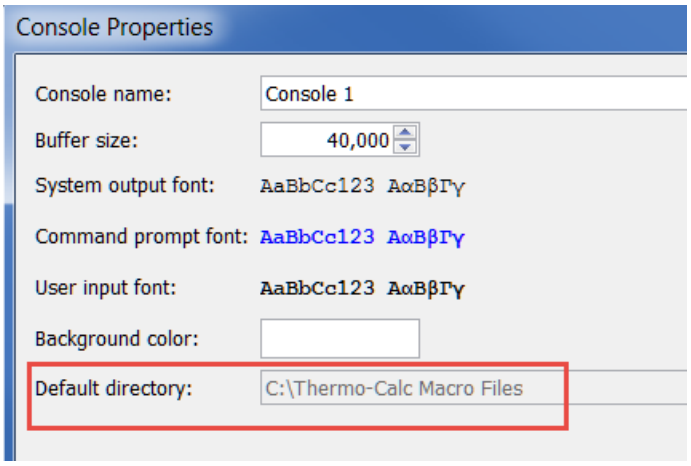
3. Click **Apply** and **OK**.
4. Launch Thermo-Calc from the shortcut where you added the parameter. You can confirm that it is set correctly from within Thermo-Calc.

How to View the File Path in Thermo-Calc

1. Launch Thermo-Calc from the short cut where you added the parameter.
2. In Console Mode, right click the **Console** window and choose **Properties**.



3. In the **Console Properties** window the **Default directory** section displays the custom file path.


Console Properties
Console name:
Console 1
Buffer size:
40,000
System output font:
AaBbCc123 AαBβΓγ
Command prompt font:
AaBbCc123 AαBβΓγ
User input font:
AaBbCc123 AαBβΓγ
Background color:
Default directory:
C:\Thermo-Calc Macro Files

Experimental Data Files (*.POP, *.DOP)



There is also another type of experimental data file (*.EXP) generated when working with DATAPLOT. See About the DATAPLOT Graphical Language.



If you are using Graphical Mode, the Experimental File Reader activity node is used to plot experimental data on one or more plots.

In order to conduct an assessment for a system, the experimental data is described with a syntax, which is similar to the way that one calculates an equilibrium in the POLY module or you edit an experimental point in the ED_EXP module. Similar to a Thermo-Calc macro file (*.TCM), an experimental data file (i.e. the *.POP or *.DOP file) is a basic text file and can be opened and edited by any text editor. For this reason, a *.POP or *.DOP file is not hardware dependent.

A POP or DOP file consists of various commands from the POLY and ED_EXP modules, as well some special commands which can only be used in such experimental data files. Various experimental information can be inputted in an *.POP or *.DOP file as different tables; the same type of experimental data are usually documented in the same table (see below).

A *.POP or *.DOP file is used in the PARROT module to provide experimental information for the optimization process, and is checked by a *syntax checker* when the PARROT command COMPILE_EXPERIMENTS is proceeded.

The special commenting identifier, i.e. a dollar sign $ which starts a line, is used to document comment lines at any position in a *.POP or *.DOP file. You may remember that this feature is universally the same as in almost all kinds of text files in Thermo-Calc software, e.g. in *.TDB, *.DAT, *.TCM, *.POP/*.DOP and *.EXP files. Such a sign and all information afterwards in the same comment line is skipped and ignored by the syntax checker.

Many POLY and ED_EXP commands can be directly used in a POP or DOP file. But there are some differences with the set of POLY or ED_EXP commands, and some specially designed commands as described in this topic can only be used in the *.POP or *.DOP files.

Frequently Used POLY Commands

Most of the commands in the experimental data file are the same as in the POLY module. The most frequently used are listed below:



The last command in an *.POP or *.DOP file must always be the SAVE command.

- CREATE_NEW_EQUILIBRIUM
- CHANGE_STATUS
- SET_CONDITION
- SET_REFERENCE_STATE
- ENTER_SYMBOL
- SAVE_WORKSPACES

Less Often Used POLY Commands

Other legal commands from the POLY module that are used less often are:



The DEFINE-COMPONENTS command must be always used as the first command in an *.POP or *.DOP file, as it automatically reinitiates the whole workspace.

- DEFINE_COMPONENTS
- EVALUATE_FUNCTIONS
- SET_ALL_START_VALUES
- SET_NUMERICAL_LIMITS
- SET_START_VALUE
- ADVANCED_OPTIONS

Frequently Used Edit Experiments (ED_EXP) Commands

Most of the special commands for the ED_EXP module are also often used in an *.POP or *.DOP file. For example:

- EXPERIMENT
- EXPORT
- IMPORT
- LABEL_DATA
- SET_ALTERNATE_CONDITION
- SET_WEIGHT

Do not use these Edit Experiment (ED_EXP) Commands



The following special ED_EXP commands are illegal and should not be used in any *.POP or *.DOP file:

- COMPUTE-ALL-EQUILIBRIA
- MAKE-POP-FILE
- READ (READ-BLOCK OR READ-WORKSPACE)
- TRANSFER-START-VALUES

Calculations

Graphical Mode vs Console Mode: Calculation Types

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About the Gibbs Energy System (GES) Module

The Gibbs Energy System (GES) module is an important Thermo-Calc Console Mode module and consists of a comprehensive subroutine package for various thermochemical calculations. The module is interactively connected with all basic and advanced modules in Thermo-Calc and the add-on Diffusion Module (DICTRA). Most users will not directly use the GES module and commands unless you perform assessments.

The GES module is in essence the Thermo-Calc calculation engine, sometimes referred to as the *calculation core*. When working in Graphical Mode you are using the GES calculation engine behind the scenes, whereas in Console Mode, and if you are performing assessments, you are directly interacting with the module. This is also applicable if you are working with any of the software development kits (SDKs).

The objective of the GES module is to provide a unified set of subroutines to be used in any application program that needs thermochemical data. All kinds of thermodynamic models for various types of substances are implemented. However, most model-dependent features are hidden inside the module, and the application programmer can use a standardized set of subroutines, i.e. using the Thermo-Calc SDKs such as TC-Python, TQ-Interface, TC-API and TC-Toolbox for MATLAB® to calculate the integral Gibbs energy or any partial derivative thereof for each phase at any composition, temperature and pressure.

There are subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any variable. You can enter and modify phase descriptions, model connections, basic thermodynamic parameters, and so on.

POLY and all other basic and special modules, as well as the add-on Diffusion Module (DICTRA), interactively call the subroutines within the GES module to calculate any thermodynamic quantities.

Calculation Engine: GES5 vs GES6



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.



To globally set the default from GES6 back to GES5, go to the **Tools → Options →** General tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. This is useful if you are using the POURBAIX module (aqueous solutions), or if you have a custom database that is not compatible with GES6. The SET_GES_VERSION Console Mode command can also be used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Equilibrium Calculations

In this section:

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The Equilibrium Calculation Module (POLY3)

An equilibrium describes what the composition of the end state of a system is, given a full specification of state variables such as temperature, pressure, initial composition, system size, etc. An equilibrium calculation is normally done in POLY-3 according to the *Global Minimization Technique*, which ensures that the most stable minimum under the specified conditions is computed.

For an equilibrium calculation to be performed, the state variables must all be set as conditions for the calculations. Such conditions include, for example, temperature, pressure, and system composition. When you calculate an equilibrium in the POLY module, you have to set these conditions manually.

Knowledge of the thermodynamic equilibrium is an important factor for understanding properties of materials and processes. With a database of thermodynamic model parameters, it is possible to predict such properties and also to obtain driving forces for diffusion-controlled phase transformations and other dynamic processes.

With the equilibrium calculation module, POLY3, it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams.

Different types of databases can be used with the POLY module, and it can be used for alloys or ceramic systems, as well as gaseous equilibria, aqueous solution involved heterogeneous interaction systems. Up to 40 elements and 1000 species can be defined into a single system for equilibrium calculations.

All normal thermodynamic state variables can be used to set as conditions in calculating equilibria, and as axes in plotting diagrams. You can set the composition or any property of an individual phase as a condition. Any state variable can be varied along an axis in order to generate a diagram. During calculations of a diagram, complete descriptions of all calculated equilibria are stored, and in the diagram any state variable can be used as an axis.

The *Global Minimization Technique* is used to ensure that the present minimum in an equilibrium calculation is the most stable minima for the specified conditions. This is based on the traditional GEM (Gibbs Energy Minimization) technique.

A direct global minimization can be performed on conditions: N, n(comp), B, b(comp), w (comp), x(comp), T, and P, but not when combined conditions as e.g. w(a)-3*w(b)=1 are used or when an activity or potential condition is used. For all other types of conditions where regular minimization converges, Indirect Global Minimization, i.e. global test and corrections, if necessary, are performed until the lowest minimum is found.

- Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of grid points provides starting combination of phases and their constitutions for

regular minimization to find the exact equilibrium solution. This solution is then subject to a global test as described below.

- Indirect Global Minimization: Under certain conditions, a direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

The full-scale and full-scope usage of the *Global Minimization Technique* has been extended from for only single-point calculations for all types of calculations (of single-points, property diagram stepping and phase diagram mapping)in Thermo-Calc.

The use of *Global Minimization Technique* may increase the computation time. The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

Global minimization is performed by default in single-point or stepping or mapping equilibrium calculations.

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases. The POLY module uses the Gibbs Energy System (GES) for modeling and data manipulations of the thermodynamic properties of each phase.

Setting Conditions for Equilibrium Calculations

Setting a condition normally involves giving a single state variable a specific value. For example, you can set the temperature to 1273.5 Kelvin (T=1273.5). Alternatively, setting a condition can involve giving a linear expression with more than one state variable a specific value. For example, you can set the mole fraction of the S component to be the same in the liquid and the pyrrohotite phases (`X(LIQ,S)-X(PYRR,S)=0`).

```
POLY_3:l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1000, P=1E5, X(C)=5E-2, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.36552E+01
 Total Gibbs energy -4.07975E+04,  Enthalpy  2.41176E+04,  Volume  7.21740E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       5.0000E-02  1.1193E-02 2.1816E-01 -1.2659E+04 SER
 FE                      9.5000E-01  9.8881E-01 6.1895E-03 -4.2279E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.5069E-01, Mass 5.3063E+01, Volume fraction 9.6312E-01  Mass fractions:
 FE  9.99844E-01  C   1.55514E-04

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 4.9313E-02, Mass 5.9230E-01, Volume fraction 3.6881E-02  Mass fractions:
 C   1.00000E+00  FE  0.00000E+00
```

The number of state variables that need to set is determined by the *Gibbs Phase Rule*. Typically, the state variables to give values to are:

- temperature (in K)
- pressure (in Pascal)
- system size in number of moles (in mole) or mass (in grams)
- the fraction of each component (in number of moles or mass)

If you fix the phase of the equilibrium and all but one of the state variables, you can discover the value of the other state variable at equilibrium.

It is possible to specify a set of conditions that does not have any equilibrium and the program detects this by failing to reach equilibrium during the calculation.

State VariableS

The following table lists some of the available state variables you can use to set conditions:

State Variable	SET_CONDITION Parameter
temperature in the system (in K)	T

State Variable	SET_CONDITION Parameter
pressure in the system (in Pascal)	P
system size (mole number in moles)	N
system size (mass in grams)	B
number of moles of a component in the system	N(<component>)
mole fraction of a component in the system	X(<component>)
mass fraction of a component in the system	W(<component>)
activity of a component in the system	ACR(<component>)
chemical potential of a component in the system	MUR(<component>)
mole fraction of a component in a phase	X(<phase>,<component>)
mass fraction of a component in a phase	W(<phase>,<component>)
activity of a species referred to a phase at ambient temperature and pressure	ACR(<species>,<phase>)
chemical potential of a species referred to a phase at ambient temperature and pressure	MUR(<species>,<phase>)
enthalpy in the system (in J)	H
enthalpy of a phase (in J/mol)	HM(<phase>)

Calculating an Equilibrium

This topic explains how to calculate an equilibrium in POLY. To calculate an equilibrium means to calculate the equilibrium composition of your system, given a full specification of conditions that reduce the degrees of freedom of the calculation to zero.



If you are running a network client installation of Thermo-Calc and cannot enter the POLY module, this may be because all the license instances on that the license server makes available have been checked out.

- POLY Module Commands

1. Define your system.

   Defining a System in Console Mode

2. Go to the POLY module. At the SYS prompt, type `GOTO_MODULE` and enter `POLY`.
3. Use SET_CONDITION followed by conditions and value assignments to set the conditions of your calculation. For example, to set temperature, pressure, initial composition and system size for a Fe-Cr-C system, you might enter the following:

   ```
   SET_CONDITION T=1200 P=1E5 W(CR)=0.18 W(C)=0.0013 N=1
   ```

   This sets the temperature (T) to 1200 K, the pressure to 1 bar (100,000 Pascal), the mass fraction of Cr to 18 mole percent, the mass fraction of C to 0.13 weight percent, and the total amount of material to 1 mole. The fraction of Fe in the system is calculated from the fractions of Cr and C. You have to set the fraction of all the components in your system except one.

4. Use COMPUTE_EQUILIBRIUM to run the calculation.
5. Use LIST_EQUILIBRIUM to see the results of the calculation.

Calculating an Equilibrium with a Fixed Phase

There are many ways to calculate equilibriums in Thermo-Calc. The following is one example.

You can calculate an equilibrium that has a certain amount of a certain stable phase. Use CHANGE_STATUS and choose `Phase` to specify the phase and the amount of that phase (in normalized mole number) that you want to set as fixed. For example, if you want to find out at what temperature a system starts to melt, enter the following:

```
CHANGE_STATUS PHASE LIQUID=FIX 0
```

You must leave the state variable whose equilibrium value you are interested in unspecified. However, if you have already specified that state variable, you can make it unspecified again by using SET_CONDITION and set that state variable to `NONE`. For example, if you have given temperature a value, you can type:

```
SET_CONDITION T=NONE
```

The calculated equilibrium includes the value of the unspecified variable at which the equilibrium enters the phase that is fixed.

For an example where an equilibrium is calculated with a fixed phase, see Console Mode example tcex07.

Calculating an Equilibrium with Suspended or Dormant Phases

You can calculate an equilibrium under the assumption that one or several phases are `SUSPENDED` or `DORMANT` using CHANGE_STATUS and choose `Phase`. For example, to specify that all phases except one should be suspended, you can first suspend all phases and then enter a single phase in the following way:

```
CHANGE_STATUS PHASE *=SUSPENDED
CHANGE_STATUS PHASE FE_LIQUID=ENTERED
```



For an example where this is done, as well as where the status of phases is set to be dormant, see the Single Equilibrium Calculation Examples.

Property Diagrams

In this section:

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Calculating and Plotting a Property Diagram 60
Calculating a Property Diagram One Phase at a Time 62
Calculating Several Properties in the Same Diagram 63

About Property Diagrams

When you calculate and plot a property diagram, there is only one independent state variable. Many different properties can be plotted as a function of this independent variable. For example, if the independent state variable is temperature, then the mole fractions of all phases can be plotted as a function of temperature. Or the composition of a specific phase may be plotted relative to temperature, or the activity of a component in the system as a whole or in a specific phase may be plotted relative to it.

A property diagram is plotted based on a series of equilibria that is computed while the value of one state variable is varied between a minimum and a maximum value. This variable is referred to as the stepping axis variable. In Thermo-Calc, first calculate one initial equilibrium, and then new equilibria are calculated at incremental steps in both directions on the stepping axis from the initial equilibrium. This continues until the stepping operation has covered the length of the axis between a minimum and a maximum value that is specified.



For an example of the calculation of a property diagram, see tcex08.

Calculating and Plotting a Property Diagram

This topic explains how to calculate a property diagram in POLY. To calculate a property diagram means to calculate a series of equilibria while the value of the stepping axis variable varies between a minimum and a maximum value. With the exception of the stepping axis variable, all the state variables that you set when you calculate the initial equilibrium retain the values when the new equilibria are calculated.

POLY Module Commands

1. Calculate an initial equilibrium in the POLY module.

2. Use SET_AXIS_VARIABLE to set the axis variable, the minimum and the maximum stepping variable values and the step length. The first parameter of SET_AXIS_VARIABLE is the axis number. Since a property diagram only has one axis variable, this is set to 1. For example, if you want to set the axis variable to temperature, and calculate an equilibrium at every 50 K between a minimum temperature of 100 K and a maximum temperature of 2000 K, enter

```
SET_AXIS_VARIABLE 1 T 100 2000 50
```



An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable. Also, the minimum stepping variable value must be smaller than, and the maximum value larger than, the value that you set the state variable to when calculating the initial equilibrium.

3. Use STEP_WITH_OPTIONS and choose `Normal` to perform the stepping operation.

   The phase regions are listed along the stepping axis, the phases contained in each region, and the number of equilibria calculated in that region. Each region is defined by the phases it contains.



The number of equilibria calculated is not just the number of steps that are performed according to the step length and the minimum and maximum values on the axis variable. This is because Thermo-Calc calculates extra equilibria when a new phase is discovered in order to determine the phase region boundary more precisely.

```
POLY_3:s-a-v 1 T 1000 2000 100
POLY_3:step
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    1000.00
...OK

 Phase Region from    1000.00     for:
     BCC_A2
     GRAPHITE
 Global check of adding phase at  1.01118E+03
 Calculated     4 equilibria

 Phase Region from    1011.18     for:
     BCC_A2
     FCC_A1
     GRAPHITE
 Calculated     2 equilibria

 Phase Region from    1011.18     for:
     FCC_A1
     GRAPHITE
 Global test at  1.09000E+03 .... OK
 Global check of removing phase at  1.15727E+03
 Calculated    17 equilibria
```

4. To plot the diagram, open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents the stepping axis variable and Y-axis represents the sum of the mole fractions of all phases (NP(*)).

Calculating a Property Diagram One Phase at a Time

There are many ways to calculate property diagrams in Thermo-Calc. One example is where you can calculate a property diagram with a separate stepping operation being performed for each phase at a time in its default most stable composition (the major constitution). This is useful if you want to create a property diagram for a heterogeneous system with both ordered phases and their disordered pairs.

To calculate a property diagram one phase at a time, use STEP_WITH_OPTIONS and when prompted choose `One_phase_at_time` to perform the stepping operation.

Calculating Several Properties in the Same Diagram

There are many ways to calculate property diagrams in Thermo-Calc. The following is another example. If you perform several stepping calculations after each other, the results of these calculations are all saved in your workspace file. This allows you to the following:

- Calculate (and then plot) missing parts of a specific property inside the first property diagram. These parts are calculated inside the range of the stepping variable with a different control condition.
- Calculate (and then plot) two or more sets of a specific property on the same property diagram for the same system. These can be calculated under different control conditions with stepping operations being performed across the same stepping axis variable range.
- Calculate phase boundary lines and then plot them in a corresponding phase diagram for the same system. This can be especially useful for some defined secondary phase-transformations. For example, if you want to find the phase boundary between BCC_A1 and BCC_B2, or the equal-Gm for two specific phases, or the equal-fraction or equal-activity for two specific phases of a certain species, then this can be useful.

Unless you have opened a new workspace file previously using SAVE_WORKSPACES , the results of the stepping calculations are saved in a RESULT.POLY3 file. To save the results of several stepping calculations in a file different from the workspace file that your results are currently saved to, then use SAVE_WORKSPACES before you perform the first stepping calculation.



SAVE_WORKSPACES overwrites and deletes the results of all previous stepping calculations.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

Phase Diagrams

In this section:

About Phase Diagrams 65
About Binary Phase Diagrams 67
About Ternary Phase Diagrams 68
About Quasi-Binary and Quasi-Ternary Phase Diagrams 70

About Phase Diagrams

Phase diagrams have two or more independent axis variables. Any state variable that has already been set can be used as the mapping variable for a mapping calculation and then as the axis variable for a phase diagram. From a mapping calculation, many types of phase diagrams can be plotted, with one of the mapped variables as one axis variable, and with other mapped variables or any varied property (state or derived variables) or entered symbol (variables, functions or table values) as the other axis variables.

All phase diagrams consist of zero phase fraction lines. There are two distinct types of phase diagrams: those with the tie-lines in the plane of the diagram and those where the tie-lines are not in the plane. The former includes binary phase diagrams and ternary isotherms. The latter includes more general isopleth diagrams with one or more fixed extensive variables (normally, this is a composition).

- The BIN and TERN modules calculate binary and ternary phase diagrams.
- The POTENTIAL and POURABIX modules calculate the more general isopleth diagrams and other related diagrams.

The following topics describe how to calculate the types of phase diagrams in the POLY_3 module. In POLY, you can calculate phase diagram for systems with up to 40 components and with thousands of phases. You can combine activity conditions and fixed phase status and fraction conditions in any way. Thermo-Calc can calculate any arbitrary 2D section through composition space.



There is no guarantee that the conditions set will result in a calculation that reaches an equilibrium.

- Binary Phase Diagram Examples
- Ternary Phase Diagram Examples
- Potential Diagram Example
- Pourbaix Diagram Examples

Calculating and Plotting a Phase Diagram

This topic describes how to calculate a phase diagram in the POLY module. The commands are described in POLY Module Commands and POST Module Commands.

1. Calculate an initial equilibrium in the POLY module.

2. Use SET_AXIS_VARIABLE to set the first axis variable, its minimum and maximum mapping value and the length of each incremental step on this axis. The first parameter of SET_AXIS_VARIABLE is the axis number and is set to 1. For example, suppose you want the mass fraction of C as your first axis variable. You want it to vary between 0 and 0.1, with the length of each incremental step being no more than 0.002. Then enter:

   ```
   SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
   ```

   An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable.

3. Use SET_AXIS_VARIABLE to set the second axis variable and specify its minimum, maximum, and step length values. The axis number is set to 2. For example, suppose you want temperature as your second axis variable and you want it to vary between 900 K and 1900 K, with an incremental step of 25 K. Then enter:

   ```
   SET_AXIS_VARIABLE 2 T 900 1900 25
   ```

4. If you want more than two axis variables, then use SET_AXIS_VARIABLE until you have set all the axis variables. You can set up to five axis variables. Axis variables 3, 4 and 5 must be set temperature, pressure or to the chemical potentials of components.

   You may want to save your workspace with SAVE_WORKSPACES before you perform the mapping calculation. This saves the axis variables you have set. However, it overwrites the results of any previous stepping or mapping calculations done.

5. Use MAP to perform the mapping calculation. The console lists the phase region boundaries and the phases contained on one side of each boundary.

```
Phase region boundary  30 at:   1.363E+03  2.012E-01
    FCC_A1
 ** GRAPHITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   1.990E+03  2.526E-01
    LIQUID
 ** GRAPHITE
Calculated.                     13  equilibria
Terminating at known equilibrium
```

6. To plot the diagram, use POST to open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents mapping axis variable 1 and the Y-axis represents mapping axis variable 2.

About Binary Phase Diagrams

Binary phase diagrams are by far the most common found in the literature and calculated by computers. However, most real systems have more than two components and thus binary diagrams are more a kind of exercise in order to calculate more realistic phase diagrams.

You can calculate many types of binary phase diagrams with POLY, but the traditional one has one composition axis and the temperature on the other axis. This is calculated by first specifying a single equilibrium by setting conditions such as

```
SET_CONDITION T=1200, P=1E5, W(C)=.02, N=1
```

This means that the temperature should be 1200 K, pressure 1 bar, mass fraction of C is 0.02 (i.e., 2 weight percent) and the system contains one mole of atoms. Note that one does not set a condition on the amount of the second component. This is simply taken to be the rest of the system.

After setting these conditions one can calculate the equilibrium by giving the command:

```
CALCULATE_EQUILIBRIUM
```

When the calculation has converged, one continues by setting the axes for the diagram calculation. In most cases, one is interested in the complete composition range but the temperature range may vary.

```
SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
SET_AXIS_VARIABLE 2 T 900 1900 25
```

This means that the axis number 1 is taken to be the mass fraction of C which may vary between 0 and 0.1 with a maximum increment of 0.002. The axis number 2 is the temperature varied between a minimum 900 and maximum 1900 K with a maximum increment of 25.

Before starting the mapping, it is a good rule to SAVE the workspaces. If this is done just before the MAP command, and the MAP command fails for some reason, the user can restart from the situation just before mapping and try to find a better start point.

```
SAVE
MAP
```

The diagram is plotted in the post-processor. The post-processor will automatically set the same axes for plotting as used for mapping.

```
POST
PLOT
```

BINARY_DIAGRAM

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Access to specific databases designed for BIN, such as TCBIN, is required.

To enter the module, at the SYS prompt type `GOTO_MODULE BINARY`. There are no other commands for this module. Follow the prompts to plot a diagram.

Syntax	BINARY_DIAGRAM
Prompts	`Database: /TCBIN/`
	`First element` `Second element`
	`Phase diagram, Phase fraction (FE), G- OR A-curves (G/A): /Phase_Diagram/`

About Ternary Phase Diagrams

There are many types of ternary phase diagrams but perhaps the most common is the isothermal section. In this case, the temperature is constant, which means that the tie-lines are in the plane of the calculation. Isothermal sections and monovariant lines on the liquidus surface can be calculated in traditional way. They can also be calculated in the TERN module, but this requires a special database (such as PTERN).

In order to set up calculation of a ternary isothermal section in the system Al-Mg-Si, do the following (after retrieving the data from the database (TDB) module):

```
SET_CONDITION T=823,P=1E5,N=1,X(MG)=.01,X(SI)=.01
```

```
C_E
```

Note that there is no condition on the amount of Al as that is the "rest". N=1 specifies that the system is closed. This calculation gives one point inside the system. Now define the axis:

```
S-A-V 1 X(MG) 0 1 0.01
S-A-V 2 X(SI) 0 1 0.01
```

Of course, you might not be interested in the whole section, and in such cases specify different lower and upper limits for the axes. Then give a SAVE command before the MAP command:

```
SAVE almgsi-823
MAP
```

The result can be plotted in the POST module. Ternary isopleths are equally simple to calculate. Use the same conditions as above if you are interested in a section of Al-Si at 1 mole percent of Mg, just define a different set of axis:

```
S-A-V 1 X(SI) 0 1 .01
S-A-V 2 T 500 2000 25
SAVE almgsi-1mg
MAP
```

In the resulting diagrams, the tie-lines are not in the plane of the diagram, thus the lever rule etc. cannot be applied. But you can calculate more elaborate sections. An interesting diagram is the section from pure Al to Mg2Si, which is almost a quasi-binary section. In order to calculate this, set up the conditions differently:

```
SET-CONDITION T=823, P=1e5, N=1, X(MG)-2*X(SI)=0, W(MG)=.01
C-E
```

Note that there is no condition on the amount of Si as this is given by the relation X(MG)-2*X (SI)=0. Also note that you can mix conditions in X and in W. Then set the axis, save the workspace and map.

```
S-A-V 1 W(MG) 0 .1 .01
S-A-V 2 T 500 1500 10
SAVE al-mg2si
MAP
```

A special type of ternary phase diagrams is liquidus surfaces. This is still not simple to calculate as a separate start point is needed for each separate line at each temperature.

However, you can easily calculate the monovariant lines where the liquid is stable together with two condensed phases:

```
SET-CONDITION T=800, P=1e5, N=1, X(MG)=0.01, X(SI)=.01
```

```
C-E
C-S P LIQ=FIX 0.3
S-C T=NONE
C-E
```

Now there should be an equilibrium where liquid is just stable. Set the axis to be the compositions.

```
S-A-V 1 X(MG) 0 1 .01
S-A-V 2 X(SI) 0 1 .01
SAVE almgsi-luni
MAP
```

TERNARY_DIAGRAM

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram.

To enter the module, at the SYS prompt type GOTO_MODULE TERNARY. There are no other commands for this module. Follow the prompts to plot a diagram.

Syntax	TERNARY_DIAGRAM
Prompts	`Database: /FEDEMO/`

	`First element:`
	`Second element:`
	`Third element:`

	`Phase diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/`
	`Temperture (C) /1000/`
	`Global minimization on: /Y/`

About Quasi-Binary and Quasi-Ternary Phase Diagrams

Quasi-binary diagrams, as well as quasi-ternary diagrams and so forth, have often been misunderstood and misused. A real quasi-binary phase diagram is for a ternary system where one component has a fixed activity or chemical potential, and a real quasi-ternary phase diagram is for a quaternary system where one component has a fixed activity or chemical potential.

A typical example of quasi-ternary system is a quaternary system Fe-Cr-Ni-C calculated at fixed carbon activity. The condition can be set as follows:

```
SET-REF-STATE C GRAPH ,,,,
SET-CONDITION T=1273, P=1e5, N=1, X(CR)=.1, X(NI)=.1, ACR(C)=.002
```

In some cases, the activity may vary in a quasi-binary section if one has a phase fixed instead (and where the phase may vary in composition). The advantage with the quasi-binary section is that the tie-lines will be in the plane of the diagram and thus the lever rule etc is obeyed.

A quasi-binary section in Ca-Fe-O when the liquid oxide is in equilibrium with liquid Fe can be specified as follows:

```
DEFINE-COMPONENTS CAO FE FEO
SET-CONDITION T=1850, P=1e5, N=1, X(CAO)=.1
CHANGE-STATUS PHASE FE-LIQ=FIX 0
```

and the mapping can be done with the following axis

```
S-A-V 1 X(CAO) 0 1 .01
S-A-V 2 T 1500 2000 25
```

However, it is a problem as FE-LIQ is not the stable phase for pure iron below 1811. One will have to calculate separate sections depending on the stable modification of Fe.

Calculating a Quasi-Binary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example where a quasi-binary phase diagram is used for calculations on a ternary system in which one component has an activity or chemical potential that is fixed (although if you have fixed a phase and the phase composition varies, then the activity or chemical potential may also vary). The tie-lines in a quasi-binary diagram are in the diagram's plane of the diagram. This means that the calculation follows the lever rule as well as other rules.

When calculating a quasi-binary phase diagram it is necessary to set a condition on either activity or chemical potential of the third component. To specify a meaningful value it is recommended that you first change the component's reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-binary Fe-Cr-O system with fixed oxygen activity, you can enter the following:

```
SET_REFERENCE_STATE O GAS ,,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is oxygen, you might enter

```
SET_CONDITION ACR(O)=0.2
```

Alternative Way to Set the Component Activity

As an alternative to set the activity of the component, you can Use CHANGE_STATUS to set a phase to fixed. For example, suppose you want to compute the iron-saturated section in "FeO"-SiO2. You then enter:

```
CHANGE-STATUS FCC=FIX 0
```

Calculating a Quasi-Ternary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example of a quasi-ternary phase diagram used for calculations on a quaternary system where one component has a fixed activity or fixed chemical potential.

When calculating a quasi-ternary phase diagram it is necessary to set a condition on either activity or chemical potential of the fourth component. To specify a meaningful value it is recommended that you first change the component's reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-ternary Fe-Cr-Ni-C system with fixed carbon activity, you can enter the following:

```
SET_REFERENCE_STATE C GRAPH ,,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is carbon, you might enter

```
SET_CONDITION ACR(C)=0.002
```

T0 Temperature Simulations

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Making a T0 Temperature Simulation 74

About T0 Temperature Simulations

The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition in a multicomponent system. The T_0-temperature is located within the two-phase field between the phases and it is the theoretical limit for a transformation without diffusion. T0 temperatures are often of interest if you want to understand how diffusionless transformations work. The T0 temperature in a multicomponent system with a fixed composition is temperature at which the tangent lines of the Gibbs energies of the two target phases are the same.

If the composition of one or two components varies, the common Gibbs energy for the two phases in partial equilibrium of a diffusionless transformation becomes a plane or surface, and the T0 temperature becomes a line or plane.



See Console Mode examples tcex 23 and tcex41.

Making a T0 Temperature Simulation

This describes how to perform a T0 temperature simulation and apply a stepping calculation to its initial result.

Before you perform a T0 temperature calculation, you must have defined your initial system and be in POLY. The initial overall composition must have appropriate settings for the desired T0 temperature calculation for the two target phases.

POLY Module Commands

1. Use SET_CONDITION to set the conditions of your calculation in the same way as when you calculate an ordinary equilibrium.
2. Use COMPUTE_EQUILIBRIUM to run the calculation. The calculation does not need to reach an equilibrium in which any of the target phases is stable.
3. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS and choose `T-zero`.
4. When prompted, specify the names of the two target phases for which the T0 temperature (where the phases' Gibbs energies are equal) is to be calculated.
5. If the T0 temperature between the two target phases is calculated, this temperature (in Kelvin) is shown in the Console window.
6. If you want to do a stepping calculation based on this initial T0 temperature calculation, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done the same way as when you calculate a normal property diagram.



When a T0 temperature simulation is run, you cannot set temperature as the stepping variable.

7. Use STEP_WITH_OPTIONS and choose `T-zero` to initiate the stepping calculation. You are prompted to specify the names of the target phases for which the T0 temperature is calculated.

   During the STEP T-ZERO calculation procedure, the calculated T0 values are presented next to the stepping variable.

   For example, part of the output might look like this:

```
Phase Region from   1.000000E-01 for:
BCC_A2
FCC_A1
1.000000E-01         940.24
9.250000E-02         941.20
2.500000E-03         977.61
7.500000E-09         979.34
```

   When the stepping calculation has finished, you can move to the POST module and plot the T0 line against the stepping composition variable or another varying axis value. Or you can impose the calculated T0 line onto a normal phase diagram.

Paraequilibrium

In this section:

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Calculating a Paraequilibrium 77

About Paraequilibrium

A paraequilibrium is a partial equilibrium where one interstitial component (such as carbon C and nitrogen N) in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements). The chemical potential for the interstitial component in two partially equilibrated phases is equal in such a case, but this is not true for the other components. In such a paraequilibrium state, it is possible to have a transformation that is partly without partitions, where a new phase of the mobile component can form with different content but where the slowly diffusing components retain their compositions.

A paraequilibrium calculation is useful when, for example, you want to study phase transformations in systems with large differences in the diffusivities of different elements. Transformations occurring under paraequilibrium states can be much more rapid than if full local equilibrium holds at the phase interface.

Calculating a Paraequilibrium

Calculating a Paraequilibrium

This topic describes both how to calculate an initial paraequilibrium with two target phases, and how to base a stepping calculation on this initial calculation.

Before you do any paraequilibrium calculations, you must have defined your initial alloy system and be in POLY. The initial overall composition must have appropriate settings for the desired paraequilibrium calculation for the two target phases.

1. Use SET_CONDITION to set the conditions of your calculation just like when you calculate an ordinary equilibrium.

2. Use CHANGE_STATUS to set the status of the chosen interstitial components to SPECIAL. For example, if C is an interstitial component, enter:

   ```
   CHANGE_STATUS COMPONENTS C=SPECIAL
   ```

   This gives you a clear picture on u-fractions of the substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that the specified components are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

3. Use COMPUTE_EQUILIBRIUM to run the calculation.
4. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS `Paraequilibrium` to perform the paraequilibrium calculation.

5. Specify the names of the target phases of the paraequilibrium state. For example, `FCC#1 BCC` and `FCC#2 M23C6`.

   Both phases must have similar interstitial/vacancy sublattices that the fast-diffusion interstitial components occupy. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system.

6. Specify the names of one or more fast-diffusing components. These components must be located on the interstitial/vacancy sublattices in both of the chosen phases.

   Interstitial components (for instance C and N combined) may have significantly different behaviours depending on how they are partitioned in different structured phases.

   If the paraequilibrium between the two specified phases is successfully calculated, then a message is displayed, for example:

   ```
   NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02 N =
   4.1548129E-03

   NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04 N =
   2.3781027E-04

   All other compositions are the same in both phases
   ```

   The first two lines show the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in each phase. These contents are expressed in u-fractions. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) are equal in the two target phases at the paraequilibrium state.

7. If you want to do a stepping calculation based on this initial paraequilibrium, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done exactly in the same way as when you calculate a normal property diagram.

8. Use STEP_WITH_OPTIONS → `Paraequilibrium` to initiate the stepping calculation. You are prompted to specify the names of the target phases of the paraequilibrium states as well as the fast-diffusing components.

The stepping calculation is performed, and the different phase regions are listed with columns for the value of the stepping variable, the amounts of the two target phases, the u-fractions of interstitial(s) in each of the two phases, and the LNACR value(s) of the interstitial component(s).

```
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.977501E-02   6.609390E-04  -2.303643E-01
   8.900000E+02    0.161    0.839   5.421135E-02   6.889794E-04  -1.689777E-02
   8.800000E+02    0.148    0.852   5.872152E-02   7.140931E-04   1.943989E-01
   8.700000E+02    0.137    0.863   6.329608E-02   7.362105E-04   4.040959E-01
   8.600000E+02    0.127    0.873   6.792661E-02   7.552871E-04   6.126989E-01
   8.500000E+02    0.119    0.881   7.260558E-02   7.713010E-04   8.206607E-01
   8.400000E+02    0.111    0.889   7.732629E-02   7.842505E-04   1.028392E+00
   8.300000E+02    0.105    0.895   8.208278E-02   7.941530E-04   1.236267E+00
   8.200000E+02    0.099    0.901   8.686971E-02   8.010431E-04   1.444633E+00
   8.100000E+02    0.093    0.907   9.168236E-02   8.049714E-04   1.653814E+00
   8.000000E+02    0.089    0.911   9.651648E-02   8.060032E-04   1.864114E+00
```



It is possible to now move to the POST module and plot some of the results of the calculation. For an example of a paraequilibrium calculation and how it can be plotted, see Console Mode example tcex23.

Potential Diagrams

In this section:

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POTENTIAL_DIAGRAM 81
Calculating a Potential Diagram 82
Calculating a Potential Diagram with Different Pressure 83

About Potential Diagrams

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

This topic describes how to calculate such potential diagrams with the POTENTIAL module, and how to later modify the pressure of such a calculation in POLY. The calculation done by the POTENTIAL module always assumes a pressure of 1 bar.

POTENTIAL_DIAGRAM

The POTENTIAL_DIAGRAM (POT or POTENTIAL) module is a potential phase diagram calculation module.

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

To enter the module, at the SYS prompt type `GOTO_MODULE POTENTIAL`.



There are no commands for this module. Follow the prompts and see About Potential Diagrams for details about how to calculate using potential diagrams.

Syntax	POTENTIAL_DIAGRAM
Prompts	`Database: /POT/` Press <Enter> and the program lists the available databases. Type one of the database names and press <Enter> to select. The following default elements are then based on the chosen database.
	`Matrix element: /Fe/`
	`First potential species: /S1O2/`
	`Second potential species: /O2/`
	`Temperature: /1000/`

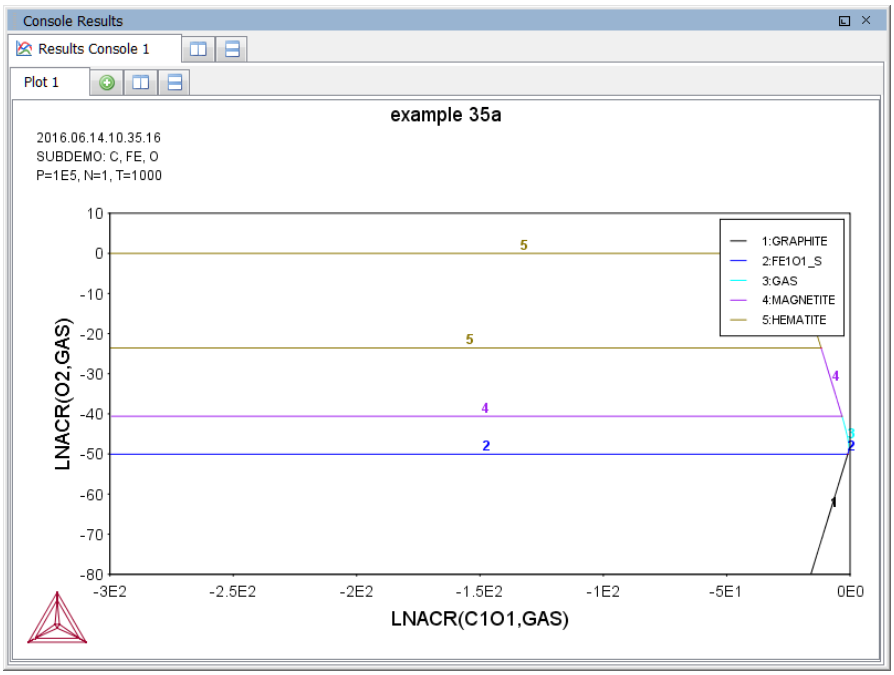
Calculating a Potential Diagram

You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulphides, sulphates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases).

1. Use GOTO_MODULE and enter `POTENTIAL`.
2. Specify which substance or solution database to use. Any substance or solution database can be used that has a gaseous mixture phase, metals (or alloys), and solids such as metalxides, sulphides, sulphates, carbonates, silicates, nitrides, and nitrates (stoichiometric or solution phases).
3. Specify the matrix element (a metal) and the two gaseous species that define you metal-gas interaction system. The names of these components must be available in the database you are using.
4. Set the temperature (in Kelvin). (The pressure is always 1 bar.)

   A potential diagram with the activities of the two gaseous species as mapping variables is calculated. These mapping variables are also set as the axis variables in the plotted diagram.

   An example diagram (Console Mode example 35).



A POLY3 file is also automatically saved in the current working directory with the default name POT.POLY3.

5. When the diagram is plotted, it opens the POST module where you can modify the plotted diagram in any way you like.

Calculating a Potential Diagram with Different Pressure

It is possible to modify both the calculation and the plotted diagram that the POTENTIAL module generates in the POLY and POST modules. You can do this by opening a POLY3-file with the results from a POTENTIAL module calculation in either POLY or POST. You can modify the calculation in the same way that you can modify any ordinary mapping calculation or phase diagram. For example, this is useful for calculating a potential diagram at a pressure other than 1 bar.

POLY Module Commands

You must have calculated a potential diagram already, and have the saved POLY3-file available.

1. Use GOTO_MODULE and enter `POLY`.

2. Use READ followed by the name of the POLY3 file that contains the results of the potential diagram calculation that you want to modify.

   A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

3. This opens the workspace file and loads the previous settings and results. The activities of the two gaseous species is now part of the conditions, and these conditions are set as the mapping variables.

4. Use SET_CONDITION to specify the pressure under which you want the potential diagram to be calculated. For example, to set the pressure to 1000 bar, enter:

   ```
   SET_CONDITION P=1e8
   ```

5. Use COMPUTE_EQUILIBRIUM to compute the initial equilibrium.

   You may also want to use ADD_INITIAL_EQUILIBRIUM to calculate some additional equilibria that the mapping calculations are based on.

6. Use MAP to perform the mapping calculations.
7. Use GOTO_MODULE and enter `POST` to set conditions for visualization and to plot the diagram.

Scheil Simulations

In this section:

About the Scheil-Gulliver Solidification Simulations 86
Scheil in Graphical Mode vs Console Mode 90
Examples of Scheil-Gulliver Calculations 91
Simulating a Scheil Solidification Process 92
State Variables for Scheil 95

About the Scheil-Gulliver Solidification Simulations



In Console Mode most of the set up for the Scheil module is via the START_WIZARD command where you are prompted to answer a series of questions. You can also perform Scheil calculations in Graphical Mode using the Scheil Calculator, which is recommended for most users. See Scheil in Graphical Mode vs Console Mode to compare.

Thermo-Calc is often used to perform equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can also be simulated.

A well-known example of a non-equilibrium calculation is the *Scheil-Gulliver solidification simulation*. In Thermo-Calc, the available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Classic Scheil Simulation

This is a Scheil simulation based on the well-known *Scheil-Gulliver* model. If this model is used without "fast diffusers" it is *Classic Scheil* simulation with the following assumptions:

- Diffusion in the liquid phase is assumed to be very fast, that is, infinitely fast.
- Diffusion in the solid phases is so slow that it can be ignored, that is, diffusion is assumed to be zero.
- The liquid/solid interface is in thermodynamic equilibrium.

In this Classic Scheil simulation the temperature is decreased step-by-step. When the temperature drops below the liquidus temperature the equilibrium amount and composition of solid and liquid phase is calculated. The solid phase is removed from the system and only the amount and composition of the liquid phase is used for the next calculation step at a lower temperature. Again, the equilibrium amount and composition of solid and liquid phase is calculated and again the solid phase is removed from the system for the next step. This procedure is repeated until the last liquid disappears.

This calculation procedure is equivalent to assuming that there is no diffusion in the solid phase and infinitely fast diffusion of all elements in the liquid phase. It has been shown to be a good approximation of the solidification of most alloys such as Ni-superalloys, Cu alloys, Al alloys, Mg alloys, and others. However, in materials with interstitial elements, such as carbon, ignoring diffusion in the solid causes discrepancies with experimental results.

Interstitial elements have much faster diffusion rates. The assumption of no diffusion in the solid phase during solidification is thus not correct at most industrial or lab-scale solidification rates.

For this reason, a variant of the Scheil simulation was developed and implemented in Thermo-Calc, where one or more elements can be defined as *fast diffusers*. See Other Options: Fast Diffusers and Scheil Simulations.

Scheil Simulation with Back Diffusion in Primary Phase

The *Scheil simulation with back diffusion in primary phase* kinetic model quantitatively takes into account the real back diffusion of all elements in the primary solid phase (typically the FCC or BCC phase). This model requires the use of both a thermodynamic and mobility database. The calculation also requires the cooling rate to be specified; a fast cooling rate allows for less time for back diffusion and the simulation result is similar to the classic Scheil-Gulliver solidification simulation. A very slow cooling rate allows for almost complete back diffusion, the solidification simulation is then close to an equilibrium calculation. It also requires that the size of the solidification domain is specified. In most cases this domain size corresponds to the secondary arm spacing, as this is where typically the liquid is trapped during solidification.



The secondary arm spacing also depends on the cooling rate. For this reason, a simple empirical relation between cooling rate and secondary arm spacing is predefined in Thermo-Calc.

For the *Scheil simulation with back diffusion in primary phase* model the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- The liquid/solid interface is in thermodynamic equilibrium.

Also see Other Options: Fast Diffusers and Scheil Simulations.

Scheil with Solute Trapping

The *Scheil with solute trapping* model simulates deviation from local equilibrium for the primary phase. It is useful for high solidification speeds, such as those seen in additive manufacturing applications and is based on the Aziz [1982] model for solute trapping and extended to multicomponent systems.

The model is based on the main assumption that the primary phase is the only dendrite forming phase affected by solute trapping.

For equilibrium- and Scheil-type solidification simulations thermodynamic equilibrium is established at the solid-liquid interface. This means that solutes are partitioned between the solid and liquid phases according to solidus and liquidus lines of the phase diagram. The assumption of thermodynamic equilibrium at the solid-liquid interface however breaks down for very fast solidification rates, that are encountered for example during additive manufacturing. Aziz [1982, Aziz; 1988, Aziz], proposed a model that links partitioning at the solid-liquid interface to solidification rate / interface velocity. Basically, the faster the solidification rate, the lower is the partitioning at the interface. Put very simply, what is thought to happen, is that the solid-liquid interface moves so quickly, that the solutes in the liquid are trapped in the advancing solid phase, thus the name “solute trapping”.

Aziz [1982] proposed a model to account for solute trapping based on balancing the overall kinetics at the solid-liquid interface. The two terms to be balanced are the velocity of the interface, that is calculated based on the cooling rate and considerations of the solid-liquid geometry (dendrite arm spacing) the interface kinetics, that follows from the trans-interface diffusion (meaning how fast solutes travel from one side of the solid-liquid interface to the other) and the change of phase from liquid to solid without changing the composition.

For a *Scheil with solute trapping* model the following assumptions are made.

- Only one primary solid phase forms dendrite, NOT necessarily the first solid phase
- Solute trapping in primary solid phase only. Other solid phases have equilibrium compositions following Scheil model
- Amounts of solid phases are dependent on solute trapping and solidification speed
- Dynamic liquidus for primary solid phase is dependent on solute trapping and solidification speed

Solute Trapping References

[1982, Aziz] Aziz, M. J. (1982). Model for solute redistribution during rapid solidification. Journal of Applied Physics, 53(2), 1158–1168.

[1988, Aziz] Aziz, M. J., & Kaplan, T. (1988). Continuous growth model for interface motion during alloy solidification. Acta Metallurgica, 36(8), 2335–2347.

Other Options: Fast Diffusers and Scheil Simulations

If a *Classic Scheil* or *Scheil simulation with back diffusion in primary phase* model is selected plus one or more *Fast diffuser* check boxes selected, then Thermo-Calc takes into account the concept of the *fast diffuser*. Typically, C is defined as a fast diffuser, but also other

elements such as N, O, or others can also be defined.



Fast diffuser does not quite define this since diffusion is not actually simulated. It is simply assumed that the “fast diffusers” distribute throughout the solid and liquid phase according to thermodynamic equilibrium. This corresponds to *infinitely fast diffusion* for the selected elements.

For a *Classic Scheil* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the solid phases, except the ones defined as “fast diffusers”, is zero.
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

For a *Scheil simulation with back diffusion in primary phase* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

The Classic Scheil simulation and Classic Scheil simulation with fast diffuser models can be considered *thermodynamic* models. There are clear limitations as a certain amount of back diffusion always takes place in the solid phase at real solidification.

You can also use the more sophisticated *Scheil simulation with back diffusion in primary phase* kinetic model. Adding the fast diffuser option to this can be useful, for example for interstitials like C in steels where these then equilibrate in all phases and not just the primary phase.

Summary

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Scheil in Graphical Mode vs Console Mode



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase

Scheil in Graphical Mode vs Console Mode

Type of Calculation	Console Mode	Graphical Mode
Classic Scheil	Use the START_WIZARD command to answer prompts	Scheil Calculator > select the Classic Scheil button on the Configuration window. Or use the Quick Start template > and select Scheil solidification simulation
Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > select the Scheil with back diffusion in the primary phase button on the Configuration window then enter the settings as needed. A mobility database is required.
Scheil with solute trapping	SOLUTE_TRAPPING command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > select the Scheil with solute trapping button on the Configuration window then enter the settings as needed.
Fast diffusers and Classic Scheil	Use the START_WIZARD command to answer the prompt `Fast diffusing components` where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > select the Classic Scheil button plus one or more of the Fast diffuser check boxes next to the composition(s) on the Configuration window then enter the settings as needed.

Type of Calculation	Console Mode	Graphical Mode
Fast diffusers and Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer the prompt `Fast diffusing components` where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > select the Scheil with back diffusion in the primary phase button plus one or more of the Fast diffuser check boxes next to the composition(s) on the Configuration window then enter the settings as needed. A mobility database is required.

Examples of Scheil-Gulliver Calculations

About the Scheil-Gulliver Solidification Simulations

tcex15 - Simulating the Solidification of a Cr-Ni Alloy

This is an example of a solidification simulation of a Cr-Ni alloy. This is a classic Scheil-Gulliver simulation.

This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- START_WIZARD
- COMPUTE_TRANSITION
- ADD_INITIAL_EQUILIBRIUM
- ENTER_SYMBOL
- ADVANCED_OPTIONS
- STEP_WITH_OPTIONS
- MAKE_EXPERIMENTAL_DATAFILE
- CHANGE_STATUS

tcex30a and 30b - Scheil Calculation for an Al-4Mg-2Si-2Cu Alloy

The Equilibrium Calculation Module (POLY3) and About the Scheil-Gulliver Solidification Simulations

These examples show two ways to do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy. In part A, you use the POLY3 module and the STEP_WITH_OPTIONS command with an EVALUATE option. Then in part B you use the SCHEIL module commands to do the same thing. Data from the COST2 database is used and included with the example in the file named *tcex30_cost2.TDB*.

tcex48 - Scheil Solidification with C Back Diffusion

This is an example of Scheil solidification with C back diffusion in solid phases. The results are compared between a simple Scheil and equilibrium calculation. The FEDEMO database is used.

tcex54 - Scheil Solidification of an Al-2.1Cu-1Si Alloy including Back Diffusion

This is an example of a solidification simulation of a Al-2.1Cu-1Si alloy. The back diffusion option in the Scheil module is used, i.e. there is back diffusion in the primary phase. The example uses both the thermodynamic ALDEMO and mobility MALDEMO demo databases included with your installation.

tcex57 - Scheil Solidification with Solute Trapping

This is an example of a solidification simulation of a Al-7.5Si-0.2Cu system. The solute trapping option in the Scheil module is used. The example uses the thermodynamic ALDEMO demo database included with your installation.



See the Graphical Mode example T_13: Scheil Solidification with Solute Trapping for an additional comparison to Classic Scheil.

Simulating a Scheil Solidification Process

- SCHEIL Module Commands
- About the Scheil-Gulliver Solidification Simulations

Simulating a Scheil-Gulliver solidification process involves calculating the liquid composition of a higher-order multicomponent system at each step of a cooling process, and resetting the liquid composition as the composition of the entire system (after having removed all amount of solid phase).

The step-by-step instructions below are intended as a simple example of setting up a calculation using the wizard in Console Mode. You can also use the macros available and briefly described in Examples of Scheil-Gulliver Calculations.

The following does not include any prompts related to using back diffusion or solute trapping. See START_WIZARD for additional details about when these options are enabled with the USE_BACK_DIFFUSION and SOLUTE_TRAPPING commands.

1. At the prompt type GOTO_MODULE SCHEIL.
2. Type START-WIZARD and press <Enter>.
3. Specify which `Database` to use. Type `?` for a list of available databases based on your license.
   - Type `FEDEMO` for this example.
4. Specify the `Major element or alloy` in your system. For example, enter `Fe` (steel/Fe-alloy), `Al` (Al-based alloy), or `Ni` (Ni-based super alloy).
   - Type `Fe` for this example.
5. Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Press <Enter> to keep the default for mass percent or type `N` to use mole percent.
   - Keep the default for this example (press <Enter>).
6. Specify the name of the `1st alloying element`. You can directly specify mass or mole percent after the name. If this is not specified, then you are prompted to enter it separately.
   - Type `Cr 5` for this example.
7. Specify the other alloying elements in the same way as you specify the first.
   - Type `C 1` for this example.
8. After you have specified your last alloying element, press <Enter>. This ends the process of defining the bulk composition of the alloy system.

> You can also specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element. As a general example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

- Press <Enter> for this example.

9. Specify the starting `Temperature (C)` in Celsius. The default is `2000`.

   This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

   - Keep the default for this example (press <Enter>).

10. At the `Reject phase(s)` prompt enter the name of the phases to reject or press <Enter> for the default `NONE`.
    - Keep the default s for this example (press <Enter>).

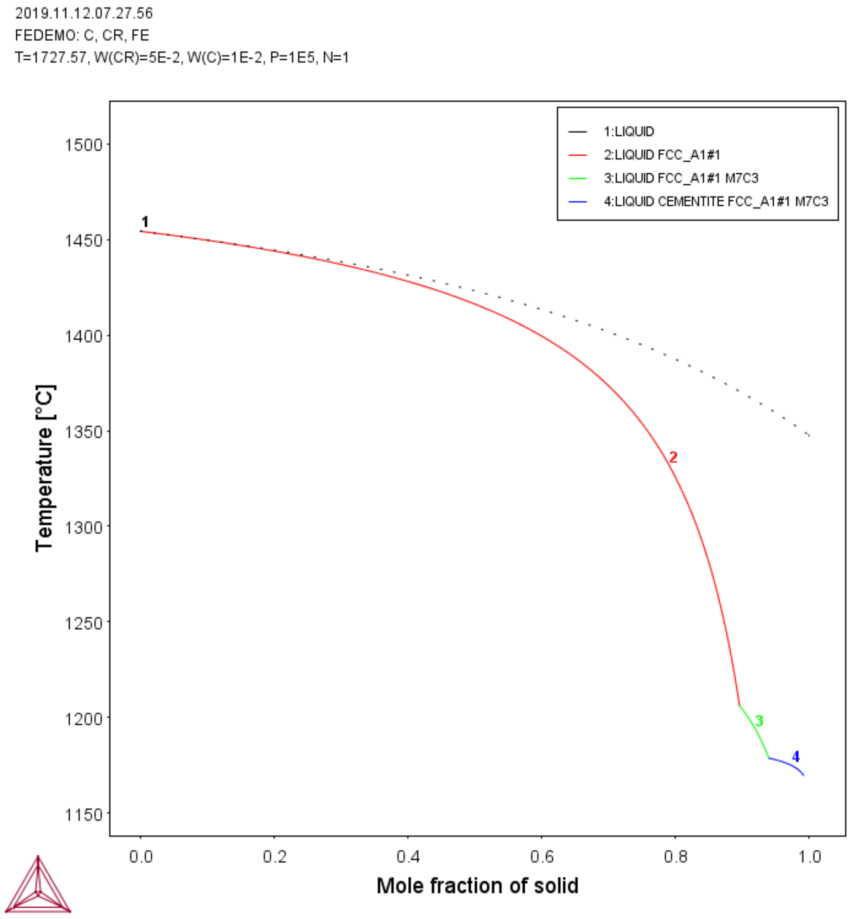
11. At the `Restore phase(s)` prompt you may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press <Enter> for the default `NONE`.
    - Keep the default for this example (press <Enter>).

12. When prompted `OK?` type `N` to go back to reconsider which phases to reject or restore. Type `Y` to continue. The thermodynamic data about the alloy system you defined is retrieved from the database.
    - Keep the default for this example (press <Enter>).

13. At the `Should any phase have a miscibility gap check` prompt, press <Enter> for the default `N` or type `Y` then specify the `Phase with miscibility gap`.
    - For this example, type `Y` then enter `FCC`as the phase with miscibility gap.

14. If you answer `Y` to the miscibility gap check, then next enter the following for `Major constituent(s) for sublattice 1` and `Major constituent(s) for sublattice 2`.
    - Enter Cr for sublattice 1 and C for sublattice 2 in this example. Then at the `Phase with miscibility gap` prompt press <Enter>. The system responds with `LIQUID PHASE NAME: LIQUID`.

15. Specify the names of any `Fast-diffusing components`. Press <Enter> for `NONE` or type all the names on the same line then press <Enter>. Keep the default for this example (press <Enter>).



After the Scheil-Gulliver solidification simulation runs, the diagram Temperature versus Mole Fraction of Solid is plotted in the Console Results window.

State Variables for Scheil

Post processing is done the same way as POLY-3: specific variables for plotting in the Scheil module are listed.

POLY Module Commands

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

Abbreviation	State variable
T	Temperature in Celsius

Abbreviation	State variable
NL/BL	Mole/mass fraction of liquid
NS/BS	Mole/mass fraction of all solid phases
NS(ph)/BS(ph)	Mole/mass fraction of a solid phase
W(ph,el)	Weight fraction of an element in a phase
X(ph,el)	Mole fraction of an element in a phase
Y(ph,el)	Site fraction of an element in a phase
NN(ph,el)	Distribution of an element in a phases
NH/BH	Heat release and Latent heat per mole/gram
CP/BCP	Apparent heat capacity per mole/gram
NV/NV(ph)	Molar volume of the system or a phase
DS/DS(ph)	Average density of the system or a phase
BT	Apparent volumetric CTE of the system

Aqueous Solutions and Pourbaix Diagrams

In this section:

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Calculating a Pourbaix Diagram 100
Plotting More Pourbaix Diagrams 102
Stepping Calculations in an Aqueous Solution 104
POURBAIX_DIAGRAM Module 105

About Aqueous Solutions and the Pourbaix Diagram

This command or module is not available with GES6.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Heterogeneous equilibrium calculations involving aqueous solutions are not different from other equilibrium calculations, but the setup of the equilibrium conditions and the reference states of the system is more complex. For example, the pH and Eh values of the aqueous solution phase are normally complex functions of bulk composition, temperature and pressure conditions.

For some simple systems, thermodynamic approximations of pH-Eh calculations can be used. But Thermo-Calc also has comprehensive thermodynamic models and databases for various non-ideal solution phases. These let you accurately calculate pH and Eh property diagrams (and many other types of property diagrams) in complex aqueous solutions in a variety of conditions.

A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

A Pourbaix diagram is a pH-Eh phase diagram where the tie-lines are not in the plane. The chemical potentials or activities of two system components (H+ and EA) are used as mapping variables and the pH and Eh quantities are normally plotted on the X- and Y-axes of the diagram. You can use many other properties as axis variables in various property diagrams for the interaction system at a specific temperature and pressure. The phase relations

between the aqueous solution and various metal forms, oxides, hydroxides, sulphides, sulphates, nitrates, silicates, carbonates and other solids, or gaseous mixtures, are represented as different fields defined by acidity and electric potential.

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases. The compositional definition and variations and the basic solvent and electron components H2O, H+1 and ZE are automatically determined by the aqueous solution phase in the Pourbaix module.



See Console Mode examples tcex40 and tcex53.

Key Components

These key components are defined as follows:

Component	Component status	Reference state	Ref-T(K)	Ref-P(Pa)
H2O	ENTERED	AQUEOUS	*	100000
H+1	ENTERED	SER		
ZE	ENTERED	REFERENCE_ELECTRODE	*	100000

Besides the aqueous solution phase, your system may also contain a gaseous mixture phase. Other neutral and charged gaseous species may also be constituents. For multicomponent systems there are normally also some interacting solid phases (stoichiometric or solution) as the so-called secondary phases. These are typically the matrix and/or precipitate phases in the alloys of interest.

Some databases have been specially developed for the Pourbaix module's diagram calculations. Such a database contains all necessary phases, i.e., an aqueous solution phase, a gaseous mixture phase, some alloy solid solution phases and some secondary solid phases. Databases developed for the Pourbaix module include *PAQ* (TCS Public Aqueous Solution Database) or *PAQS* (TGG Public Aqueous Solution Database).



If such a dedicated Pourbaix module is not used, then an aqueous solution database such as *TCAQ* (TC Aqueous Solution Database), *AQS* (TGG Aqueous Solution Database), or any user-specified aqueous databases can be used.

This database contains at least the AQUEOUS and REFERENCE_ELECTRODE phases. The aqueous solution database needs to be appended with additional required data and phases, such as interacting alloy (solid) solution phases and secondary (solid and liquid) phases. Additional data is from one or more databases, such as SSUB/SSOL/TCFE or other substances/solutions databases.

Calculating a Pourbaix Diagram

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases.

When calculating a Pourbaix diagram, you need to have a database with an aqueous solution phase (that is, a phase with water as the dissolving solvent and with aqueous cation/anion and complex species as the dissolved solutes). Due to restrictions of aqueous solution models (SIT, HKF, Pitzer) used in the Thermo-Calc software, the aqueous solution database must be designed in the same Thermo-Calc database format as that used in the PAQ, PAQS, TCAQ and AQS databases for the aqueous solution phase.

Pourbaix diagram calculations are done in the advanced Pourbaix module.

How to Calcuate a Pourbaix Diagram

1. At the `SYS` prompt, enter GOTO_MODULE POURBAIX.
2. At the `Need any instruction on the POURBAIX module?` prompt, press <Enter> to skip or enter `Y` to learn more.
3. Press <Enter> at the prompt `Enforce a PAUSE after plotting when running a MACRO?`.
4. Press <Enter> to accept the default `1` to `Start a completely new POURBAIX diagram calculation` or enter `3` to `Open an old file and make another POURBAIX calculation`.

   To choose `3`, you must have already done a Pourbaix calculation and have it saved in a POLY3 file. The new calculation uses the same system definition as the previous calculation, but the other conditions, such as the bulk composition, temperature and pressure, can be modified in the next step.

5. Type `Y` or `N` to set whether to `Consider the GAS phase` (gaseous mixture phase) in the calculation.

   The gaseous mixture phase should at least contain H2O, O2 and H2. If a GAS phase is not considered, then only the interactions between the aqueous solution phase and various solid phases (alloy phases and secondary phases) are calculated. Such a

calculation may not accurately present all the heterogeneous interactions. Some secondary phases are therefore usually needed. Such phases exist in the PAQ or PAQS Public Aqueous Solution Databases. They can also be appended from the SSUB/SSOL/TCFE or other appropriate substances/solutions databases.

6. Type `Y` or `N` to set whether to `Use single database` (`Y`) or a multiple database (`N`).

   If you choose to use a single database, at the `Combined Database: /PAQ2/` prompt specify a database that is specially developed for the Pourbaix module's diagram calculations.

   If you choose to use a multiple database, then you are prompted to specify an aqueous solution database and to append any additional required data and select necessary phases, such as various interacting alloy (solid) solution phases, and secondary (solid and liquid) phases, for example.

7. Specify all your solutes and the molality of each solute when prompted to do so. This can be done in terms of elements (such as Fe, Ni, Na, Cl, C or S) or arbitrary complex species (such as NaCl, CO2, CoCl3, Fe0.93S, NaSO4-1, or H2SO4). You can enter the element/species and the molarity on one line (for an example, NaCl 2.5).

   The definition of your system and its initial bulk composition is now presented.

   The first letter of the element abbreviation must always be upper case. Any second letters must be lower case. When you have finished your specification, press <Enter> when asked to specify `Next solute`.

8. Type `Y` to confirm the defined system and its bulk composition.

   The thermodynamic data for your system is now retrieved from the database(s) chosen.

9. Answer the questions that you are prompted regarding various parameters of your calculation. You are asked to do any of the following:
   - `Rejectphase(s)` or `Restore phases(s)`
   - Check for miscibility gaps on any phase (`Should any phase have a miscibility gap check?`)
   - `Enforce the Global Minimization Technique in calculations?`
   - Save all functions, variables and tables in POLY3 file?

- `Set numerical limits` on the calculation
- Confirm defined conditions?
- Accept the default settings for two mapping variables

10. The Pourbaix calculation starts. Answer the question `Any missing phase boundary you could possibly think of?` Type `Y` or `N` to set whether you want to add starting points to the calculation. If you suspect that the calculation has missed some phase boundaries, this may help the program to detect them.
11. Answer questions about how the diagram is plotted and how to save the results of your calculation. You are asked to do any of the following:
    - Change the pH/Eh steps for smoother curves?
    - `Zoom in` on a specific region of the diagram
    - `Change the curve-label option for the diagram`
    - `Add label-texts onto the Pourbaix diagram`
    - `Change the subtitle of the diagram`
    - `Change the axis-texts`
    - `Further refine the diagram in the POST Module`
    - Print the diagram (save a `Hard copy of the diagram`)
    - `Save the X-Y coordinates of curve on a text file`
    - `Modify the diagram`
    - Calculate and plot another Pourbaix diagram (`Any more diagram?`)

Plotting More Pourbaix Diagrams

When you have calculated a Pourbaix diagram, you can plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

The variables can be plotted along the X- and Y-axes. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram. In the table, *AQsp* refers to the name of a specific aqueous species. The asterisk (*) can be used as a wild card character for all such species. If neither *AQsp* nor * is entered in parenthesis, then all species are searched.

You must have plotted a Pourbaix diagram to plot a diagram with other variables than Ph and Eh on the Y-axis and the X-axis. You can either plot such additional diagrams directly after having finished the plotting and saving/printing of a Poubaix Ph-Eh diagram or by choosing option `2` (Open an old file and plot other property diagrams) when you enter the POURBAIX module and opening a POLY3 workspace file.

Abbreviations for Aqueous Solution Variables

Abbreviation	Variable
pH	Acidity
Eh	Electronic Potential (V)
Ah	Electronic Affinity (kJ)
Pe	Electronic Activity (log10ACRe)
IS	Ionic Strength
TM	Total Concentration
Aw	Activity of Water
Oc	Osmotic Coefficient
MF(AQsp)	Mole Fractions of Aqueous Species
ML(AQsp)	Molalities of Aqueous Species
AI(AQsp)	Activities of Aqueous Species
RC(AQsp)	Activity Coefficients of Aqueous Species

How to Plot an Aqueous Solution Diagram

1. Type `Y` when prompted whether to plot any more diagrams, or select option 2 when you enter the POURBAIX module.
2. Specify which variable you want the X-axis to represent. Use the abbreviation specified in the preceding table. When you specify the name of an aqueous species, you can use the asterisk (*) to select all species.
3. Specify which variable you want the Y-axis to represent. The diagram is then automatically plotted.

4. Answer questions about how the diagram is plotted and how to save it. You are asked to do any of the following:
    a. change the axis-type (linear, logarithmic or inverse) on the X-axis or Y-axis
    b. zoom in on a specific region of the diagram
    c. change the curve-label option for the diagram
    d. add label-texts onto the Pourbaix diagram
    e. change the subtitle of the diagram
    f. change the axis-texts
    g. refine the diagram in the POST Module
    h. print the diagram (save a hard copy)
    i. save the X-Y coordinates of curve on a text file
    j. modify the plotted diagram
    k. calculate and plot another aqueous solution diagram

Stepping Calculations in an Aqueous Solution



Performing the stepping calculation overwrites all the previous settings and stepping results on the POLY3-file. To avoid this, use SAVE_WORKSPACES to create a new workspace.

When you have calculated a Pourbaix diagram, you can use the saved results of the calculation (the POLY3 file), and make a property diagram based on stepping calculation.

Since the program normally sets the calculated initial equilibrium point as the starting point, the minimum value for the stepping variable must be specified as smaller or equal to the specific initial condition, and the maximum value as larger or equal to that condition. If pH is set as the stepping variable, the program automatically calculates the equilibrium constant in logarithmic (log10Ka) of the electrolysis reaction H2O (water) = H+ + OH- for the real aqueous solution under the current temperature-pressure-composition conditions, and thus this constant log10Ka value is considered as the highest pH in specifying the maximum value along stepping. Subsequently, confirm or modify an increment factor with a default value; for pressure and mole of a component, specify the step in logarithmic (log10P or log10N).

State Variable Abbreviations

You can use any of these state variables as a stepping variable.

State Variable	Abbreviation
Temperature (K)	T
Pressure (bar)	P
Acidity	pH
Electronic potential (V)	Eh
Mole number of a dissolving component (such as Fe, Na, Cl, or NaCl) in 1 kg of water.	N(Comp) (for example, `N(Fe)`)

How to Do a Stepping Calculation

You must have plotted a Pourbaix diagram before making a stepping calculation on an aqueous solution.

1. Use GOTO_MODULE POURBAIX to enter the POURBAIX module.
2. Type `4` to open an old file and make another STEPPING calculation.
3. Choose which POLY3 file to load.
4. Specify the conditions of the calculation by answering the questions that follows.

   The system definition is the same as in the previous Pourbaix calculation, but you can modify conditions such as bulk composition, temperature and pressure, and change some component definitions if necessary.
5. Specify which variable to use as the stepping variable (see the preceding table), its minimum and maximum value, and the length of each incremental step.

   The settings and stepping results are written to the opened POLY3 file, and a first default property diagram is plotted.

POURBAIX_DIAGRAM Module



This command or module is not available with GES6.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Getting started with the Pourbaix module

After you enter the POURBAIX_DIAGRAM module, you are asked if you want to have step-by-step instuctions to help walk you through the module.

```
Need any instruction on the Pourbaix module? /N/: Y
```

If you answer `Y` a series of notes are displayed. The following is a more comprehensive summary of these same notes.

WHAT IS A POURBAIX DIAGRAM?

The Pourbaix diagram is a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modeled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).

WHAT DATABASE SHOULD I USE?

At least one database is required that contains an aqueous solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc databases.

CHOOSING A CUSTOM AQUEOUS SOLUTION DATABASE

You can also use a custom database but it must be in the Thermo-Calc TDB format. Due to the restrictions of aqueous solution models used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ2) for aqueous solution phases.

Among other things, keep the following requirements in mind:

The ELECTRON is defined as an special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electro-potential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;

The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;

The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.

Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O1, O2 and H2; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!

All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a GASeous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above).

Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the PAQ2 or as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for GASeous mixture phase and for varous solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.

The advanced POURBAIX module is designed so that it requires you to just answer some necessary questions, rather than to go through the other Console Mode modules (i.e., TDB, GES5, POLY3 and POST) although you still enter commands at the prompts. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the

calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.

The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-POLY3-POST calculation.

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE *<FILE NAME>*.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Enforce a Pause

After the initial set of information is displayed, you are asked:

```
Enforce a PAUSE after plotting when running a MACRO? /N/
```

- If you choose `Y` a pause is always enforced after each diagram is plotted;
- If you choose `N`, all the command-lines (answers) for the session continue without stopping or until the SET_INTERACTIVE_MODE line in the macro file is reached.

Whenever running a Thermo-Calc macro (TCM) file, you may want to pause after a specific diagram is plotted on screen. This gives you the flexibility to:

- Print it (of EMF/PS format) to a printer
- Convert it (of EMF format) to (PDF) graphical files;
- Save it as an EMF graphical file;
- Dump it as a PNG or BMP graphical file;
- Set background colour for the current diagram
- You can also set the default font/size and change plot layers for sequential plots.

Pourbaix Main Options

If you answer `Y` to the Pause prompt above, these options are displayed:

1. Start a completely new Pourbaix diagram calculation.
2. Open an old file and plot other property diagrams.
3. Open an old file and make another Pourbaix calculation.
4. Open an old file and make another stepping calculation.

POURBAIX_DIAGRAM Commands for Options 1 to 4

Tabulation Reactions

In this section:

About the Tabulation Reaction Module 111

Tabulating a Reaction 112

Tabulating a Substance or Solution Phase at Fixed Composition 113

About the Tabulation Reaction Module

The TABULATION_REACTION (TAB) module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

The TAB module begins by evaluating the most stable species of a substance in either a homogeneous state or in a reaction. Results are presented in a table or plotted as a graph.

▶ Tabulating a Reaction

A reaction tabulation presents you with the following properties, on rows representing different temperature levels:

- Heat capacity change / Delta-Cp (Joule/K) in column 2.
- Enthalpy change / Delta-H (Joule) in column 3.
- Entropy change / Delta-S (Joule/K) in column 4.
- Gibbs energy change / Delta-G (Joule) in column 5.

In the case of a tabulation of a substance or solution phase at a fixed composition, the properties presented are the heat capacity, enthalpy, entropy and Gibbs energy, rather than the degree of change in those properties.

▶ Tabulating a Substance or Solution Phase at Fixed Composition

You can add a 6th column to the table that shows the values of a property or user-defined function of your choice.

T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)
298.15	-4.44006E+01	-9.18800E+04	-1.98115E+02	-3.28120E+04
300.00	-4.43267E+01	-9.19621E+04	-1.98389E+02	-3.24452E+04
400.00	-3.92294E+01	-9.61533E+04	-2.10482E+02	-1.19604E+04
500.00	-3.34122E+01	-9.97861E+04	-2.18613E+02	9.52022E+03
600.00	-2.77768E+01	-1.02842E+05	-2.24200E+02	3.16779E+04
700.00	-2.26324E+01	-1.05358E+05	-2.28088E+02	5.43040E+04
800.00	-1.81080E+01	-1.07390E+05	-2.30808E+02	7.72568E+04
900.00	-1.41889E+01	-1.09000E+05	-2.32710E+02	1.00438E+05
1000.00	-1.08095E+01	-1.10245E+05	-2.34025E+02	1.23779E+05
1100.00	-7.77802E+00	-1.11169E+05	-2.34908E+02	1.47229E+05
1200.00	-5.07556E+00	-1.11807E+05	-2.35464E+02	1.70750E+05
1300.00	-2.93467E+00	-1.12203E+05	-2.35782E+02	1.94314E+05
1400.00	-1.19414E+00	-1.12407E+05	-2.35934E+02	2.17901E+05
1500.00	2.55400E-01	-1.12452E+05	-2.35966E+02	2.41497E+05
1600.00	1.49022E+00	-1.12363E+05	-2.35909E+02	2.65091E+05
1700.00	2.56484E+00	-1.12159E+05	-2.35785E+02	2.88676E+05
1800.00	3.51909E+00	-1.11854E+05	-2.35611E+02	3.12246E+05
1900.00	4.38259E+00	-1.11458E+05	-2.35397E+02	3.35797E+05
2000.00	5.17775E+00	-1.10980E+05	-2.35152E+02	3.59325E+05

Tabulating a Reaction

A tabulation of a given chemical reaction provides you with data about the rate of change of the standard tabulation properties at various levels of temperature. You can also add a column for a property of your choice to the table.

1. Use GOTO_MODULE TAB to enter the TAB module.

2. If you want to add one thermodynamic functions to the tabulation calculation, which is present in a sixth column in the table, use ENTER_FUNCTION.

   You are prompted to enter the name of the column that is given at its head, and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

3. Use TABULATE_REACTION followed by a formula that specifies of the reacting species and products to perform the tabulation calculation. The name of the elements must be entered in upper case letters only. Terminate the chemical reaction with a semi-

colon. For example, you can enter:

```
TABULATE_REACTION 3H2+N2=2N1H3;
```

Elements that are designated with a single letter must be followed by a stoichiometry factor, even if this factor is 1. `CO` hence be interpreted as Cobalt rather than as carbon monoxide. Carbon monoxide is entered as `C1O1` or `O1C1`.

4. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

   The tabulation calculation is performed and you are given a table that shows the various properties at each temperature level within the range defined.

   If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column of you chose (on the Y-axis) against temperature (on the X-axis). When this graph is plotted, you are now in the POST module, where you can modify the graph in various ways.

Tabulating a Substance or Solution Phase at Fixed Composition

A tabulation of a substance or solution phase at fixed composition provides you with data about the standard tabulation properties at various levels of temperature for a given chemical reaction. You can also add one extra property column of your choice to the table.



It is important to have already defined the system and retrieved thermodynamic data from a database before using the TAB command.

1. Use GOTO_MODULE TAB to enter the TAB module.

2. Use SWITCH_DATABASE to switch to a database that contains solution-based data, such as TCFE for example.

   You cannot use the default SSUB database when tabulating solution phases at a fixed composition.

3. If you want to add one thermodynamic function to the tabulation calculation, which is present in a sixth column in the table, use ENTER_FUNCTION.

   You are prompted to specify the column header and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

4. Use TABULATE_SUBSTANCE followed by the name of the substance or solution phase to perform the tabulation calculation.
5. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and a table shows the various properties at each temperature level within the defined range.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column you chose (on the Y-axis) against temperature (on the X-axis).). When this graph is plotted, you end up in the POST module, where you can modify the graph in other ways.

Results

In this section:

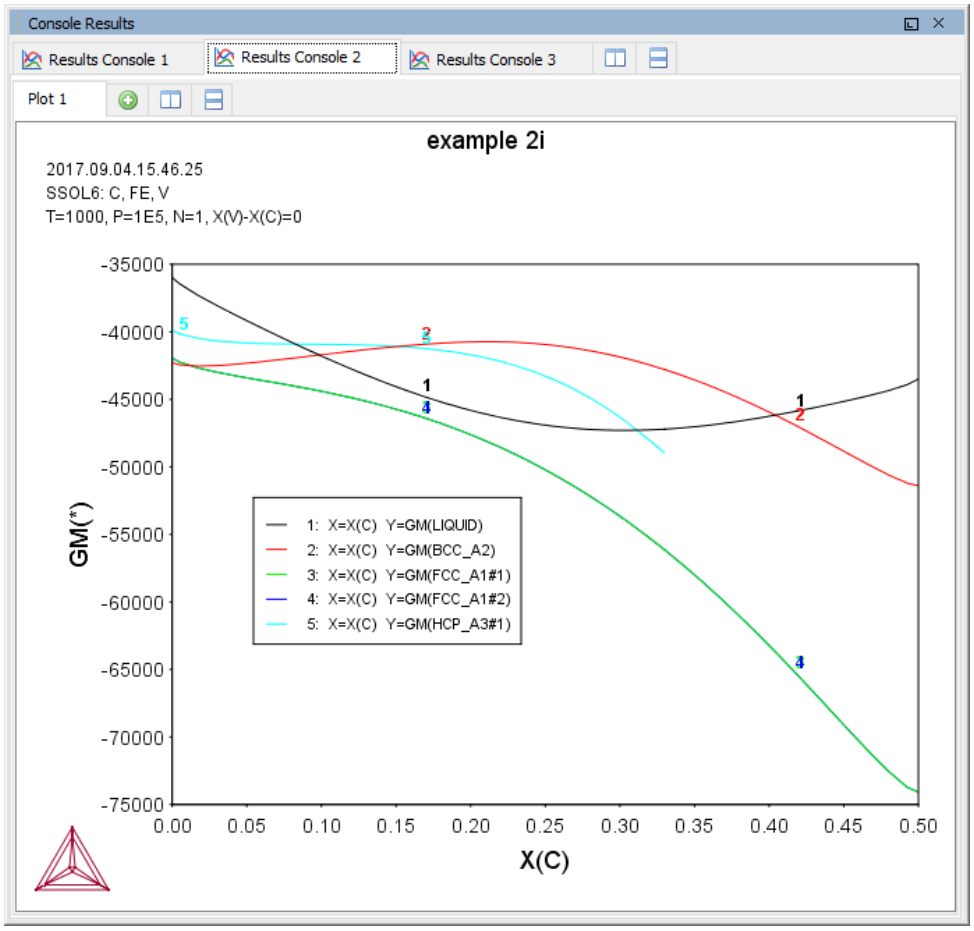
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Console Mode Results

The results of a calculation in Thermo-Calc can be plotted by the post-processor module, also called the POST module. The diagram is displayed in the **Console Results** window.

In the POST module, you can define and plot various kinds of diagrams based on a calculation. You can modify diagram type, which variables to plot on each axis and between which minimum and maximum values, append experimental data from an EXP-file, change labels and symbols in the diagram, zoom in on (and out from) a certain region in a diagram, etc.

If you calculate a property or phase diagram in POLY, then you have to open the POST module yourself. If your calculation was performed by a response-driven module such as SCHEIL or POURBAIX, then the plotting of a diagram based your calculation is part of the dialogue of questions and answers you have in that module (but under the hood, the response-driven module is actually utilizing the POST module to get the plotting done).



Example of output to the Console Results window.

Using the POST Module

Use the POST module after a STEP_WITH_OPTIONS or MAP calculation to generate *graphical* or *tabulated* presentations on screen or into files.

The graphical files are available in different formats (e.g. PS, EMF, PNG, BMP, PDF, JPG, TIF) or data forms (e.g. EXP, TAB and WRL). The graphical output can be phase diagrams, property diagrams, diffusion profiles and other types of plots. The tabulated presentation is into a basic text file (TXT) or a spreadsheet (e.g. an MS Excel file with an extension of .XLS).



The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

Within the POST module, you can choose any state variable, any derived variable, or any entered symbol (functions or variable) as the X/Y-axis.

When a diagram is plotted, appearance parameters for defining a high-standard graph can be further specified, e.g. curve labelling options, diagram titles and subtitles, plot size, axis length, axis types, axis-tic type, tie-line status, automatic or manual scaling and zooming, semi-automatic or manual labelling on phase boundaries and phase regions, graphic formats, text fonts, colours, raster plot, etc.

You can append experimental data onto a plotted diagram. You can also save the coordinates onto a textual file, which can be edited and used as an experimental data file to be merged onto another diagram or as a part of a setup file for PARROT-module assessment.

Phases can be suspended or restored in a plotted diagram. The reference states for components can also be modified for the resulted diagrams. Moreover, you can translate a plotted property diagram (after a stepping calculation) into a tabulated form, such as a simple list on screen or a textual file, and a spreadsheet .

Plotting Diagrams

Plotting a diagram is to graphically represent how several variables (typically two variables) co-vary. Each axis in a property diagram or a phase diagram represents the value of one variable. The default variables represented by the X- and Y-axes are the following:

- If you plot a diagram based on the results of a mapping operation (a phase diagram), then by default the X- and Y-axes represent the mapping axis variables 1 and 2 (set using SET_AXIS_VARIABLE in POLY).
- If you plot a diagram based on the results of a stepping operation (a property diagram), then by default, the X-axis represents the stepping variable (set using SET_AXIS_VARIABLE) and the Y-axis represents the sum of the mole fractions of all phases (that is, NP(*)).

POLY Module Commands

How to Plot a Diagram

To plot a diagram, you must have already made a stepping or mapping operation in POLY (or in some cases, made a calculation as part of some opening a response-driven module), and you must have entered the POST module.

The POST command is available inside POLY. Use POST to enter the POST module

1. If you want to directly plot your diagram with the default variables represented by the X- and Y-axes, type `Plot` and press <Enter>. This plots a property or phase diagram with the default variables represented at each axis. If you do not want to plot your diagram with these default variables, go to the next step.
2. Use SET_DIAGRAM_AXIS to set which variables to plot on the X-axis and the Y-axis. For example, if you want to plot a phase diagram with pressure on the Y-axis and temperature on the X-axis, type:

```
SET_DIAGRAM_AXIS X T
SET_DIAGRAM_AXIS Y P
```

3. Use PLOT_DIAGRAM to plot your diagram.

Saving and Printing the Output in Console Mode

Global Settings: Graphical and Console Mode Plotting

Output can refer to results in the form of tabulated data in a table or a diagram.

The terms *diagram* and *plot* are interchangeable. The commands in Console Mode generally use the term diagram and in Graphical Mode it is also called a plot (e.g. the Plot Renderer).

Commands to Save and Print Diagrams

Use the following commands to create diagrams, which then display in the **Console Results** window. From this window, you can right-click the diagram and choose **Save as** or **Print**. You can also use the following commands for these actions.

PLOT_DIAGRAM

After you use the SET_PLOT_FORMAT command to define the default graphic device (the printer) you can use a PLOT_DIAGRAM command to either save the calculation output to a file or display the output in the **Console Results** window.

DUMP_DIAGRAM

DUMP_DIAGRAM is an alternative command used to create output. After a diagram is displayed to the **Console Results** window with the PLOT_DIAGRAM command, you can save (dump) it to a file using this command.

MAKE_EXPERIMENTAL_DATAFILE

Use MAKE_EXPERIMENTAL_DATAFILE to save all the data about the plotted diagram in an EXP-file. An EXP-file is a plain text file that describes the diagram in the DATAPLOT graphical language. Note that information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

- *DATAPLOT User Guide* included with this documentation set.

PRINT_DIAGRAM

First use PLOT_DIAGRAM to create output that displays in the **Console Results** window. Then after entering the PRINT_DIAGRAM command, the **Print** window opens where you can choose additional settings for a hard copy of the diagram.

Commands to Save Tables

Tables or tabulated data can be listed in the **Console** window. You then use commands to save the text to different file formats (txt, html, or xls) where you can then print the information.

- LIST_DATA_TABLE: Use this command to output to the screen or to file.
- TABULATE

Saving Diagrams

You can save the output in a variety of file formats. For JPG and PNG images you can also adjust the image quality.

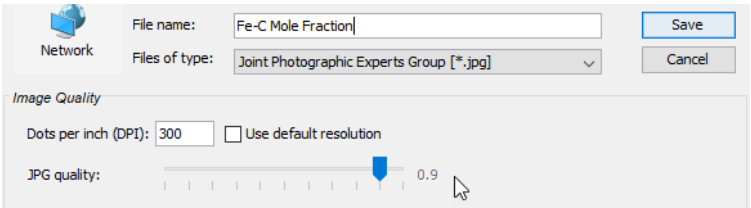
In Console Mode, the diagram is output to the **Console Results** window after using the PLOT_DIAGRAM command.

In Graphical Mode, the diagram is output to the **Results** window after performing a tree that includes a Plot Renderer.

1. In the **Results** window, right-click the diagram and select **Save as**.

   In the Graphical Mode **Configuration** window you can also click the **Save Diagram** (or **Save table**) buttons to open the **Save** window.

2. In the **Save** window:
   a. Navigate to where you want to save the diagram.
   b. Enter a **File name**.
   c. From the **Files of type** list choose **png** (the default), **jpg**, **ps**, **pdf**, **gif**, **svg**, or **emf**.
   d. For PNG and JPG files only, under the **Image Quality** section, choose to improve the resolution of the image. For JPG files you can also adjust the file size.
      - To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** check box. Then enter a numerical value in the **Dots per inch (DPI)** field.
      - For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.



   e. When you are ready, click **Save**.

Printing Diagrams

In the **Console Results** window, right-click the diagram and choose **Print**. Select additional settings as required on the **Print** window.

Use the LIST_DATA_TABLE command to save to file and then print the file.

Modifying Diagrams

Modifying a diagram amounts to changing the settings that determine how the POST module presents the calculated results and plots a new diagram. Suppose that you have already plotted a binary phase diagram with the mapping axis variables temperature and mole fraction of one of your components (the Fe component, say) on the X- and Y-axes. If you then want to modify your diagram so that the Y-axis instead represents, say, the mass fraction of Fe rather than the mole fraction, then you use SET_DIAGRAM_AXIS to set diagram axis `Y` to `w(Fe)`, and then use PLOT_DIAGRAM.

There are many ways in which you can modify your diagram and how it is presented. Any modification made in the plot settings is taken into account the next time you use PLOT.

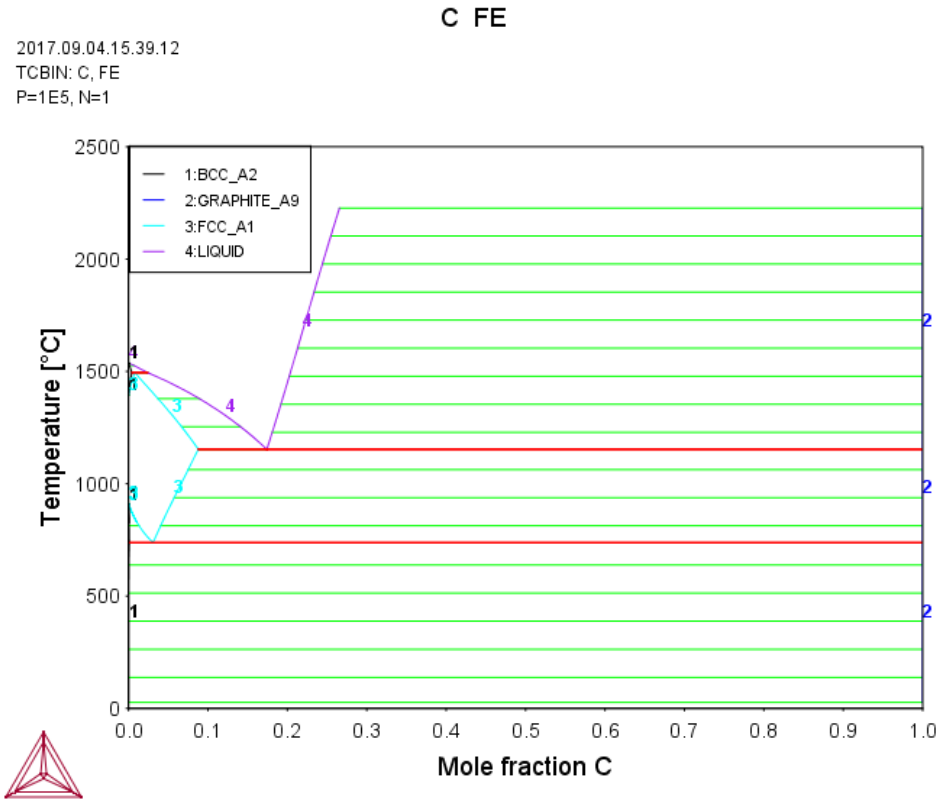
Example Commands

The following are some of the modifications you can make. Use:

- SET_TITLE to set add a title or to change an already existing title. The title is displayed above the plotted diagram in the Console Results window.
- ADD_LABEL_TEXT to add a label text that starts at a certain X- and Y-coordinate. If you have plotted a phase diagram, then you can let Thermo-Calc set the label text that specifies the names of the stable phases at that coordinate.
- SET_AXIS_TYPE to set whether the scale of an axis is linear, logarithmic or inverse.
- SET_DIAGRAM_TYPE to plot a triangular diagram with the X-axis on the triangle's base and the Y-axis on the triangle's left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
- SET_SCALING_STATUS to modify the range of values that are displayed on an axis. In effect, you can use it to zoom in or out of the diagram. For example, to set the scale of the X-axis to range from 0 to 0 .3, type:

  ```
  SET_SCALING_STATUS X N 0 0.3
  ```

  The `X` specifies which axis to change the scaling on, the `N` turns off Thermo-Calc's automatic scaling, and `0` and `0.3` specifies the minimum and maximum values on the scale. You can turn on automatic scaling again by setting the second parameter to `Y`.
- SET_LABEL_CURVE_OPTION to label each set of curves that have the same stable phases with a certain digit. A legend is also added, where you specify which phases each digit designates.


C FE
2017.09.04.15.39.12
TCBIN: C, FE
P=1E5, N=1
1:BCC_A2
2:GRAPHITE_A9
3:FCC_A1
4:LIQUID
Temperature [°C]
Mole fraction C
2500
2000
1500
1000
500
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Loading Saved Diagrams

If you have previously saved a diagram in an EXP-file, then you can load and superimpose the diagram on another diagram. Both the following command requires you to specify which prologue and dataset(s) that are loaded from an experimental data file.

Use APPEND_EXPERIMENTAL_DATA to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, the labels on the diagram are not changed when you plot the additional data from the EXP-file, irrespectively of the data in that file.

Use QUICK_EXPERIMENTAL_PLOT to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, these settings are overwritten with the axes settings from the EXP-file.

Working with the Console Mode Output

Pause, Resume or Stop Output to the Console Window

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To stop the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

Controlling Console Output

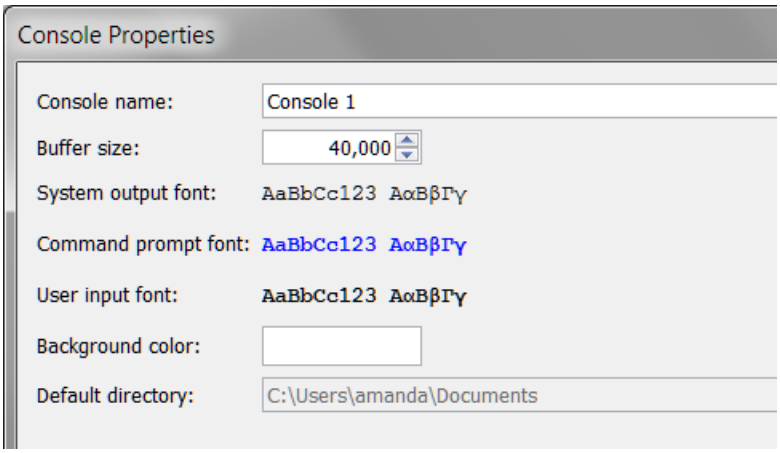
In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To terminate the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

In Console Mode, sometimes the output overflows the window text buffer. This is how to increase the buffer size.

1. Right-click the Console tab header in the Console window (if this is the first Console tab, it is labeled **Console 1**).

2. Click **Properties**, and increase the **Buffer size** in the Console Properties window.


Console Properties
Console name:
Console 1
Buffer size:
40,000
System output font:
AaBbCc123 AαBβΓγ
Command prompt font:
AaBbCc123 AαBβΓγ
User input font:
AaBbCc123 AαBβΓγ
Background color:
Default directory:
C:\Users\amanda\Documents

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ABOUT

The ABOUT command lists basic information about the development history and ownership of the Thermo-Calc software as well as version information.

BACK

- GOTO_MODULE.

Use the BACK command to switch control back to the most recent module. Going from the POST module, BACK goes only to the TAB or POLY module (from where the POST module is entered).

CLOSE_FILE

Close an opened text file.

Syntax	CLOSE_FILE
Prompt	`Unit number: <Unit number>` A unit number given in an OPEN_FILE command must be specified.

DISPLAY_LICENSE_INFO



You can also access this same information from the top menu. Choose **Help → Show License Info**.

Use this command to launch a license diagnostics program implemented in the SYS module. It detects the license information for the Thermo-Calc installations on the current client computer (and on the connected license server), and lists the details, including the current status of available license file and all its included license features for the current installation (s), as well as the Safenet Environment Variables and detailed Local (Client) Information, on screen or into a textual file (*.TXT).

This is useful for a list of license details, and to obtain basic technical support by sending the *.TXT file to support@thermocalc.com. If you are running a network client installation of Thermo-Calc, you can see how many of the client example licenses that are currently checked out and how many of them are left. You can also see which clients computers it is that have checked these client example licenses out.

Syntax	DISPLAY_LICENSE_INFO
Prompt	`Output to screen or file /Screen/: <Mylicenseinfo.txt>` Press <Enter> to display a list of license information or into a *.TXT file under a specific file name which can later on be opened and edited by any basic text editor.

EXIT

Use the EXIT command to leave the program and return to the operating system. Use a SAVE command before exiting otherwise all data and results are lost (in either the GIBBS, POLY, PARROT or REACTOR module).

GOTO_MODULE

Switch between modules. The name of the module must be typed. To get a list of available modules, press the <Enter> key.

Syntax	GOTO_MODULE
Prompt	`Module name: <Module name>`
	If the <Enter> key is pressed without typing a unique module name (or typing a ? mark) it prompts for the `MODULE NAME` and lists the available modules.

HELP (? and ??)

Enter ? or ?? to get text help about the current prompt (whether this is the prompt of a module, or a prompt that requests you to specify the value of some parameter).



For some commands and prompts, more detailed help is given when two ?? are entered.

HELP

Lists the available commands or explains a specified command. Specifying a unique command displays an explanation on screen. Typing a command abbreviation that is not unique lists all matching commands. Get the command information by typing a unique abbreviation or the complete command name.

Syntax	HELP
Prompt	`Command: <Command name>` *Command name* is the name of the command (one of the-module commands) to get help. If the <Enter> key is pressed without typing a command name, then all the available commands are listed.

HP_CALCULATOR

The HP-CALCULATOR commend is the QBA simple interactive calculator using reverse Polish notations.

Available OPCODEs (HPC codes) are listed by entering the command HELP.

Use the BACK command to quit and go back to the SYS module.

Input are numbers, + - * / and ^ and OPCODEs. Several numbers an operations can be given on one line. The content of the X register is displayed after each operation.

For example, to compute 2*EXP(1.5**3-30000/(8*1273)), you should input the following:

```
30000 8/1273/chs 1.5 3 ^ + exp 2 *
```

INFORMATION

Get basic information about topics related to the module you are in.

Syntax	INFORMATION
Prompt	`Which subject /Purpose/: <Topic name>` Specify a subject (or its abbreviation as long as it is unique). Enter a question mark `?` for a list of topics.

MACRO_FILE_OPEN



Some of the information in this topic is related to the add-on Diffusion Module (DICTRA).

The macro file functionality is a way to predefine sequences of Thermo-Calc commands stored in a macro file (a basic text file usually with the default extension *.TCM or*.DCM for DICTRA) and then executing all of the sequences using this command (preceded by the macro file name). This command can be used within various modules (i.e. SYS, POLY, PARROT, TAB and DICTRA_Monitor).

Syntax	MACRO_FILE_OPEN
	`<Name of a macro file *.tcm>` An **Open** window displays to specify the filename of the macro file (*.TCM) with the macro command, so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** *.TCM for Thermo-Calc (Console Mode) calculations and *.DCM for DICTRA simulations, cannot be changed. Click **Open** or **Cancel** to continue. A window such as **Save**, **Open**, or **Print** opens if the macro file contains commands to: • set log files (these have a file extension .TCM) • save or read GIBBS, POLY or PARROT workspaces • switch user databases • compile experiments (from existing *.POP files) • create new *.PAR files • append *.EXP files • plot diagrams, etc. If required, opening these windows can be avoided by issuing the file names (preferably with file-type extensions; if the files are not in the current working area where the macro is located, the appropriate and complete paths of the files should also be specified) and sometimes with the required options after the corresponding commands or parameters/options. For details, see the related commands and modules. When using a macro file that intended to plot graphs on screen, but the command SET_PLOT_FORMAT is used to alter the plotting environment from the default value, it is important to first use the command SET_PLOT_FORMAT again to change back to the default value.

This is useful when the same or similar calculations are made frequently with small changes [in terms of system definitions, data manipulations, conditions (for single points, stepping or mapping calculations), plotting settings, etc.). For example, use this feature when calculating phase/property diagrams during an assessment of thermodynamic data.

A macro file can be automatically generated in Console Mode if in the SYS module the SET_LOG_FILE command is used and a log file name (with a file extension *.TCM) is given before any other SYS, DATA, TAB, GIBBS, POLY, POST, PARROT, or ED-EXP command or any special-module command (e.g. BIN, TERN, POTENTIAL, SCHEIL, POURBAIX, or REACTION). Such a log file generated in Console Mode is a text file. You can use a text editor (such as Notepad++) to remove unnecessary command lines, modify some commands, settings and definitions, add some pause points, add comment lines that start with @@, and so forth. Then save it as a macro file with the standard file extension TCM.

Experienced users can also write/edit an appropriate macro file for calculations/simulations, using any basic textual editor outside the Thermo-Calc program.

All commands can be used in a macro file.



The file can be terminated with EXIT or interrupted with SET_INTERACTIVE.

Within a macro file you can use comment-lines (for describing the problems and for explaining commands and inputs/outputs), which should always start with the @@ signs in the beginning of each comment-line. Such comment-lines help to document the macro file, while these are not considered as command lines and thus do not affect the proceeding of all the normal commands in modules when the file is called by Thermo-Calc.

You can put multiple-line comment-blocks in a macro file between the @ (" and "@)" signs. The former sign indicates where the comment begins and the latter sign indicates where the comment ends. A comment-block begins from a line started with the *begin comment* sign @ (and ends with the *finish comment* sign @); all the lines written in between are ignored, and the line started with @) is also ignored.

Another use for a macro file is to allow you to interact at some specific points, using the "@?" sign starting a text line (note that the text describing the expected user-specification/input should be written as a continuous string without any empty space), for user's on-time specifications of arguments/parameters or inputs of parameter-values that are requested by a certain command. The macro temporally stops at the "@?" sign, prompt on screen the text given after "@?", and waits for the specified argument/parameter/value. Thermo-Calc then uses specified argument/parameter/value as the input(s) for the associated command. For example, you can input the values of lower and higher temperature limits for the second axis-variable as follows:

```
GO POLY-3
SET-AXIS-VAR 2 T  @?Low-temperature-limit:
@?High-temperature-limit:
```

You can have macro-variables denoted by the signs of @#n (for definition) and ##n (for usage); and up to nine variables inside a single macro file. Such a macro-variable can be assigned with its desired value, as for example:

```
@#3First-element?
```

This writes the text (note that the text describing the expected user specification/input is written as a continuous string without any empty spaces) after the "@#3" sign as prompted on screen and then wait for a specification. The input is assigned to the macro-variable ##3, which is directly called in different parts within the current macro file.

For example, the content of the macro-variable `##3` is inserted in the command:

```
DEFINE-SYSTEM ##3
```

It is also useful in more complicated commands, such as:

```
SET AXIS VAR 1 x(##3) 0 1,,,
```

This command sets the mole fraction of macro variable 3 as axis 1.

A macro file can have any number of pauses at the `@&` signs, for the purpose of checking the details/results of executing certain commands when running the macro file. However, you can also prevent the software from temporarily stopping at any pause by typing any character (except for the `Y` character for confirming a Yes answer to a command prompt) after specifying the name of a macro file.

A macro file can have a maximum of five nested levels, i.e. a macro file can call another macro file, and if one sub-level macro is terminated by the command it resumes at the next command in the previous macro. If it is terminated by `end-of-file`, the Thermo-Calc (Console Mode) software stops.

This feature is especially useful for alloy design that requires many (hundreds) of calculations/simulations on similar material system/processes (specified in many different but appropriately-documented macro files that are organized in up to five levels) during a certain period of time (e.g. in an evening), you can run the main macro (on the top level) at a certain time (e.g. before leaving the office) and afterwards (e.g. next morning) you can systematically and efficiently check/compare/analyse the results (saved as graphical files, and/or EXP, TXT, XLS… files).

By adding the SYS command SET_ECHO at the beginning of a macro file (or in the primary macro file on the top level if any sub-level(s) of macro files are used), it is useful to automatically display the complete/detailed meaning of various commands in all the sequential operations in the software, all enforced according to the macro file(s).

OPEN_FILE

A text file is opened for use in other commands where a unit number is necessary. The program automatically assigns a unit number.

Syntax	OPEN_FILE
Prompt	`File name: <File name>` A legal file name must be specified.

SET_COMMAND_UNITS

This command is useful for reading inputs already prepared by a textual editor on a file. Such inputs can be a table of values or a large number of parameters. The file must be opened with OPEN_FILE.



The first two lines of an input file are skipped before any input is read.

Syntax	SET_COMMAND_UNIT
Prompt	`Input unit number /5/: <Input unit number>` Specify the input unit number returned from an OPEN_FILE command. The next command is taken from the file connected to this unit number. The last command on such a file must be EXIT or SET_INTERACTIVE when you are in POLY, POST or SYS module, in order to go back to read input from the keyboard. The default value is the current input unit.
	`Output unit number /6/: <Output unit name>` Specify the output unit number returned from an OPEN_FILE command.

SET_ECHO



This command is not applicable if macro files are not used.

Add the SET_ECHO command at the beginning of a macro *.TCM file (or to the primary macro file on the top level if any sub-level(s) of macro files are used).

Automatically displays on screen the complete details of various commands in all the sequential operations in the software, that are enforced according to the macro file(s).

SET_GES_VERSION

This command enables switching between the two versions of the Gibbs Energy System (GES) calculation engine. As of Thermo-Calc version 2019b, GES6 is the default. Also see About the Gibbs Energy System (GES) Module.



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Syntax	SET_GES_VERSION
Prompt	`USE GES VERSION 5 OR 6 /6/:` The default is version 6. If you change the version to GES5, it is set for the current session of Thermo-Calc only. If you launch a new Console window, the version resets to GES6.
	 To globally set the default from GES6 back to GES5, go to the **Tools → Options →** General tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. This is useful if you are using the PARROT module (optimization) or if you have a custom database that is not compatible with GES6.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

SET_INTERACTIVE

Use the SET_INTERACTIVE command to reset the input and output units to the initial values, i.e. keyboard and screen. Add this as the last command to the macro files.

SET_INTERACTIVE_MODE

Use the SET_INTERACTIVE_MODE command to reset the input and output units to the initial values, i.e. keyboard and screen.



Remember to add this as the last command to your macro files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.

SET_LOG_FILE

Use it to save, in a basic text file, everything typed into Thermo-Calc. When having problems executing a command sequence, this command can be used to save the command typed onto a log file with the file extension *.TCM.

This command also makes the system echo the full command for all commands typed. This feature is useful when demonstrating the system since the abbreviated commands are often difficult.

The saved log file can then be edited as a macro file by using a basic text editor. This is useful to run the macro file(s) for similar calculations (the same system but slightly varied temperature-pressure-composition conditions), or run the example macro files.

Macro Files

Syntax	SET_LOG_FILE
Prompt	A **Save** window opens to specify a file name for the *.TCM file, so that the path (in the **Save in** field) and **File name** can be specified. If a log file with the same name exists in the current working directory, it is overwritten. The **Files of type** (i.e. TCM) cannot be changed. Click **Save** or **Cancel** as applicable.

SET_PLOT_ENVIRONMENT

Use this command to set the plot devices to save or print plots to, which varies for by installation type.



This command must be terminated with an empty line or two commas.

Syntax	SET_PLOT_ENVIRONMENT
Prompts	`Default plot device number /Default number/: <Device number>` The number given is unique for each type of graphical device. The default graphical device number should normally be selected. A question mark `?` gives you a list of all available graphical devices used.
	`Pseudo file name: <Pseudo-file name>` The name given here is a symbol which can be used to refer to a physical graphics device when asked for graphical output file.
	`Plot device number /1/: <Device number>` The number that specifies the type of graphical device.

	`Plot file name: <File name or printer name>`
	The name of the graphical device on system level (name of file or printer).
	Example
	`SET_PLOT_ENVIRONMENT 1 lasp 5 a0tr,,`
	This example sets the default plot device number to `1`, and defines an alias named `lasp` with plot device `5` and connected to a printer named `a0tr`.

SET_TC_OPTIONS

Predefine the default values of three general options for performing all the sequential single-points, stepping and mapping calculations.

Syntax	SET_TC_OPTIONS
Prompts	`Use_global_minimization /Y/:` By default it global minimization is used where possible (depending on the conditions setting). A global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. Enter N to prevent global minimization being used to reach the equilibrium.
	`Global_test_interval /0/: <An integer value>` The integer number determines how often the global minimization should be used during calculations with STEP_WITH_OPTIONS and MAP. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during step calculations, and only at node points during map calculations. Any other positive integer number, n, suggests it performs global minimization tests at every n^{th} step during step and map calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The software is initially configured with 0 (zero) as the default value, but such a configuration for the default value can be changed by this option.
	`Automatically_add_initial_equilibria /Y/:` When ADD_INITIAL_EQUILIBRIUM is not used before a map calculation, a mesh of INITIAL_EQUILIBRIUM is automatically added before the mapping procedure itself takes place. This mesh is only available when the two independent axis-variables have already been defined by the POLY command.
	`Set_axis_variable` If Y is entered, the POLY module always enforces the automatic procedures for adding initial equilibrium points during mapping. For N, no initial equilibrium points are then added during mapping.

STOP_ON_ERROR

Useful for batch jobs in order to prevent that an erroneous sequence of commands to the program causes waste of computer activity.

Syntax	STOP_ON_ERROR
	Give the preferred argument (ON or OFF) after the STOP command. If the default argument ON is given, the program terminates after an illegal or ambiguous command. It is possible to reset the effect of this command by giving the argument OFF.

Database (TDB) Module Commands



These commands are related to the DATABASE_RETRIEVAL module, which is also known as the TDB module.

Search the online help for step-by-step instructions to define a system.

In this section:

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DEFINE_SYSTEM 158

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LIST_SYSTEM 161

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SET_AUTO_APPEND_DATABASE 164

SWITCH_DATABASE 165

AMEND_SELECTION



This command is for the DATABASE_RETRIEVAL (TDB) module.

Use this command after defining the elements, species or the system (with the commands DEFINE_ELEMENTS, DEFINE_SPECIES, or DEFINE_SYSTEM). The prompts allow changes to the predefined system. By answering Y or N, each of the selected elements, species or phases can be accepted or rejected (although this is not the case for the constituents or the entire system).

Syntax	AMEND_SELECTION
Prompt	`Keep <Name1> No/Quit/Yes/` `Keep <Name2> No/Quit/Yes/`
Options	`Keyword-- Elements/Species/Phases name&` Names of the pre-defined or pre-selected elements/species/phases

APPEND_DATABASE



This command is for the DATABASE_RETRIEVAL (TDB) module.

Appends data to the current set of data already read from another database. The syntax is the same as for the SWITCH_DATABASE command.

This command enters all additional functions and parameters to already existing phases, e.g atomic mobilities, phase constituents, excess models, G0 and interaction parameters.

This command is most commonly used to read mobility data from stand-alone mobility databases.

This command should be used with some caution if thermodynamic data is appended and the application is run with Gibbs Energy System version 5 (see SET_GES_VERSION in the SYS module). It can change calculated values in an unexpected way. This can happen e.g. if the appended database has the same function name as a function in the data retrieved from a database opened with SWITCH_DATABASE.

Syntax	APPEND_DATABASE
Prompt	`New database name /XYZ/:` The name of either an existing database (e.g. FEDEMO) or USER.

DATABASE_INFORMATION



This command is for the DATABASE_RETRIEVAL (TDB) module.

Use the DATABASE_INFORMATION command to obtain a short description of the current database. This can include information on covered systems, used models, valid ranges for parameters in temperature and composition, major applications, and so on.

DEFINE_ELEMENTS

This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of elements. All possible species that can be formed by the given elements are retrieved from the database. The names of elements must be separated with a space or comma. It is possible to use a wildcard * after a common part of element names so that all the elements, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 40 elements can be defined into a single system.

Also see Defining a System in Console Mode for step-by-step instructions to define a system with this command.

Syntax	DEFINE_ELEMENTS
Prompt	`Element& <Element1, Element2, …>` A list of elements to be defined into the system.
	When appending database(s), this command, or DEFINE_SPECIES or DEFINE_SYSTEM must be repeated with the same or similar elements as defined in the first switched database.

DEFINE_SPECIES

This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of species. Only those species given are retrieved. The different names of species must be separated with a space or comma. It is possible to use a wildcard * after a common part of species names so that all the species, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 1000 species can be defined in a single system.

Defining a System in Console Mode

Syntax	DEFINE_SPECIES
Prompt	`Species& <Species1, Species2, …>` A list of species to be defined in the system.
	When appending database(s), this command, DEFINE_ELEMENTS or DEFINE_SYSTEM must be repeated with the same or similar elements as defined in the first switched database.

DEFINE_SYSTEM



This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of either elements (equivalent to DEFINE_ELEMENTS) or species (equivalent to DEFINE_SPECIES). Certain databases have a default value of the keyword (as either ELEMENTS or SPECIES) reflecting what is most appropriate when defining a system.

The different names of elements or species must be separated with a space or comma. It is possible to use a wildcard * after a common part of elements or species names so that all the elements or species, which start with that common part and are available in the currently switched or appending database, are defined in the system.

When appending database(s), this command (or DEFINE_ELEMENTS or DEFINE_SPECIES) must be repeated with the same or similar elements as defined in the first switched database. Different databases might contain different elements and have different species definitions: avoid defining elements/species that are missing in the appending database(s). Otherwise, the program indicates these missing elements/species, and ignores them in subsequent steps. But additional elements/species, and additional phases not available in the first switched database can be defined and retrieved from the appending database(s). Up to 40 elements and 1000 species can be defined in a single system.



Also see Defining a System in Console Mode for step-by-step instructions to define a system with this command.

Syntax	DEFINE_SYSTEM
Prompt	`Elements: <Element1, Element2, …>, or Species: <Species1, Species2, …>`
Options	**Description**
`Species or Elements`	Default keyword.
`Element&`	Specify a list of elements for the defining system.
`Species&`	Specify a list of species for the defining system.

GET_DATA

This command is for the DATABASE_RETRIEVAL (TDB) module.

Enter the defined system's elements, species, phases, and the connected parameters obtained from either the primary switched or additionally appending database(s) to the GIBBS and/or DICTRA workspace. Then use the GET_DATA command to get all information concerning a defined system from the databank.

Only after executing this command can you go to any of the application programs such as GES, POLY or DICTRA and use the retrieved data. When appending database(s), this command must be repeated in order to obtain the additional system definitions, parameters and functions.

LIST_DATABASE



This command is for the DATABASE_RETRIEVAL (TDB) module.

List all elements, species, phases or phase constituents in the database.

Syntax	LIST_DATABASE
Options	**Description**
`Keyword`	One of the keywords Elements, Species, Phases or Constituent must be used to indicate what to list
`Elements`	All available elements, the reference state, atomic mass, H298-H0 and S298. Some elements have spaces in the column for the reference state. This implies that there are no parameters stored for this element.
`Species`	All available species together with the stoichiometric factors.
`Phases`	All available phases together with the number of sublattices and the number of sites in each sublattice.
`Constituent`	All available phases, the number of sublattices, the number of sites in each sublattice and the species dissolved in each phase. Species in different sublattices are separated with a colon (:). It is important to realize, for example, a phase can consist of Fe, Mo, V, and Cr, and its thermodynamic parameters can come from the binary systems Fe-Mo, Fe-V, Fe-Cr, and Mo-Cr. These data can give a relatively good description of the corners of the Fe-Cr-Mo system, but would most certainly give a bad one for the system Mo-Cr-V, due to the fact that the interaction parameters are, by default, set to zero, which originates from binary systems not included in the database.

LIST_SYSTEM

This command is for the DATABASE_RETRIEVAL (TDB) module.

List all elements, species, phases or phase constituents in the defined system. It works only after a system is defined.

Syntax	LIST_SYSTEM
Keyword	One of the keywords `Elements`, `Species`, `Phases` or `Constituent` must be used to indicate what to list. ▶ LIST_DATABASE

REJECT

This command is for the DATABASE_RETRIEVAL (TDB) module.

Reject elements, species, phases or phase constituents that can form from the defined elements and species. Phases/species/constituents that are possible to form in the defined system are removed from the list of system phases/species/constituents (shown by the command LIST_SYSTEM). Phases/species/constituents that are not included in the list cannot be entered without first being restored. The different names must be separated with a space or comma. You can use a wildcard * after a common part of names so that all the elements/species/phases/constituents that start with that common part and are available in the currently switched or appending database, are rejected from the defined system.

This command can also reject a defined system, and thus reinitiate the entire DATA module memory and GES workspace.

Syntax	REJECT
Prompt 1	(Keyword = Elements or Species or Phases) `If keyword: <Name1, Name2, …>`

Prompt 2	(if keyword = Constituent)
	`Phase: <Phase name>`
	`Sublattice number: <Sublattice number in the phase>`
	`Constituent: <Constituent(s) in the sublattice of the phase>`

Prompt 3	If keyword = SYSTEM the DATA module is reset to its initial state; GIBBS is reinitiated and data already entered to GES is lost.
Options	**Description and additional information**
`Keyword`	One of the keywords `Elements`, `Species`, `Phases`, `Constituent` or `System` must be used to indicate what is rejected.
`Name&`	Names of the pre-defined elements/species/phases/constituents/system
`Elements`	The given elements are rejected.
`Species`	The given species are rejected, making it impossible to form them from the defined elements.
`Phases`	The given phases are rejected, making it impossible to form them from the defined elements or species.
`Constituent`	The given constituent in one phase are rejected. Add the following when prompted: `Phase`: The name of the phase containing the constituent to be rejected. `Sublattice number`: The sublattice where the constituent enters (the first sublattice is 1). The question is omitted if there exists only one possible sublattice. `Constituent`: The name(s) of the constituent(s) to be rejected.

RESTORE



This command is for the DATABASE_RETRIEVAL (TDB) module.

Restore already explicitly rejected elements, species, phases or constituents; it is the opposite of the command REJECT although it does not restore a completely rejected system.

Phases/species/constituents that are possible to form from the defined elements or species are entered to the list of system phases/species/constituents (shown by the command LIST_SYSTEM). Phases/species/constituents that are not included on the list can now be added to the list. The different names must be separated with a space or comma. It is possible to use a wildcard * after a common part of names so that all the elements/species/phases/constituents, which start with that common part and are available in the currently switched or appending database, are restored in the defined system.

Syntax	RESTORE
Prompt1	(if keyword = ELEMENTS or SPECIES or PHASES) `Keyword: <Name1, Name2, …>`

Prompt2	(if keyword = CONSTITUENT)
	`Phase: <Phase name>`
	`Sublattice number: <Sublattice number in the phase>`
	`Constituent: <Constituent(s) in the sublattice of the phase>`

Options	**Description and Information**
`Keyword`	One of the keywords `Elements`, `Species`, `Phases` or `Constituent` must be used to indicate what is rejected.
`Name&`	Names of the pre-defined elements, species, phases, and constituents
`Elements`	The given elements are restored.
`Species`	The given species are restored and thus possible to form from the defined elements.
`Phases`	The given phases are restored and thus possible to form from the defined elements or species.
`Constituent`	The given constituent in one phase are restored. Add the following when prompted: `Phase`: The name of the phase containing the constituent to be restored. `Sublattice number`: The sublattice where the constituent enters (the first sublattice is 1). `Constituent`: The name(s) of the constituent(s) to be restored.

SET_AUTO_APPEND_DATABASE

This command is for the DATABASE_RETRIEVAL (TDB) module.

Enforce an automatic action that appends thermodynamic data from a chosen database regarding the system to the data you already have about the system from the current database (that is, the default database or the database last chosen with SWITCH_DATABASE or APPEND_DATABASE).

This is useful to simultaneously retrieve both thermodynamic and mobility data for a defined system when performing a DICTRA module simulation.

This command should be used before defining a system (with the commands DEFINE_ELEMENTS, DEFINE_SPECIES, or DEFINE_SYSTEM) and retrieving the data with the GET_DATA command from the primary switched database.

Syntax	SET_AUTO_APPEND_DATABASE
Prompt	`Database name /XYZ/: <Additional database name>`
Option	`Additional database name` The name of an existing database or a User database that corresponds to the automatically-appending database.

It works in a way that is similar to the APPEND_DATABASE<DATABASE-NAME> command sequence, but only the phases that are also available in the primary switched database are appended. There is no possibility to manually list, reject and/or restore any phase that is available in the appending database. When retrieving data with GET_DATA afterwards, all the phases that exist in the appending database but not in the primary switched database are automatically rejected. The prompt is kept as for the primary switched database, `TDB_XYZ`: (where `XYZ` stands for the name of the primary switched database) until the execution of GET_DATA.

Therefore, to selectively append more phases from a secondary database to a system that is defined and retrieved from a primary switched database, then APPEND_DATABASE and sequential commands (such as DATABASE_INFORMATION, DEFINE_SYSTEM, DEFINE_ELEMENT, DEFINE_SPECIES, LIST_SYSTEM, REJECT, RESTORE and GET_DATA) should be used instead, before this command.

Although it is impossible to manually list, reject and restore any phase from the appending database, the DATA module automatically ignores all the phases that do not exist in both the primary switched database and the appending database, and append the data for the phases (that are also available in the primary switched database) from the appending database, as informed on screen when executing GET_DATA afterwards.

SWITCH_DATABASE



This command is for the DATABASE_RETRIEVAL (TDB) module.

Switch (or change) from the current database to a new one. It also reinitializes the entire module.

The database can be either a standard database (the ones in `tc_initd.tdb`) or a so-called user database. To open your own (user) database, type `USER` followed by the path to the user `.TDB` file or press <Enter> and select it in the window that opens.

Syntax	SWITCH_DATABASE
Prompt	`New database name /XYZ/:` The name of either an existing database (e.g. FEDEMO) or USER.

POLY Module Commands

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ADD_INITIAL_EQUILIBRIUM

This command is for the POLY module.

Add initial equilibrium points from which a phase diagram is calculated (through the MAP command).

For each initial equilibrium the first stage of the mapping varies the value of the given axis variable condition, changing it in the given direction. When a phase change is found it is saved as a start equilibrium, and if the symbol ">" was used, it continues the search until the end of the axis variable.

If no axis variable conditions differ between initial equilibria then the map results in several overlaid diagrams, in accordance with the selected conditions and the values.

The ADD_INITIAL_EQUILIBRIUM default command implicitly makes the MAP command search for phase changes according to settings set by ADVANCED_OPTIONS STEP_AND_MAP command. Default for STEP_AND_MAP are three initial equilibrium equidistantly along each axis variable, along the edge of the axis variable rectangle.

By default these default start points are used in MAP. If any ADD_INITIAL_EQUILIBRIUM is used these default start points are not used. They are again used if the command ADD default is used together with another ADD_INITIAL_EQUILIBRIUM command.

The ADD command with the default direction scans along the axis variables and generates start points each time the scan procedure crosses a phase boundary. In addition, it generates four start points, scanning cross the middle of each axis, if there is any solubility line that does not reach the axes. At the MAP command, a search for lines in the diagram is made along each direction of the axis variables in the diagram.

In this way, it should guarantee that all possible phase boundary lines in a phase diagram are found. It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the POLY module remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria by appending a > after the direction at the ADD command. For example:

```
Direction /Default/: 2>
Direction /Default/: -2>
```

This generates one start point for each set of phase change in the positive direction of the axis 2 (or negative direction of the axis 2); this ensures finding all possible phase boundary lines (not just the first one) along such an axis direction.

This is particularly useful when you have a phase diagram with several lines with no intersection. It is thus possible to calculate e.g. an isopleth for a much more limited composition range. It is also useful for calculating CVD diagrams and Pourbaix diagrams.

Syntax	ADD_INITIAL_EQUILIBRIUM
Prompt	`Direction /Default/: <Direction code>` Direction code(s): • `1` or `2` for positive direction of axis 1 or 2, respectively. • `-1` or `-2` for negative direction of axis 1 or 2, respectively. • `Default` for MAP to start looking for phase changes from each corner of the axis variable rectangle. The direction is important when the initial equilibrium point is in a single-phase region or when the diagram is an isopleth (tie-lines not in the plane of calculation). In such cases, the program will search for a line in the diagram (i.e., a line where the amount of a phase is zero) in the given direction.

Normally, this command is not needed to calculate a property diagram (with the STEP_WITH_OPTIONS → `NORMAL` command-sequence), as the STEP procedure starts from the current equilibrium state already calculated. In many cases, the ADD_INITIAL_EQUILIBRIUM command is not required for MAP commands either.

In order to calculate a simple property diagram, set the equilibrium conditions and the stepping axis variable, and then give a STEP command. But if a phase diagram has disconnected lines, ADD_INITIAL_EQUILIBRIUM may still be needed to add two or more initial equilibria so that the MAP calculation starts from such initial equilibria at the specified directions to find all phase boundary lines.

This command becomes unnecessary in most cases, as the MAP routines that by default use the Global Minimization Technique handles all the initial equilibrium points in a robust and automatic way. Therefore, you do not need to have a good guess of the starting point and to add any initial equilibrium point prior to the calculations of various types of phase diagrams. However, if preferred, use this command to add any initial equilibrium points in certain directions, the POLY module uses the specified starting point(s) and corresponding user-added initial equilibrium point(s) for a mapping calculation; in such a case, the automatic procedure in the rewritten MAP routines are not enforced while the Global Minimization Technique can still be applied. Similar situations occur when a specific database, in which there are some definitions of initial-equilibrium adding direction(s) for accessed binary and/or ternary subsystems in its ACCESSED_SYSTEM section, is used in the BINARY or TERNARY module for calculating a binary or ternary phase diagram.

All the initial equilibrium points generated by ADD_INITIAL_EQUILIBRIUM (previously and presently; saved in the current POLY workspace) can be easily listed on screen with LIST_INITIAL_EQUILIBRIA. A certain initial equilibrium point (including its conditions and equilibrium results) can be loaded into the current equilibrium, if needed, with LOAD_INITIAL_EQUILIBRIUM. Any specific or all of the initial equilibrium points can be deleted from current POLY workspace, if desired, with DELETE_INITIAL_EQUILIBRIUM.

ADVANCED_OPTIONS

This command is available with the POLY and ED-EXP modules.

Syntax	ADVANCED_OPTIONS
Prompt	`Which option? /Step_and_Map/:  <Option>`

Several options are available after you enter this command at the prompt. The default is STEP_AND_MAP.

```
POLY:advanced-options
Which option? /STEP_AND_MAP/:?
 EQUILIBRIUM_CALCUL       NEW_COMPOSITION_SET      STABILITY_CHECK
 GLOBAL_MINIMIZATION      OUTPUT_FILE_FOR_SHOW     STEP_AND_MAP
 IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM          T-ZERO TEMPERATURE
 KEEP_COMP_SET_NUMBERS    PHASE_ADDITION           TOGGLE_ALTERNATE_MODE
 LIST_PHASE_ADDITION      PRESENT_PHASE
 MAJOR_CONSTITUENTS       SHOW_FOR_T=
Which option? /STEP_AND_MAP/:
```

- EQUILIBRIUM_CALCUL
- GLOBAL_MINIMIZATION
- KEEP_COMP_SET_NUMBERS
- LIST_PHASE_ADDITION
- MAJOR_CONSTITUENTS
- NEW_COMPOSITION_SET
- OUTPUT_FILE_FOR_SHOW
- PARAEQUILIBRIUM
- PHASE_ADDITION
- PRESENT_PHASE
- SHOW_FOR_T=
- STABILITY_CHECK
- STEP_AND_MAP
- TOGGLE_ALTERNATE_MODE
- T-ZERO_TEMPERATURE

AMEND_STORED_EQUILIBRIA



This command is for the POLY module.

This command gives information about the calculated blocks (and phase regions included in blocks) after the STEP or MAP calculation(s). It allows you to list all or part of the calculation results, to suspend all or parts of the calculation results that are redundant or where metastable equilibria are calculated, and to restore all or parts of the calculation results (if having been suspended by another AMEND_STORED_EQUILIBRIA command).

The workspace for storing equilibria may overflow during stepping or mapping, and is then written to a file as blocks. Each block usually contains one or more ranges of equilibrium regions.

Use one these options:

- L to list the calculated equilibria (all or a specified block)
- S to suspend everything (all blocks and their regions)
- Q to suspend each set of equilibria individually (specified blocks and/or regions)
- R to restore everything (all blocks and their regions)

Syntax	AMEND_STORED_EQUILIBRIA
Prompts	`Name: <Name of a defined table>` List (L) the calculated equilibria, suspend everything (S) or suspend each set of equilibria individually (Q), or restore everything (R).
	`Block /*/: <Block number>` Specify a block number in the option L, S, Q or R. Or include all the blocks in the amending option, by accepting the wildcard * (press <Enter>). For L, a block (if a block number is specified) or all the blocks (if the wildcard * is accepted/used), with the regions and the equilibrium details, that are calculated during stepping or mapping is listed on screen or in a textual file. For Q, each ranger in a block (if a block number is specified) or in all blocks (if the wildcard * is accepted/used) then choose:

	`S(uspend) K(eep) /K/: <S or K>`
	For S or R, if a block is specified, you are asked what region in the block should be suspended or restored. However, if the wildcard * is accepted/used, you are asked the following:
	`Really suspend all /N/:`
	`Really restore all /N/:`
	In both cases the default is N and you are prompted for which block(s) and which region(s) in a certain block to execute the S or R action.
	`Really suspend all /N/:`

Syntax	AMEND_STORED_EQUILIBRIA
	Y suspends everything. `Really restore all /N/:` Y restores everything.
	`Range: <Range(s) of region>` Specify one or more ranges to be suspended (the `S` option) or restored (the `R` option). The wildcard * suspends or restores all ranges in the specified block. In order to know the ranges the LIST command must first be used.
	`S(uspend) K(eep) /K/: <S or K>` The Query suspend option (`Q`) asks for each region in a certain block if it should be suspended or kept. Suspended regions are not included on sequentially generated plots.
	`Output file: /Screen/: <File name>` This prompt is only for listing (the `L` option), and after it the command is terminated. The file name must be given here; or accept the default Screen (terminal) by pressing <Enter>. A list of stored equilibria as various blocks (with all their ranges) are shown out on screen or the file.

CHANGE_STATUS



This command is available with the POLY and ED-EXP modules.

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the SUSPENDED or DORMANT phase-status. Another important applications is to calculate paraequilibria by setting some components to the SPECIAL component-status.

For a component and for a species, the status can be one of the following:

- `ENTERED`: the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED`: the component(s) or species are not considered in the calculation.
- `SPECIAL`: the specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).



Only component(s) can have the status SPECIAL, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_ STATUS command.

Syntax	CHANGE_STATUS
Prompts	`For phases, species or components? /Phases/: <Keyword>` *Keyword* = phase or species or components
	`Phase name(s): <Name(s) of the phase(s)>` For `phase` as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be assigned to the phases can also be given on the same line if preceded with an equal sign (=).

Syntax	CHANGE_STATUS
	An asterisk, *, can be used to denote all phases. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended phases. In the same way, *D means all dormant phases, and *E means all entered phases.
	Name(s): <Name(s) of the Species or Component(s)> For species or components as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of phase as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =. An asterisk, *, can be used to denote all species or components. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended species or components. In the same way, *E means all entered species or components.
	Status /Entered/: <New status> The new status to be assigned must be given. For species, the values ENTERED or SUSPENDED can be used. For the POLY module, using the Entered or Suspended status here has the same result as using the commands MAKE_COMPONENT_ENTERED and MAKE_COMPONENT_SUSPENDED. The exception is that any existing conditions that depend on a suspended component are removed when using the MAKE_COMPONENT_SUSPENDED command. For components, the status ENTERED, SUSPENDED or SPECIAL can be given. SPECIAL means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the *ufractions* or other normalized fractions of system components. For phases, the status ENTERED, SUSPENDED, DORMANT or FIXED can be given. DORMANT means the same as suspended but the driving force is calculated. FIXED means that it is a condition that the phase is stable at a certain amount. For example, for the ufractions, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status SPECIAL. This is assigned by the CHANGE_STATUS command: Change_Status comp C=special.
	Start value, number of mole formula units /0/: <Initial amount> For ENTERED phases, an initial amount of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.
	Number of mole formula units /0/: <Equilibrium amount> For FIXED phases, the equilibrium amount of the phase [always using an initial estimation being the NPF(phase) value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.

Syntax	CHANGE_STATUS

Note when specifying a FIXED phase status

Special attention should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below.

The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the CHANGE_STATUS command to set a relevant condition, e.g. `CHANGE_STATUS phase <phase>=fix <amount>` where the fixed <amount> is roughly the same as the F-suffixed quantity `NPF(phase)`.

The `NPF(phase)` quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other `F`-suffixed state variables [e.g. GF(phase), HF(phase) and DGF(phase)] cannot be directly applied in any POLY command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: `NPFabc = NP(abc)/NA` or `NPFabc = NPM(abc)/NA*N`. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1 NA = 1
FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1 NA = 1
BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3 NA = 1
SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18 NA = 30
```

If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modeled by the Two-Sublattice Ionic Liquid Model, i.e.:

```
IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q,7
```

then the evaluation of its NA value becomes even more complicated:

```
NA = p + q*yC2 + q*yN2 + q*yO2 + q*yFeO2 3/ 2
```

where the stoichiometric coefficients *p* and *q* are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

There is no strange thing when using a zero value [i.e. `0`] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.

However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations.

Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a

Syntax	CHANGE_STATUS
	liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. N=1). When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [NA>1; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF(phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper `NPF(ION_LIQ)` value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of N/[$p + q^*y$C2 + q^*y_N2 + q^*y_O22 + q^*y_{FeO}2 3/ 2].

Examples

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_Status comp C=special
```



The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statues:

- `ENTERED`: the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.
- `SUSPENDED`: the phase(s) are not considered in the equilibrium calculations.
- `DORMANT`: the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.

- `FIXED`: it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMPUTE_EQUILIBRIUM

This command is for the POLY module.

The full equilibrium state is calculated for the given set of conditions. The Global Minimization Technique is by default enforced in this command (C_E), while it can be disabled temporarily (for the current single-point equilibrium calculation) if using C_E – or C_E * command-combination, or permanently (for all the sub sequential single-point calculations or stepping/mapping calculations within the current TCC run) if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the ADVANCED_OPTIONS → `MINIMIZATION_OPTION` command-sequence.

Syntax	COMPUTE_EQUILIBRIUM
Prompt	The C_E command can be used, in order to enforce the ordinary POLY minimization routines in an equilibrium calculation; this is because of that the ordinary C_E command is now associated with the Global Minimization Technique, and only after the Global Minimization If technique is permanently switched off the C_E command makes no difference from the C_E – command-combination. Only certain types of equilibrium conditions [e.g. `T`, `P`, `N`, `N`(`<component>`), `X`(`<component>`), `B`, `B`(`<component>`), and `W`(`<component>`)] are fully supported in the Global Minimization mode (called *Direct Global Minimization*); and when other types of equilibrium conditions are used, after the initial POLY, a Global Minimization test and corrections are performed until the lowest minimum is found (called *Indirect Global Minimization*). If there is any problem with convergence, you may try the C_E * command-combination. The character * enforces the command to use an advanced technique to obtain a complex equilibrium. However, after a successful C_E *calculation, you may repeat the C_E command and can check the status of phases, species or components (with LIST_STATUS → CPS command-sequence) and equilibrium conditions (with LIST_CONDITIONS) and list out the calculation results (with LIST_EQUILIBRIUM), because such actions may tell you how to further modify various settings for your current calculation. This command-combination is not that useful anymore, because the Global Minimization Technique that is always associated with the C_E command is even more powerful and more precise in finding the most-stable equilibrium state in a complex heterogeneous interaction system; therefore, the C_E * command-combination is functional and can be used only after the Global Minimization mode has already been disabled temporarily or permanently. Some phases that are not stable in the current equilibrium state may not have their most favorable composition after this command, and thus their driving forces may not be correct. You can force the program to correctly calculate the driving forces of metastable phases, by giving repeated C_E commands until the number of iterations (that is shown on screen after this command) is reduced to 2. Also see the POLY command SET_NUMERICAL_LIMITS which can set the approximate driving force for metastable phases option on or off in all the subsequent POLY calculations within the current TCC run.

Syntax	COMPUTE_EQUILIBRIUM
	 If an equilibrium state for the defined system is not found, an error message is given. You can try repeating this command a few times, or change some of settings for the numerical limits, for starting variables and starting values, for starting constitutions of certain phases and for reference states of certain components, or to verify some of the defined conditions.

COMPUTE_TRANSITION



This command is for the POLY module.

This command is a combination of the CHANGE_STATUS, SET_CONDITION and COMPUTE_EQUILIBRIUM commands. It allows a direct calculation when a new phase may form by varying one of the already-set conditions. It can be used only after at least one equilibrium is calculated successfully; otherwise, you are informed on the necessity of first making an equilibrium calculation to find out the stable phases under the current conditions.

When this command is used, the program calls the command CHANGE_STATUS to temporarily change the phase status of a specified phase as FIXED at the *zero* amount, and at the same time to temporarily release one of the existing equilibrium conditions (which is chosen by you). The program calculates a new equilibrium in which that specific phase is stable but its equilibrium amount in the system is zero. The released condition is then assigned with a calculated value that ensures the calculated equilibrium. After wards, the program automatically changes the phase status of that specific phase back to ENTERED, and resets the temporarily released condition as one of the conditions and assigns it with the value that is calculated to ensure the zero-amount formation of that specific phase.

This command is useful to find melting temperature, boiling temperature, or solubility limits, and generally when you want to set the most optimal conditions for calculating an equilibrium where a specific phase becomes stable. It can also be used when you want to know exactly how far away the defined conditions are from the value that can ensure a zero-amount of a specific phase in the system when other conditions remain the same.

After a successful calculation, you can issue a COMPUTE_EQUILIBRIUM calculation to assure the calculated transitional equilibrium is a really stable one, and can also use LIST_EQUILIBRIUM to see the details of transitional equilibrium state.

Syntax	COMPUTE_TRANSITION

Prompts	`Phase to form: <Phase name>`
	
	A new `phase name`, e.g. `BCC` that is expected to form, is specified here. This changes the status of this new phase to be `FIXED` as `0` amount, and the program shows the information such as:
	
	`You must remove one of the these conditions`
	
	`P=100000, T=800, N=1, X(FE)=.5  DEGREE OF FREEDOM 0`
	
	If the key word `ANY` is used when prompted for `Phase to form` (instead of a specific phase name), it is possible to find out any new phase to be formed, in a given varying direction sign and at an estimated change of the released condition: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). Such calculations can be repeated if required. This feature is useful to find out all possible phase transformations along a certain released condition.

Syntax	COMPUTE_TRANSITION
	`Give the state variable to be removed /T/: <One condition>` `One condition` must be removed, in order to calculate the transition equilibrium where the specified (or any) new phase to be formed at a calculated value of this released variable.

	Therefore, the message may display (after a successful calculation) if, for example, `X(Fe)` is entered:
	
	`To form BCC the condition is set to X(FE)=.48605791769`
	
	This calculated value is assigned as the parameter of that removed condition, in this case, the `X(FE)` variable. If the LIST_CONDITIONS command is typed this message displays:
	
	`P=100000, T=800, N=1, X(FE)=4.86057918E-1`
	
	`DEGREES OF FREEDOM 0`
	
	If the key word `ANY` (instead of a specific phase) is given as the phase name when it is prompted for Phase to form, the line is prompted for a given varying direction sign and an estimated change of the released condition before the calculation of transition equilibrium:

	`Estimated change (with sign) /1/: <+/-#>`
	
	A given varying direction sign and an estimated change of the released condition, in this case as `X(FE)`, must be given here: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). For example, if a combination of -0.02 is input, this message may display (after a successful calculation):
	
	`To form BCC_A2#1 the condition is set to X(FE)=.493708756187`
	
	This calculated value is then assigned as the parameter of that removed condition, in this case, the `X(FE)` variable. The message is shown if the LIST_CONDITIONS command is typed:
	
	`P=100000, T=800, N=1, X(FE)=4.93708756E-1`
	
	`DEGREES OF FREEDOM 0`

CREATE_NEW_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

During data-assessments using the ED_EXP module (a submodule of PARROT), you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

Syntax	CREATE_NEW_EQUILIBRIUM
Prompts	`Equilibrium number /2/: <A new equilibrium number>` Each equilibrium in the POLY workspace is identified by a unique integer number. Such an equilibrium number can be recalled with SELECT_EQUILIBRIUM.
	`Initiation code /2/:` When an equilibrium is created, you can choose to `ENTER` all components and phases (initiation code 2), `ENTER` the components only (initiation code 1) or `SUSPEND` everything (initiation code 0). No other values are legal. The entered components and phases can later be changed with CHANGE_STATUS.

DEFINE_COMPONENTS

This command is available with the POLY and ED-EXP modules.

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.

This implies a command REINITIATE_MODULE and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	`Give all new components / existing components/: <New components>` The `new components` must be specified all on one line. These replace the existing component definitions. The number of components cannot be changed with this command. Use CHANGE_STATUS instead.
	To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements. The new components do not have to be present as species.

DEFINE_DIAGRAM

This allows automatic calculation and plotting of a diagram with a single command. It is the same as the DEFINE_MATERIAL command up to when the first equilibrium is calculated. The alloy OPTION feature is also available in this command to specify alloying compositions for a special alloy predefined by the OPTION keyword in a selected database (e.g. the TCNI Ni-based Superalloys Database).

Use this command to calculate all types of phase diagrams after specifying all composition value and an initial temperature (if temperature is used as an axis). However, for binary and ternary diagrams, the special BIN and TERN modules may be preferred.

It then lists all the independent variables for the defined system (i.e. temperature and the components) and asks for a variable as the X-axis. You must also specify a maximum and minimum for the X-axis. The second axis (Y-axis) can be another composition (or the temperature if that is not on the X-axis) from the independent variable list. The program then calculates and plots a *phase diagram*, as there are two independent quantities on the axes.

Alternatively, select a dependent quantity as the Y-axis variable from the second list on screen (e.g. the amount of all phases, composition of a specific phase, or fractions of a component in all phases), and the program calculates and plots how this quantity depends on the condition on the X-axis. This is a *property diagram*.

This command ends up within the POST module monitor. You can refine the calculated phase diagram or property diagram.

Moreover, many more property diagrams with axes other than compositions can also be plotted (after the calculation), using SET_AXIS_VARIABLE in the sequent POST monitor.

Syntax	DEFINE_DIAGRAM

Prompts	These prompts are given:
	`Same elements as before /Y/?`
	`Mole percent of <Element> /##/: <Value>`
	or
	`Mass percent of <Element> /##/: <Value>`
	`Database /ABCDE/: <Database name>`
	`Major element or alloy: <Element name>`
	`Composition in mass (weight) percent? /Y/:`
	`1st alloying element:  <Element name>`
	`Mass (weight) percent: <Amount of the above specified element>`
	`2nd alloying element: <Element name>`
	`Next alloying element: <Element name>`
	`Mass (weight) percent: <Amount of the above specified element>`

Syntax	DEFINE_DIAGRAM

	`Temperature (c) /1000/: <Temperature of interest in oc>`
	`Reject phase(s) /none/: <List of phase(s) to be rejected>`
	`Restore phase(s) /none/: <List of phase(s) to be restored>`
	`OK? /Y/: <Y or N>`
	`Should any phase have a miscibility gap check? /N/:`
	`Phase with miscibility gap: <phase name>`
	`Major constituent(s) for sublattice #: /aa/: <Constituent(s)>`
	`Phase with miscibility gap: <Phase name>`
	The first equilibrium is calculated, as with DEFINE_MATERIAL. Then a list of all independent conditions suitable to be chosen as X/Y-axis variables is given by the program.

	`Quit? /Y/: <Y or N>` This question is asked only when the axis variables are already defined, or if DEFINE_DIAGRAM is used. It then offers an opportunity to quit (Y) the calculation or to continue (N) the calculation but by defining other axes.
	`Give the number of the condition to vary /1/: <A condition index>` Select one of the independent conditions by giving its index on the condition list as the X-axis variable.
	`Minimum value /XXX/: <minimum value for X-axis>` Specify the minimum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value.
	`Maximum value /YYY/: <maximum value for X-axis>` Specify the maximum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value. Then another list with some dependent quantities is given by the program, which can be selected as the Y-axis variable.
	`Give the number of the quantity on the second axis /#/: <##>` Select one of the independent conditions or dependent quantities as the Y-axis variable, by giving its corresponding index given on the condition lists.  It must be different from the X-axis variable already selected. If selecting one of dependent quantities (by giving the corresponding number from the second list) as the Y-axis, then a property diagram is to be automatically calculated (through a normal stepping procedure) and generated. For `composition of a phase` the phase name is asked for further specification subsequently. If selecting any of the other independent variables (conditions) on the first list as the Y-axis, then a phase diagram is automatically calculated (through a mapping procedure) and plotted.
	`Name of phase: /ABC/: <phase name>` This is prompted only in case of that the `composition of a phase` is selected as the Y-axis variable. The phase name for which the composition varied along with X-axis variable should be specified.

Syntax	DEFINE_DIAGRAM
	`Multiple start points? /Y/:` By default, the program automatically generates and uses multiple start points for mapping the defined phase diagram.
	`Save file /Result/: <File name>` The file name where the calculations are stored (saved as a *.POLY3 file) should be specified; the default file name is `RESULT.POLY3`.  Linux and Mac are case sensitive so ensure you enter `.POLY3`.

DEFINE_MATERIAL

This command is for the POLY module.

Read data for a system from a database in the POLY module. It is convenient to use for alloys when there is a major component and the amount of the other elements is known in mass (weight) fraction. The command reads the system from the specified database, sets the composition and temperature (and pressure equal to 1 bar) and calculates the equilibrium state before the prompting for a new command. You can list the results with LIST_EQUILIBRIUM or set a new composition or set axis for a STEP or MAP command.

You cannot append data from different databases in this way. Use this command with data from a USER database.

Syntax	DEFINE_MATERIAL
Prompts	`Same elements as before /Y/?` This question is asked only if some data is already read from the database, or if the command DEFINE_MATERIAL or DEFINE_DIAGRAM is used. It then offers a convenient way to change the composition and temperature with one command. This command only works properly in cases where the composition of the material system is already defined as in the mole-percent or mass-percent unit.

	`Mole percent of <Element> /##/: <Value>`
	
	or
	
	`Mass percent of <Element> /##/: <Value>`
	
	If you have decided to use the same materials system (available in the current POLY3 workspace) by accepting the default (Y) to the previous prompt `Same elements as before /Y/?`, one of the alternative prompts display for each of the components in the defined system, depending on how the composition is defined (either in mole-percent, or in mass-percent).
	
	Prompts are repeated until all the defined components are completed. Then, the program prompts to specify the temperature condition.

	`Database /ABCDE/: <Database name>` The database with the description for the material must be given, or press <Enter> if using the current database. It is possible to give a USER database.
	`Major element or alloy: <Element name>` The material must have a major element, usually the element which is present in the largest amount. The fraction of this element is not set but is the rest. In some databases there are the alloys predefined. An alloy has a default major element and have limits of the amounts of the alloying elements. If you stay within these limits the calculation gives reasonable results.

Syntax	DEFINE_MATERIAL
	`Composition in mass (weight) percent? /Y/:` By default the input is taken as mass percent. Choose N to change to mole percent.  Composition should be given in PERCENT not FRACTION, as it is required for the `W` and `X` state variables in the SET_CONDITION command.
	`1st alloying element: <Element name>` The first alloying element must be given. All alloying elements are asked for in a sequence. These can be given in any order. You must know if you are present as assessed systems in the database. There is no error or warning messages if data are missing. Check the documentation of the database selected. If an alloy is selected, a list of legal alloying elements and their maximum percent is listed on-line.
	`Mass (weight) percent: <Amount of the above specified element>` The amount of the alloying element in mass (weight) percent. Using DEFINE_MATERIAL you cannot use the normal flexibility for conditions, but all must be given in mass percent. However, you can after wards change the conditions using SET_CONDITION.
	`2nd alloying element: <Element name>` The second alloying element must be given. If only one, press <Enter>. If an element name is given then the program asks for its mass fraction.
	`Mass (weight) percent: <Amount of the above specified element>` The amount of the above specified alloying element in mass (weight) percent.
	`Next alloying element: <Element name>` Continue giving elements and mass (weight) fractions until all elements specified. When all alloying elements and their compositions (as in the above prompt) are specified, press <Enter> as answer to this question to finish the materials definition.
	`Temperature (C) /1000/: <Temperature of interest in oC>` POLY makes the first calculation after retrieving the data for this temperature. By pressing <Enter> to accept the default temperature. The value should be given in Celsius (°C).  The pressure is set to 1 bar.
	`Reject phase(s) /None/: <List of phase(s) to be rejected>` This is a question generated by the database allowing you to select the phases. Normally, all phases should be included when you press <Enter>. If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line. It is possible to reject all phase by giving an asterisk *. If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore those that should be included. The question is repeated until you press <Enter> after rejecting all unwanted phases or an asterisk *.
	`Restore phase(s) /None/: <List of phase(s) to be restored>`

Syntax	DEFINE_MATERIAL
	You can restore phases that are accidentally or deliberately rejected. It may also be possible to restore some hidden phases. If phases are to be restored the name of the phases must be supplied. Several phase names can be specified in one line. It is possible to restore all phase by giving an asterisk *. The question is repeated until you press <Enter> after restoring all desired phases.
	`OK? /Y/:` By default, all phases to be selected from the database have the thermodynamic data retrieved and the references from the chosen database are listed. Enter N if there are any errors or you want to amend the selection then you are returned to the prompt about rejecting phase(s).
	`Should any phase have a miscibility gap check? /N/:` The database usually creates two or more composition sets for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase, specify this here. It costs some computation time and may make the subsequent MAP or STEP more difficult to converge. If you do not want to have any phase with a miscibility gap in the calculation, press <Enter>. Then, DEFINE_MATERIAL starts calculating the equilibrium, and is terminated.
	To set such a phase with miscibility gaps in the calculation, answer Y. Then the software asks questions about the phase names and their constitutions, such as: `Phase with miscibility gap: <Phase name>` You must supply the phase name, which has a miscibility gap under the specified system and conditions.
	`Major constituent(s) for sublattice #: /AA/: <Constituent(s)>` The software shows a default constituent in the sublattice `#(1,2,3,…)`, according to the existing phase definition in the chosen database. You can specify one or more major constituents for the sublattice # in the phase. This question is repeated until all sublattices are specified.
	`Phase with miscibility gap: <Phase name>` You can supply another phase name with a miscibility gap under the specified system and conditions, and answer the questions concerning the major constituent(s) in associated sublattice (s). By pressing <Enter>, the command starts calculating the equilibrium, and then terminates.
	 It is also possible to use this command to select an alloy from a specific database (e.g. the TCNI Ni-based superalloys database). Such alloys are predefined by the OPTION keyword inside the database, and have their default major elements and composition limits of their alloy elements. Such alloys available in the selected database (at the prompt `Database /ABCDE/` can be listed on the screen if typing a ? mark on the prompt `Major element or alloy`. When a specific predefined alloy (instead of a major element) is selected, the major element is staked from the alloy definition and shown on the screen (with a message like `Alloy found with major element NI`).

Syntax	DEFINE_MATERIAL
	You can only specify alloying elements and the compositions (weight percent or mole percent). Typing a ? at any of the prompts for the alloying element names, e.g. `1st alloying element`, `2nd alloying element`, lists all the alloying elements and the composition limits in the alloy. If the composition of an alloying element is outside of its limit, there is a message (such as `Amount above limit: 30.0000`) and a prompt `Override limit ? /N/`. If you decide to enforce the override by answering `Y` on this prompt (i.e. accepting the over-limit alloying composition), another warning message (such as `Amount of major element below limit: 70.0000`) and prompt `Override limit ? /N/`. Then further decide if enforcing the overriding: if Y then accepting the major element's composition below the limit; if N then using the predefined major element composition limit.

DELETE_INITIAL_EQUILIBRIUM



This command is for the POLY module.

Delete ONE specific initial equilibrium point or ALL of the initial equilibria. The initial equilibria are used as starting points for all the sub-sequential MAP and STEP calculations.

- ADD_INITIAL_EQUILIBRIUM.

Syntax	DELETE_INITIAL_EQUILIBRIUM
Prompt	`Number /All/: <Number of an initial equilibrium>`
	Specify the number of an initial equilibrium (as a specific numerical value e.g. 3, or ALL) to be deleted from the POLY3 workspaces. It is recommended to use LIST_INITIAL_EQUILIBRIA to figure out the numbers for all the existing initial equilibrium points that have already been added (*manually* through ADD_INITIAL_EQUILIBRIUM, or *automatically* by some other POLY commands) and stored in the current POLY3 workspace. By default, ALL the initial equilibrium points are deleted.

DELETE_SYMBOL



This command is available with the POLY and ED-EXP modules.

Use the DELETE_SYMBOL command to remove symbols i.e. constants, variables, functions or tables.

Syntax	DELETE_SYMBOL
Prompt	`Name: <Name of a symbol>` Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.

ENTER_SYMBOL

This command is for the POLY module.

There are also GES and POST module commands with the same name.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command STEP_WITH_OPTIONS) or mapping calculation (enforced by MAP). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using EVALUATE_FUNCTIONS before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.



See example 44 for an example of using variables and functions.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Syntax	ENTER_SYMBOL
Prompt	`Constant, Variable, Function or Table? /Function/: <Keyword>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION` or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER_CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable

Syntax	ENTER_SYMBOL
	with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST.  There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`Name: <Name of the symbol>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.  For different types of symbol (constant, function, variable or table), the questions have different prompts.

	`Function: <Definition for a function or variable>`
	Functions and *variables* are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).
	Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS` and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).
	Examples of function expressions:
	• `GM(LIQUID)`: The Gibbs energy of liquid per mole component
	• `H.T/4.184`: The heat capacity of the system in calories
	• `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
	• `T-273.15`: The temperature in Celsius
	`&: <Continuation of the definition for the symbol>`
	The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.

	`Value: <Value for a constant>` A *constant* can only be assigned a numeric value once.
	`Value or expression: <Value of expression for a variable>`

Syntax	ENTER_SYMBOL
	A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

	`Variable(s): <Variable(s) in a table>`
	
	A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.
	
	Example:
	
	`ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)`
	
	Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.
	
	To show the temperature in Celsius in a table, give the command ENTER_FUNCTION `TC=T-273`; and then use the symbol `TC` in the table.
	
	`& <Continuation of the definition for the table>`
	
	The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press `<Enter>` again.

EQUILIBRIUM_CALCUL

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Use this command to decide how to perform the POLY minimization (i.e. the traditional Gibbs energy minimization). The *Global Minimization Technique* is used by default for various single point equilibrium calculations and for stepping or mapping calculations.

To permanently turn off the Global Minimization Technique (for all sequential calculations throughout the current run), use the GLOBAL_MINIMIZATION command and set the options to use only the local POLY minimization. You can also make other adjustments to control the steps in reaching Gibbs energy minima in an equilibrium state, for example.

When enforcing the Global Minimization Technique in the equilibrium calculations, you can further adjust how to assign grid points and to handle compositional set(s) for solution phases during stepping/mapping. In order to improve convergence, and because the Global Minimization Technique uses the normal POLY optimization routine for some calculations, you can also change how to control the steps in reaching Gibbs energy minima in an equilibrium state.

Settings for the Minimization of an Equilibria

The following prompts show how the POLY optimization does the local POLY minimization to reach the minimum of an equilibrium state.

```
Force positive definite phase Hessian /Y/:
```

Choose `Y` or `N` to determine how to reach the minimum of an equilibrium state in a normal POLY optimization procedure. This is related to the special quantity, the phase stability function `QF (phase)`, for all kinds of phases in an equilibrium state [a phase stability function for a phase is negative when the phase composition is inside a spinodal, and positive everywhere else].

If the composition of a solution phase is inside its spinodal, the enforcement of positive definite eigenvalues of a Hessian matrix (i.e. when `Y` is selected) makes the step be taken towards the minima rather than the local maxima. Furthermore, if an eigenvalue (for a phase) of the Hessian matrix is near `0.0`, the step size is large this sets a lower limit to this eigenvalue, reducing the step-size and improving the convergence.



The POLY command sequence SHOW_VALUE `QF(phase)` shows the size of the lowest eigenvalue of a phase in an equilibrium state.

If you answer:

- `Y` , it helps the local POLY minimization to converge (if there is a problem), especially if `QF(phase)=0` for phases.
- `N` the local POLY minimization routine is applied.

For each phase in a defined system, the molar Gibbs energy of the phase is a function of the temperature-pressure condition and its composition:

$$G_m(X) = G_m(T, P; y_1, y_2, \ldots, y_n)$$

Compute a Hessian matrix, which describes the curvature of the Gibbs energy curve of this phase at the defined composition X:

$$\partial^2 G_m / \partial y_i \partial y_j$$

Diagonalize this matrix and call the Eigenvalues as `e1,e2,...,en` . The `QF(phase)` quantity for this phase is the lowest of these eigenvalues divided by the same values for a corresponding ideal phase:

$$QF(ph) = \min(\{e_1, e_2, \ldots, e_n\}) / \min(\{se_1, se_2, \ldots, se_n\})$$

Here, `se1,se2,...,sen` are the Eigenvalues for the ideal phase. Therefore, for an ideal phase, the `QF(phase)` should always be `1.0`.

`Control stepsize during minimization /Y/:`

Choose `Y` or `N` to determine whether to introduce a control of step size while reaching the minimum of an equilibrium state in a normal POLY optimization procedure. If you choose `Y` it might help the POLY optimization to converge, especially if some site fractions are less than `1E-4`.

EVALUATE_FUNCTIONS

This command is available with the POLY and ED-EXP modules.

The value of one or more or all entered functions or variables are evaluated and listed.

Syntax	EVALUATE_FUNCTIONS
Prompt	`Name(s): <Name(s) of defined function(s)>` The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated. Variables are evaluated only if these are explicitly named.

GLOBAL_MINIMIZATION

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Designed to decide how to perform the so-called Global Minimization in the POLY module. By default, the POLY module uses the Global Minimization technique for various single-point equilibrium calculations and for stepping or mapping calculations. You can use this to permanently (for all sequential calculations throughout the current software run) turn off the Global Minimization technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization technique in the equilibrium calculations, you can adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

The following prompts affect how the Global Minimization is done. Settings for global minimization:

```
Use global minimization as much as possible /Y/:
Use global minimization for test only? /N/:
Maximum number of gridpoints per phase /2000/: <Integer number>
Use global minimization as much as possible /Y/:
```

Choose Y or N to decide if using the Global Minimization Technique from start of calculation or not. The default value on start-up may be changed by SET_TC_OPTIONS in the SYS module.

If Y the calculation is done when possible (depending on the condition settings), and a Global Minimization test is always performed when an equilibrium is reached. This costs more computer time but the calculations are more accurate.

If N the calculation is not used to reach the equilibrium state. `Use global minimization for test only?` determines if the Global Minimization test is made against the calculated equilibrium states obtained by the Ordinary POLY Minimization calculation.

```
Use global minimization for test only? /N/:
```

If Y a calculated equilibrium state obtained by the Ordinary POLY Minimization calculation is tested against the Global Minimization Technique after it is reached; and if found it as unstable, there is an error message.

If N the Global Minimization Technique is never tested for or done for all sequential calculations throughout the current TCC run. This implies that Global Minimization Technique is permanently turned off, and that consequently only the Ordinary POLY Minimization routine is used.

`Maximum number of gridpoints per phase /2000/: <Integer number>`

Specify the maximum number of grid points that are computed for each of the phases in the currently defined system, during the calculations enforced by the global minimization. More grid points give a higher robustness and take more computation time. The total number of computed grid points in all phases is limited to `2E6`.

KEEP_COMP_SET_NUMBERS



This is available with the ADVANCED_OPTIONS command in the POLY module.

- ADVANCED_OPTIONS
- COMPUTE_EQUILIBRIUM

This setting affects the COMPUTE_EQUILIBRIUM command and turns on/off the functionality to keep the composition set numbers from the previous equilibrium calculation. The setting is on by default.

To turn the setting on or off enter the ADVANCED_OPTIONS command in POLY, then enter this option and either press <Enter> to keep the default Y or enter N at the prompt:

```
Keep composition set numbers /Y/:
```

If this setting is on, performing the COMPUTE_EQUILIBRIUM command keeps the composition set number for any phases that were also present in the last result from COMPUTE_EQUILIBRIUM.



The composition set numbers are kept when the constitution of a phase in the new equilibrium result is similar to the constitution of one of the composition sets of that phase in the previous result. Making major changes to the conditions between calculations makes it therefore less likely that the composition set numbers are kept. The major constituents, given in the thermodynamic database, are used if no previous result exists.

LIST_AXIS_VARIABLE



This command is for the POLY module.

Syntax	LIST_AXIS_VARIABLE
	Lists all the axis variables for a stepping or mapping calculation that have already been set by SET_AXIS_VARIABLE.

LIST_CONDITIONS



This command is available with the POLY and ED-EXP modules.

All the conditions that are set by the SET_CONDITION command and the command-sequence CHANGE_STATUS PHASE =FIXED <0 or 1 or alike>, are listed. The current conditions are also listed by the LIST_EQUILIBRIUM command. The degree of freedom in the defined system is also shown.

- If this is zero, you can perform a COMPUTE_EQUILIBRIUM command.
- If it is larger than zero, some more conditions are required, and you must further set additional ones, using SET_CONDITION or CHANGE_STATUS.
- If it is negative, then too many conditions are defined and the unnecessary ones conditions need to be removed using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or the CHANGE_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

Syntax	LIST_CONDITIONS
Example	P=100000, T=800, N(NI)=1E-1, N=1 FIXED PHASES FCC_A1=1 LIQUID=0 DEGREE OF FREEDO 0

LIST_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a text file.

You can also execute this command if no calculation is made or if the calculation fails. Make sure to interpret the results accordingly.

Syntax	LIST_EQUILIBRIUM
Prompt	`Output to screen or file /Screen/: <File name>` The name of the text file where the list of the calculation results shall be written.
	`Options /VWCS/: <Option(s)>` Select the output units and formats by optionally specifying a combination of these letters. • *Fraction order:* `V` means VALUE ORDER; `A` means ALPHABETICAL ORDER. • *Fraction type*: `W` means MASS FRACTION; `X` means MOLE FRACTION. • *Composition*: `C` means only COMPOSITION; `N` means CONSTITUTION and COMPOSITION. • *Phase*: `S` means including only STABLE PHASES; `P` means including ALL NON-SUSPENDED PHASES.
	Default options are `VWCS`. If the output fraction type should be in mole fraction (rather than mass fraction), then give `VXCS` or type `X` (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase). If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type `L_E,,,` or `LIST_EQUILIBRIUM ,,,` LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See CHANGE_LEGEND for details.

LIST_INITIAL_EQUILIBRIA



This command is for the POLY module.

List all the equilibria added with ADD_INITIAL_EQUILIBRIUM.

Syntax	LIST_INITIAL EQUILIBRIA
	All the initial equilibria are used for the MAP (and STEP) calculations.

LIST_PHASE_ADDITION



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

The values set as additional contributions (given by PHASE_ADDITION) to Gibbs energy *G*m (J/mol formula unit) to all the phases (stoichiometric or solution) are listed at the current calculated equilibrium.



LIST_PHASE_ADDITION has no additional prompt.

LIST_STATUS

This command is for the POLY module.

There is also an ED-EXP module command with the same name.

List the status of components, species or phases.

Syntax	LIST_STATUS
Prompt	Specify what to list: `Option /CPS/:`*<keyword(s)>* keyword = C or P or S, or any combination • `C`: list component status • `P`: list phase status • `S`: list species status • `CS`: list both components and species Default is `CPS`.
	The results depend on the key word specified in the options for CHANGE_STATUS, a table with the current status of phases or species or components, or the combinations, is shown: • For components, the statuses and reference states are listed. • For species, only the status is listed. • For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed.
	The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.

LIST_SYMBOLS



This command is for the POLY module.



There are also POST and ED-EXP module commands with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

LOAD_INITIAL_EQUILIBRIUM



This command is for the POLY module.

Copies all conditions and calculated results from a specific added initial equilibrium to the current equilibrium. The current conditions and calculation results are lost, and the newly loaded initial equilibrium point gets into the POLY workspace.

Syntax	LOAD_INITIAL_EQUILIBRIUM
Prompt	`Number: <Number of an initial equilibrium>` Specify the number of an initial equilibrium to be loaded as current. The number can be found with LIST_INITIAL_EQUILIBRIA.

MAKE_COMPONENT_ENTERED



This command is for the POLY module.

The MAKE_COMPONENT_ENTERED command sets the status for the components to be ENTERED in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium states. ENTERED means that the component(s) are included in the calculation and these are stable if that minimizes the total energy.



This command has the same results as when using CHANGE_STATUS `Entered` option.

Syntax	MAKE_COMPONENT_ENTERED
Prompts	`Name(s) <Name(s) of the components>` The names of the components to set to ENTERED (all on one line). A comma or space must be used as separator. An asterisk, "*", can be used to denote all components.

MAKE_COMPONENT_SUSPENDED



This command is for the POLY module.

The MAKE_COMPONENT_SUSPENDED command sets the status for the components to be SUSPENDED in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium states. SUSPENDED means that the component(s) are not considered in the calculation. Any conditions that depend on the suspended components are automatically removed.



Removing relevant conditions is unique to this command and does not occur when suspending components with the CHANGE_STATUS command and `Suspended` option.

Syntax	MAKE_COMPONENT_SUSPENDED
Prompts	`Name(s) <Name(s) of the components>` The names of the components to set to SUSPENDED (all on one line). A comma or space must be used as separator. An asterisk, "*", can be used to denote all components.

This command is useful when an element has a very low amount because you can now ignore it in the calculation instead of reading the entire system from the database. The command is also of use when working in an API with many calculations.

MAJOR_CONSTITUENTS

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Use this to set the major constituent(s) of a composition sets in a miscibility gap of a solution phase. Normally, the major constituents are specified when a new composition set is created by the NEW_COMPOSITION_SET option; but for the first composition set, this option may be needed before using NEW_COMPOSITION_SET.

The following prompts are to specify the major constituent(s) on each of the sublattice sites for a composition set of a certain solution phase:

```
Phase name: <name of a phase>
```

Specify the name of the solution phase with a new set of major constituents.

```
Composition set number /1/: <#>
```

The default value for the composition set number (#) is usually /1/ as the other composition sets are given major constituents when creating them. Each phase has initially one composition set.

```
Major constituent(s) for sublattice 1: /XX/: <YY>
```

The major constituents (YY) on each sublattice of a solution phase can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This question is repeated for each sublattice in the phase.

MAP

This command is for the POLY module.

This command starts the mapping procedure for making a calculation of phase diagrams in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Syntax	MAP
	A phase diagram consists of mapped phase boundary lines/curves; on one side of each such phase-boundary line/curve, the amount of one specific stable phase is zero (i.e. the zero-fraction lines). From a single MAP calculation, many different types of phase diagrams in the defined multicomponent heterogeneous system can be plotted, with some desired properties (that vary along the calculated phase-region boundaries) plotted as X/Y-axis variables. All different types of phase diagrams are generated by the mapping calculations through this command.

Normally, you need to have calculated at least one initial equilibrium point and have also defined at least two independent varying variables (i.e. the controlling conditions in the system) that are set with SET_AXIS_VARIABLE. You can also have three, or four or maximum five independent varying variables that are defined by the SET_AXIS_VARIABLE command).

This lists the current values of each of the independent axis variables for each of the calculated equilibrium points along each of the mapped phase boundaries, and also lists the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command while it can be disabled if having decisively switched it off (or possibly in some special modules) through changing the minimization option using the ADVANCED_OPTIONS → MINIMIZATION_OPTION command-sequence. You can choose how often to do a Global Minimization test (via the Global Test Interval option) in the ADVANCED_OPTIONS STEP_AND_MAP command-sequence.

During a MAP calculation, the values of mapped axis-variables for presenting each phase boundary (lines/points) of the calculated phase-regions are listed, and the corresponding stable-phase sets are shown up.



You can terminate the mapping of a line by pressing a single <Ctrl-A> (Windows) or <Ctrl-C> (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at a certain stage during a calculation procedure enforced by this command, these messages display on screen:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use SET_NUMERICAL_LIMITS to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

In particular, for phase diagrams with tie-lines in the plane (i.e. most binary systems and ternary isotherms), there is a MAP procedure which checks for the best phase to use as axis variables in order to ensure reasonable increments between the tie-lines. This produces smoother curves and also gives a better stability in finding adjacent phase-regions.

Complex miscibility gaps of various solution phases are automatically detected during a mapping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a Global Test Interval value and confirming the `Automatically add initial equilibria` in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as `FCC_A1#2`, `FCC_A1#3`, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable. The advanced mapping procedure (enforced by the Global Minimization Technique) inside the Thermo-Calc software (both the Console Mode and Graphical Mode) can efficiently and effectively handle complex miscibility gaps in multicomponent heterogeneous systems.

To get a complete phase diagram, sometimes it may be necessary to have multiple starting equilibrium-points, and/or to have added multiple initial-equilibrium points (through ADD_INITIAL_EQUILIBRIUM) inside various phase-region boundaries under certain direction(s).

NEW_COMPOSITION_SET



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

A solution phase that can exist with two (or more) different compositions simultaneously must have two (or more) composition sets in its phase descriptions. Normally the database creates as many composition sets as is necessary but use this command to add or delete more composition sets. A complex solution phase in a defined multicomponent system can have up to 9 different composition sets for the purpose of appropriately handling its possible miscibility gap(s) under various temperature-pressure-composition conditions.

This option is unnecessary if the Global Minimization Technique is in use, as it can automatically detect all possible miscibility gap(s) for complex solution phases (normal or disordered/ordered phases) and then automatically add required composition sets for such phases in the defined system.

This option can automatically create composition sets also for disordered phase when it is executed for the ordered phase.

If you have your own data file, this option must be used to indicate that a solution phase can have a miscibility gap (or may exhibit some complex phase separations as to more than two composition sets), unless that the possibly-additional composition set(s) for the solution phase must have already been added inside the TDB file (through a TYPE_DEFINITION command to amend composition-set) or been manipulated through the GIBBS module (using the AMEND_PHASE_DESCRIPTION COMPOSITION_SET command-sequence). This option asks for default major constituents for the new sets and it is important that this is set correctly, otherwise the test for miscibility gaps may fail.

The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:

```
Phase with miscibility gap: <Name of a phase>
```

Specify the name of the phase with miscibility gap.

```
New highest composition set number /2/: <#>
```

The default value is usually one higher than the current value. Each phase has initially one composition set. If a lower value is given, composition sets are deleted. You cannot take away the first composition set.

A message displays to show that you need to specify the composition for the composition set # (2,3,…).

```
Major constituent(s) for sublattice 1: /XX/: <YY>
```

The major constituents (`YY`) in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This prompt is repeated for each sublattice in the phase, sometimes even for all sublattices in the first composition set if such major constituents have not been specified.

OUTPUT_FILE_FOR_SHOW



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

The name of a text file is asked for and all the results output from the command SHOW_VALUE is written to this file.

When you use this command, a window opens with a default name for the file `tc_show.dat`. Choose a location to save the file and click **Open**.

PARAEQUILIBRIUM

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

This calculates a paraequilibrium between two specific phases in an alloy system with one or more interstitial component(s) as fast diffusion species. Under the paraequilibrium state, two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components (such as C, N, O, S, etc., as individual or combined)], along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with SET_AXIS_VARIABLE.

To ensure a successful point calculation of paraequilibrium state between two specific phases in a defined alloy system, it is important that you first have made a single-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviors as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Note the following:

- Always check if the chosen phases A and B have the exactly same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).
- Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and staring bulk composition for the system.
- Always set the status of the chosen interstitial components as SPECIAL using the POLY command: CHANGE_STATUS`Component <interstitial component> = SPECIAL`. By doing this, you get a clear picture of u-fractions of various substitutional and interstitial components, which are different from the overall composition in the

system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

Settings

```
Name of first phase:  <Phase A>
Name of second phase: <Phase B>
```

The names of the two target phases A and B, between which the paraequilibrium state is to be calculated, must be entered subsequently or on the same (first) line at once then separated by an empty space, e.g. `FCC#1 BCC` or `FCC#2 M23C6`.



You need to understand what you are dealing with in terms of calculating a paraequilibrium state between the two specified phases.

Specifically, there are four distinguished cases to understand: (1) both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component (s) occupy; (2) the choice on the target phase pair must be reasonable for the defined system and specified initial overall composition; (3) both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or (4) it is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

```
Fast diffusing component: /c/: <interstitial component(s)>
Fast diffusing component: /none/: <interstitial component(s)>
```

The name(s) of the fast-diffusing component(s) (C as the default single component) must be given at the above prompts subsequently or at the same (first) prompt. It is possible to specify more than one interstitial component as fast diffusion species.

Note the following:

Such specified interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: these must be located on the interstitial/vacancy sublattices in both chosen phases;

If there is only one fast-diffusing component which is carbon, press the <Enter> key to accept the default input at the first prompt; if the single fast-diffusing component is another element (e.g. N), type its name at the first prompt;

If there are two or more fast-diffusing components (e.g. C and N), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as C N);

To finish the input of fast-diffusing elements, accept NONE at a repeated prompt, i.e. by pressing <Enter> key to start the paraequilibrium point calculation;

If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus canceled entirely.

If the paraequilibrium state between the two specified phases is successfully calculated, the messages displays e.g.

```
NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02  N = 4.1548129E-03
NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04  N = 2.3781027E-04
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant
```

The first and second lines list the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in a specific phase expressed in the so-called u-fractions [u-f(phase,C) and u-f(phase,N)], for the phase A (in this case as FCC) and phase B (in this case as BCC), respectively. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) in both the target phase A and target phase B are the same at the current paraequilibrium state, while these are not shown on screen. The last line indicates that after this advanced-option calculation the LIST_EQUILIBRIUM command is irrelevant and does not list the paraequilibrium state for the system at the current condition.

However, if the single-point calculation of the paraequilibrium state between the two specified phases has failed, these messages display:

```
*** Error 4 in ns01ad
*** Numerical error
```

This implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component (s). Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.

PHASE_ADDITION

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Sometimes it is interesting to add a constant contribution to the Gibbs energy of a phase (stoichiometric or solution). This can be done in the Database module (DATA) or Gibbs Energy module (GIBBS), for a stoichiometric phase, or for a pure end-member in a solution phase. However, if the addition is related to the equilibrium state, for example, strain energies or surface energies, interfacial energies, or deformation energies, it may be more convenient to have this quantity related to the equilibrium state rather than the thermodynamic data.

Give a value of an addition to the Gibbs energy of a phase. The value should always be constant (implying that the addition is not a function of phase composition or temperature-pressure conditions in the equilibrium state) and always be given in the unit of J/mol formula unit of the phase.

The following prompts are to specify the additional energy term (always being a constant) of a given phase.

```
Phase name: <Name of a phase>
```

Specify the name of the (stoichiometric or solution) phase with the addition.

```
Addition to G per mole formula unit: <xxxxx>
```

The value (`xxxxx`) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature-, or pressure-dependent.

POST

The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

- POST Module Commands
- Using the POST Module

Syntax	POST
	Switches to the POST module, which has its own command set.

PRESENT_PHASE



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Specify the name of the present phase a the name of the phase that should be present at all calculated equilibria:

```
Present phase:
Phase name: <Name of a phase>
```

READ_WORKSPACES



This command is used in both the POLY and GES (GIBBS) modules.

Workspace Files

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with SAVE_WORKSPACES. Such a *.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	`File name` is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3, otherwise type the whole POLY-file name.  A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters. A window opens so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. POLY3) cannot be changed. Click **Open** to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.
	When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type `READ,,` or `READ_WORKSPACE ,,`

REINITIATE_MODULE



This command is for the POLY module.

This command makes sure that the whole POLY module (and thus the entire POLY workspace) is reinitiated to the state as it was when first entered.

Syntax	REINITIATE_MODULE
	All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.

SAVE_WORKSPACES



This command is available for both the POLY and GES (GIBBS) modules.

Workspace Files

You can save the current status and workspaces, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on a *.POLY3 file. The workspaces are saved to a file with this command. This is useful so you have access to the workspace for later use or when you need to terminate the current Console Mode session.

- In the Gibbs (GES) module workspace, all thermochemical data are stored.
- In the POLY module workspace, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GES workspace.
- When you are in a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings are saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called `POT.POLY3` ; the POURBAIX module saves a file called `POURBAIX.POLY3` and so forth.



After a SAVE_WORKSPACES command, you can always come back to exactly the state you had when you issued the command by giving a READ_WORKSPACE command. For example, after saving the POLY and GIBBS workspaces to a file, you can leave the program and at a later time READ the file and continue from the saved state.

Important Information About Map and Step Commands



A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Syntax	SAVE_WORKSPACES
Options	A `file name` must be specified. The default extension of the POLY workspace file is *.POLY3 but you can have any other file extension.  Linux and Mac are case sensitive so ensure you enter `.POLY3`. A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** cannot be changed. If there is already a file with the same file name under the directory a warning message displays. Click **OK** to overwrite the current POLY or GIBBS workspace onto the existing file. Click **Cancel** to return to the module. You can use the SAVE command with an unspecified name (i.e. through `SAVE , , ,` command-sequence) to save the POLY or GIBBS workspace.  When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Console Mode session or in a previous run (which is READ into the current POLY3 workspace), you can type `SAVE, , Y` or `SAVE_WORKSPACE , , y`. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.

SELECT_EQUILIBRIUM



This command is available with the POLY and ED-EXP modules.

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.

Syntax	SELECT_EQUILIBRIUM
Prompt	`Number /Next/: <Choice on equilibrium>` Options: `FIRST`, `LAST`, `NEXT`, `PREVIOUS` or `PRESENT`. Most commands affect only the `PRESENT` equilibrium. However, the REINITIATE_MODULE and DEFINE_COMPONENTS commands remove all the stored equilibria.

SET_ALL_START_VALUES

This command is available for the POLY and ED-EXP modules.

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

Syntax	SET_ALL_START_VALUES
	`T /XXXX/: <Temperature in K>` If the temperature is not a condition, supply a guess of its final value (in K).
	`P /100000/: <Pressure in Pa>` If the pressure is not a condition supply a guess of its final value (in Pa).
Prompts	`Automatic start values for phase constitutions? /N/: <Y, N or F>` • For N, enter an initial amount of each entered phase and the major constituents or site fraction of each constituent. • For Y, the program automatically sets the start values for phase constitutions in all possible phases. • `F` is for force. In some cases the calculation fails because impossible conditions are set, e.g. `W(C)=1.5` `[W(C)` is mass fraction and must thus be less than unity. The program tries to fulfill this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set `W(C) to 0.015`, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, choose `F`.
	`Should <phase> be stable /N/: <Y/1 or N/2>` A guess if this phase should be stable or not is requested. All entered phases are prompted for this question and next two. You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No). The `phase` name may have a hash sign # followed by a digit, e.g. `BCC_A2#2`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.
	`Major constituent(s): <Name of major constituent(s) in the phase>` The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving $ the constituent is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.

Syntax	SET_ALL_START_VALUES
	`Y(<phase>,<constituent>) /.XXXXXXXXXX/: <.YYYYY>` The current value (`.XXXXXXXXXX`) is default. You can accept the default by pressing <Enter> or give a new value (`.YYYYY`). The phase name or constituent name may have a hash sign # followed by a digit, e.g. `Y(BCC_A2#2,FE), Y(BCC_A2#2,C#2)`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.

SET_AXIS_VARIABLE

In order to calculate a diagram, set at least one axis variable in a stepping calculation, or at least two axis variables in a mapping calculation. For property diagrams, one axis is enough; for phase diagrams two or more are necessary. Any condition that can be set to calculate an equilibrium can be used as an axis variable (with its lower and upper limits and step length) by using SET_AXIS_VARIABLE, and the POLY program does, after a STEP or MAP command, vary the value of the condition between the limits set on its related axis variable. As an extraordinarily unique and powerful feature of the Thermo-Calc software, up to five independent axis variables can possibly be used in a mapping calculation of a multicomponent heterogeneous system; however, the axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.

Syntax	SET_AXIS_VARIABLE
	`Axis number /#/: <An axis number>` Specify a number between 1 and 5. The axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.
Prompts	`Condition /None/: <One condition>` Here the condition that should be varied along the axis must be given. The condition is specified as in SET_CONDITION, for example `W(C)` for mass fraction of carbon. By accepting `NONE`, the axis is removed.
	`Min value /0/: <Min value>` Specify the minimum value of the axis condition.
	`Max value /1/: <Max value>` Specify the maximum value of the axis condition.
	`Increment /.025/: <Step length>` Specify the maximum step length. By default, this is 1/40 of the total axis length.

You can give SET_AXIS_VARIABLE without having set a condition on the axis variable. Under such circumstances, the relevant condition is automatically created and the value set between the minimum and maximum axis limits; however, as a side effect, the POLY module creates two conditions, `P=1e5` and `N=1` (these have not been defined as a condition yet), in case you set an axis variable which is not already a condition.

You can use a logarithmic axis during calculations. This is useful for low fractions like in a gas phase where `1e-7` to `1e-2` might be an interesting range. The pressure is also suitable for logarithmic step. You specify the logarithmic axis by giving an asterisk * after the increment value.



The increment in this case is treated as a factor.

For example,

```
S-A-V 1 P 1E5 1E25 5*
```

This makes axis 1 a logarithmic axis where the difference between two calculated values makes a factor 5.



The factor must be larger than 1.0.

In some cases, such as when the DEFINE_DIAGRAM command is used or a special advanced module (e.g. BIN, TERN, POT, SCHEIL or POURBAIX) is called, some axis variables are automatically set by the program, not necessarily by this command.

SET_CONDITION

This command is available with the POLY and ED-EXP modules.

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the M/W/V/F-suffixed state variables (for normalization) and R-suffixed state variables (with respect to chosen reference states), can be used as conditions. In addition to temperature and pressure conditions, a multicomponent system can have mixed types of conditions. You should repeat this command for a multicomponent system until the degree of freedom in the defined system becomes zero. When a FIXED phase status is used on a specific phase (use CHANGE_STATUS), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax	SET_CONDITION

	Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.
	
	Example
	
	`SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2`
	
	or
	
	`SET_COND T=1273, P=1E5`
	`SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2`
	
	In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.

Prompt	`State variable expression: <State variable name or linear expression> or a linear expression of state variables.` Some of the state variables that can be used in conditions are: • T: temperature in the system (in K) • P: pressure in the system (in Pascal) • N: system size (mole number in moles) • B: system size (mass in grams) • N(<component>): mole number of a component in the system • X(<component>): mole fraction of a component in the system • W(<component>): weight fraction of a component in the system • For the SET_CONDITION command this is ACR(<component>): activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is ACR(<phase>,<component>) (activity of a component in a phase) • For the SET_CONDITION command this is MUR(<component>): chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is MUR (<phase>,<component>) (chemical potential of a component in a phase)

Syntax	SET_CONDITION
	• X(<phase>,<component>): mole fraction of a component in a phase • W(<phase>,<component>): weight fraction of a component in a phase • ACR(<species>,<phase>): activity of a species referred to a phase • MUR(<species>,<phase>): chemical potential of a species referred to a phase • H: enthalpy in the system (in J) • HM(<phase>): enthalpy of a phase (in J/mol) There are many state variables that can be used in conditions. For more information, enter an INFO STATE_VARIABLES command. A condition is normally a value of a single state variable with its value. ***Example*** T=1273.15 P=1E5 X(C)=.002 W(CR)=0.5 ACR(CR)=0.85 X(FCC,C)=.001 H=-250000 HM(BCC)=-225000 A condition can also be a value of a linear expression involving more than one state variable. For example, X(LIQ,S)-X(PYRR,S)=0 This means that it is a condition that the mole fraction of S component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.  After the equal sign only a numeric value is allowed in the expression.
	Factor: <A factor for the state variable, or a continuation> This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is: 2*MUR(FE)+3*MUR(O)=-35000 This means that it should be a condition that two times the chemical potential of FE plus three times the chemical potential of O should be -35000 J/mol.
	State variable: <A specified state variable, or a continuation> This question is prompted if a single state variable name has not given in either the prompt State variable expression or Factor, or a state variable expression is given but the expression is incomplete, for example, T- or 2*MUR(FE)+, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).

Syntax	SET_CONDITION
	`Value /X/: <A numeric value, a constant or a variable>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed; for example `T=NONE` takes away the temperature condition.

SET_INPUT_AMOUNTS

Specify how a system is made up from mixing of various substances. It is useful with a substance database. In the C-H-O-N system, you can, for example, give:

```
S-I-A N(H2)=10, N(H2O)=25, N(C1O2)=5, N(N2)=100
```

The POLY module automatically converts this into conditions for the current set of components. In the case when the elements are defined as the components, the command above is equivalent to

```
SET-CONDITION N(H)=70, N(O)=35, N(C)=5, N(N)=200
```

Syntax	SET_INPUT_AMOUNTS
Prompts	`Quantity: <N(<specie>) or B(<specie>)>` You can give the amount also preceded with an equal sign `=` [e.g. `N(H2)=10` or `B(H2O)=1000`], or press <Enter> for the next prompt on the amount of the quantity.
	`Amount: <Value of the quantity>` Specify the numerical value of the quantity.  You can give negative amounts in the SET-INPUT-AMOUNTS command.

SET_INTERACTIVE



In the POST module this is called SET_INTERACTIVE_MODE.

Use the SET_INTERACTIVE command to use it in demonstration or macro files to stop the execution of the command file and pass over input focus to the keyboard.

SET_NUMERICAL_LIMITS



This command is available for the POLY, Scheil and ED-EXP modules.

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`Maximum number of iterations /500/:` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`Required accuracy /1E-6/:` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`Smallest fraction /1E-12/:` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is `1E-12` for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30` (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system).
	`Approximate driving force calculation for metastable phases /Y/:` Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. By default, the metastable phases are included in all iterations but these may not have reached their most favorable composition and thus their driving forces may be only approximate.

Syntax	SET_NUMERICAL_LIMITS
	 If it is important that these driving forces are correct, choose N to force the calculation to converge for the metastable phases. This may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.

SET_REFERENCE_STATE

This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials, and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature, and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials, and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC (O2,GAS), LNACR(O2,GAS).

For the POST module, and after calculating with the STEP_WITH_OPTIONS or MAP commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. MUR(comp), MUR (comp,ph), ACR(comp), ACR(comp,ph) or the common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`Component: <Name of the component>` The name of the component must be given.
	`Reference phase: <Name of a phase used as the new reference state>`

Syntax	SET_REFERENCE_STATE
	Enter the `Name of a phase` for the system.  For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed. If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy. The following are example using temperature. Pressure is used in the same way: • In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C. • If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1. • Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state.
	`Temperature /*/: <Temperature for the reference state>` Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.  The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.
	`Pressure /1E5/: <Pressure for the reference state>` Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.

	Examples
	
	`S-R-S Fe SER`
	`S-R-S Cr FCC * 100000`
	`S-R-S H2O AQUEOUS * 100000`
	`S-R-S ZE REF_ELECTRODE * 100000`

SET_START_CONSTITUTION



This command is available with the POLY and ED-EXP modules.

This command is similar to SET_ALL_START_VALUES, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
Prompts	`Phase name: <Name of a phase, and possible major constituent(s)>` Specify the name of a phase for which the constitution shall be set. If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A $ means keeping the same constitution, and `NONE` means to give individual site-fractions.
	`Y(<Phase>#<Composition_set>,<Constituent>#<Sublattice>) /xxx/: <SF>` The site fraction (`SF`) of the constituent shall be given. The default value `xxx` is the last calculated one.

SET_START_VALUE

This command is available with the POLY and ED-EXP modules.



This command is not often required as the automatic start values can be handled for most problems.

Set a start value of an individual variable.

Syntax	SET_START_VALUE
Prompts	`State variable: <Name of a state variable>` The state variable must be given.
	`Value` Specify the value to be assigned the state variable as start value.

SHOW_FOR_T=



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Display various thermodynamic properties (state variables, derived/partial variables or entered symbols) of the currently calculated (stable/meta-stable) equilibrium state but under a different temperature condition. This is useful for knowing, for example, a volume-related property of a frozen (stable/meta-stable) equilibrium state at a certain temperature, where the equilibrated phase assemblage and all the phase compositions are not adjusted while only the temperature condition is changed.

Use this option carefully. You must have successfully calculated a real equilibrium state under one temperature condition (normally the temperature for the last heat treatment). This can then be used to obtain the value(s) of any specified state variable(s) or derived/partial variable(s) or defined symbol(s) for thermodynamic properties of the entire system, of components, or of phases for the currently-defined system (being in a frozen state) under another temperature (normally at room temperature). No real equilibrium is re-calculated through this option, and thus the phase amounts and compositions in the system are the same as at the last real equilibrium calculation.

Settings

```
Temperature (K) /298.15/: <temperature_in_K>
```

Specify the new temperature condition (in K) under which the values of some specific state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system (being in a *frozen* state) is shown on screen.

```
State Variable or symbol /VM/: <State variable or symbol name(s)>
```

Specify the name(s) of the desired state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system. More than one state variable or symbol of interest can be simultaneously specified on the same line. For example, you can choose to show the values of VM or GM (i.e. molar volume or molar Gibbs energy of the entire system), or of VM(*) or HM(*).T (i.e. molar volumes or isobaric heat capacity of all phases), or of ACR(*), DGM(*) and LNACR(*,FCC) [i.e. activities of all system components, driving forces for all phases, and activities (in logarithm) of all system components in the FCC solution phase], under the new temperature condition (being in a frozen state).

SHOW_VALUE

This command is available for the POLY and ED-EXP modules.

Show the current value of any state variable, function or variable.

Syntax	SHOW_VALUE
Prompt	`State variable or symbol: <Name(s) of state variable(s) or symbol(s)>` A single or several state variables or symbols (entered functions or variables) can be specified.
	The wildcard * can be used to denote all phases or all components. You can use the dollar-sign `$` to denote all stable phases. Thus, the command SHOW W(*,*)lists the mass fraction of all phases, whereas `SHOW W($,*)` lists the mass fraction of all stable phases. If you `SHOW` a function, all functions are evaluated using the current values of the state variables. But if you `SHOW` a variable, it retains its value from the time it was `ENTERED` or last `EVALUATED`. Therefore to save a value from one calculation to another, `ENTER` it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.

STABILITY_CHECK

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

In some composition ranges of a multicomponent system, it often happens that an unstable solution phase region locates inside a miscibility gap, and the stability limit (the *spinodal curve* or *spinodal*) may be not easy to find. A system inside a spinodal is thermodynamically unstable with respect to compositional fluctuations, and the system may experience the *spinodal decomposition* (i.e. decomposing to a mixture of regions with the two stable compositions, one on each side of the miscibility gap).

This option makes it possible to automatically check internal stability of both stable and unstable phases in all subsequent single-point equilibrium and MAP/STEP calculations. It can find out if any phase is subject to spinodal decomposition during the subsequent calculations. If there is an unstable phase located inside a miscibility gap in a calculation, it gives a warning so that you suspend the unstable phase, or use FORCED automatic start values for phase constituents (i.e. SET_ALL_START_VALUES → `FORCE` command-sequence), or create other composition sets; you can also ignore the warning message if you know that the unstable phase is not formed in the current calculations.

Settings

```
Stability check on? /Y/:
```

```
Check also for unstable phases? /Y/:
```

If the automatic stability-check option is switched on choose to also check the stability for unstable phases. The default is Y and if an unstable phase is found to be located in a miscibility gas during a subsequent single-point equilibrium or MAP/STEP calculation, a warning message informs you to selectively make adjustments in the calculation settings [e.g. suspending the unstable phase, or using FORCED automatic start values for phase constituents by the S_A_S_V F command-sequence, or creating other composition sets, etc.]. By answering N the stability check is enforced only to stable phases in the system.

STEP_AND_MAP

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

STEP_AND_MAP is the default ADVANCED_OPTIONS choice and is used to determine how to perform Global Minimization test and how to handle initial equilibrium points.

Settings for MAP and STEP:

```
Global test interval /0/: <Integer number>
```

Settings for MAP:

```
Automatically add initial equilibria /Y/:
Number of mesh along an axis /3/: <Integer number>
Use inside meshing points /N/:
Global test interval /0/: <Integer number>
```

The integer number determines how often the Global Minimization should be used during STEP_WITH_OPTIONS and MAP calculations. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n, suggests it performs a Global Minimization test at every n-th step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The Thermo-Calc software is installed with 0 (zero) as the default value, but such a configuration for the default value can be changed by using SET_TC_OPTIONS in the SYS module.

```
Automatically add initial equilibria /Y/:
```

When ADD_INITIAL_EQUILIBRIUM is not used before MAP, a mesh of initial equilibrium points are added before the mapping itself takes place. This mesh is only available when two (2) axes are already defined. The default on start-up may be changed by SET_TC_OPTIONS in the SYS monitor.

```
Number of mesh along an axis /3/: <Integer number>
```

An integer for how many intervals of initial equilibrium points to be added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, center, and end of each axis-variable forming 2 intervals.

```
Use inside meshing points /N/:
```

If N the INITIAL_EQUILIBRIUM mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If Y, the initial equilibrium points added are also added to the inside edge.

STEP_WITH_OPTIONS

This command is for the POLY module.

The STEP_WITH_OPTIONS (short name, STEP) command initiates the stepping procedure to make a calculation of property diagrams in a multicomponent heterogeneous system. A property diagram is usually stepped under one defined independent stepping axis-variable, and is often constructed by the defined independent mapping axis-variable against a chosen property (for the system, or for a specific phase, or for a certain species).

In the POLY module, it is possible to compute a series of equilibria with one condition as the stepping axis variable. This is achieved by first calculating a single equilibrium, and then selecting one of the conditions as the axis variable. The minimum and maximum value and the incremental step along the axis must also be given. By default, the global minimization technique is used .

A property diagram consists of property lines that change (normally) along with the stepping axis-variable. From a single STEP calculation, many different types of property diagrams in the defined multicomponent heterogeneous systems can be plotted. Various types of property diagrams are generated by the stepping calculations.

About Property Diagrams

Normally, before the command can be invoked, you need to have already calculated an initial equilibrium point and set one independent variable (i.e. the controlling condition in the system) . This is done using SET_AXIS_VARIABLE. You then list the current values of the axis variable for each calculated equilibrium, as well as the corresponding information when the set of stable phases changes.

By default, the global minimization technique is enabled, You can turn this off by using the command-sequence ADVANCED_OPTIONS → GLOBAL_MINIMIZATION.

You can choose how often to do a global minimization test using the command-sequence ADVANCED_OPTIONS → STEP_AND_MAP → GLOBAL TEST INTERVAL.

Syntax	STEP_WITH_OPTIONS
Prompt	`Option? /Normal/: <A chosen option, N, I, S, O, E, M, T, or P>` N = Normal, I = Initial equilibria, S = Separate phases, O = One phase at a time, E = Evaluate, M = Mixed Scheil, T= T0, and P Paraequilibrium

Normal (N)

When you accept the default, Normal (N), it allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). Only the step axis value is changed between each step.

When you repeat the STEP → NORMAL command-sequence, you can make several stepping calculations while still keep all the stepping-calculation results in the current POLY3 workspaces.



The calculation results are saved in the default `RESULT.POLY3` file or you can specify to save it in the `<MyName>.POLY3` file. This is as long as there is no SAVE_WORKSPACES command before the second set of command sequences (STEP → NORMAL). Repeated stepped results can be restored into the same current POLY3 workspaces/file.



Linux and Mac are case sensitive so ensure you enter `.POLY3`.

The addition of several steps enables you to generate special types of property diagrams and to calculate and plot special phase boundary lines on phase diagrams, such as:

- The missing part(s) of a specific property [that are calculated under another controlling condition inside the range of the stepping-variable] on the same property diagram.
- Two or more sets of a specific property [that are calculated under different controlling conditions and stepped over the same stepping-variable range] on the same property diagram for the same system.
- Calculate some special phase-boundary lines [especially for some defined secondary phase transformations or alike, e.g. the BCC_A1 <--> BCC_B2 phase-boundary, or equal-Gm for two specific phases, or equal-fraction or equal-activity for a certain species in two specific phases, that shall be calculated under different controlling-conditions and also be stepped over different stepping variable(s)], and then plot (or impose) them onto a corresponding phase diagram (which can be resulted from several such STEP → NORMAL calculations or even from a separate MAP calculation) for the same system.

Initial_Equilibria (I)

An initial equilibria is added at each calculated point. This can be useful, for instance, to generate a set of isothermal calculations.

When you choose `I`, an initial equilibrium is stored at each calculated equilibria. It is intended to generate a matrix of calculated initial equilibria, first stepped under a STEP INITIAL_EQUILIBRIA command-sequence and then repeated by another STEP NORMAL command-sequence (or even continued by a MAP command).

For example, you can first use the temperature condition as the stepping axis-variable with this option, which calculates a number of initial equilibrium points and automatically adds each one as an initial equilibria for another STEP → NORMAL command-sequence (or even for a MAP command). Before the second STEP command (i.e. the STEP → NORMAL command-sequence), you can chose a compositional condition as the new stepping axis-variable; then the STEP → NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two STEP commands together give a matrix of values.

Separate_Phases (S)

In this way, you can calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase, etc.).

One_Phase_at_Time (O)

This option is recommended for STEPPING heterogeneous systems with both ordered phases and the disordered pairs.

When you choose O, the stepping calculation is conducted individually for one phase at a time. That is, it is stepped over the whole stepping variable range, but the stepping is repeated for all the entered phases in the defined system. This is particularly useful to properly step in composition for an equilibrium heterogeneous system with both ordered phases and the disordered pairs. Thus, instead of calculating for the same composition for each of the phases at each composition step, it starts the stepping in each of the phases in the default most-stable compositions (the major constitutions).

Evaluate (E)



For Scheil-Gulliver simulations it is recommended you use the SCHEIL module.

Evaluate E is an advanced option and is useful when additional conditions (instead of the stepping variable) require changing during a stepping calculation. It allows a stepping calculation in a single axis with simultaneous evaluation of one or more variables after each step. As variables can be used as conditions, it means that you can change the conditions during the stepping. After a successful EVALUATE calculation, you can go to the POST module to manually define and plot property diagrams.



The variables given are evaluated after each step, which may change other conditions. This can be useful to perform the Ordinary ScheilGulliver Approach (non-equilibrium transformations) for simulating alloy solidification without back diffusion of fast-diffusing interstitial components in solid phases. However, it is recommended you use the SCHEIL module.

Specify the prompt:

`Variable name(s): <Variable name>`

The names of the variables that shall be evaluated after each step must be typed here.



The miscibility gap test is automatically used during stepping (see ADVANCED_OPTIONS) if a phase has two or more composition sets.

The miscibility gap test means that you can start calculating from high temperatures in a steel where the MC carbide is not stable. During the calculation, the MC carbide first becomes metastable with a composition different from the metallic FCC phase and later also becomes stable.



See Console Mode example tcex30A.

Mixed_Scheil (M)



For Scheil-Gulliver simulations it is recommended you use the SCHEIL module.

This is an advanced stepping calculation designed for the Extended Scheil-Gulliver Approach (partial-equilibrium transformations) to simulate alloy solidifications with back diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in solid phases is performed. It also will consider BCC-->FCC phase transformation (practically for steels) along the alloy solidification process.

To ensure a successful stepping calculation of mixed Scheil-Gulliver simulation of solidification process of a defined alloy system with a certain initial overall composition, it is important to note the following:

- For solution phases with possibility of miscibility gap existence, you have appropriately added the necessary composition set(s);
- You have already set the temperature condition as the stepping SET_AXIS_VARIABLE command, with minimum and maximum temperature points as well as an appropriate s temperature step for the cooling process).
- There must be a composition condition for each of the back diffusion components (i.e. fast-diffusing interstitial components, such as C, N and/or other elements) that are already defined in terms of mole-fraction or mass-fraction, e.g. `X(C)` and `W(N)`. Otherwise, a stepping calculation with this option can fail.

- An initial equilibrium in which the LIQUID mixture phase is the only stable must be calculated. This is why it is good to start with a relatively high temperature condition for the initial equilibrium calculation. It is always necessary to reject or suspend the GAS mixture phase (if it exists) before the C-E and STEP commands, to avoid its formation along with LIQUID.
- In cases where fast-diffusing interstitial components are specified as back diffusion components, you can choose to `allow BCC>FCC` phase transformation (practically for steels) during the alloy solidification process.

These are the prompts for this option:

```
Fast diffusing components: <Fast diffusion interstitial(s)>
```

Specify one or more interstitial component(s) as the back diffusion component(s).

- If there is only one fast-diffusing interstitial component (e.g. C or N), type its name;
- If there are two or more fast-diffusing interstitial components (e.g. C, N and S), always type the names on the same line at once (separated by an empty space in between, e.g. C N S);
- If there is no fast-diffusing interstitial component to be considered, type `NONE` to ignore back diffusion entirely, meaning a normal Scheil-Gulliver simulation is performed.



Such specified back diffusion interstitial component(s) must be appropriately defined according to the phase constitution definitions of some major alloy solution phases (e.g. FCC, BCC, HCP, etc.). These are located on the interstitial/vacancy sublattices in such alloy solution phases; otherwise, such a Scheil-Gulliver simulation may not make sense at all.

```
Allow BCC -> FCC ? /Y/:
```

By default the BCC-->FCC phase transformation is allowed. This is usually a typical phenomenon along the cooling processes of steels/Fe-alloys.

During the calculation the simulated solidification path, including the locally-equilibrated phase assemblage (region), captured temperature condition (`T` in K), remaining liquid phase (`NL`, mole fraction), overall formed solid phases (`NS`, mole fraction) and latent heat formation (`NH`, J/mol) along the cooling process are shown after the information on starting temperature point of the alloy solidification process, e.g.

```
  Solidification starts at  1743.15 K
  Phase Region from   1.744150E+03 for:      LIQUID
  Phase Region from   1.742525E+03 for:
```

```
      LIQUID
      FCC_A1#1
        1742.5250          0.9960          0.0040          -1.1824
        1742.4000          0.9795          0.0205        -202.1585    . . . . . .
Phase Region from   1.733150E+03 for:
      LIQUID
      BCC_A2
      FCC_A1#1
        1733.1500          0.3294          0.6707       -8032.6240
        1733.0250          0.3237          0.6763       -8095.1490    . . . . . .
```

After a successful calculation, you can go to the POST module to manually define and plot property diagrams for the alloy solidification process according to the chosen Scheil-Gulliver model, or to impose existing relevant experimental information or other types of calculated solidification results [e.g. Scheil-Gulliver simulation with or without considering fast-diffusing interstitial component(s), full-equilibrium approach, or Diffusion Module (DICTRA)-type simulation with moving-boundary conditions] onto the same plotted property diagrams. Normally, the solidus temperature (`T` in Celsius) is set as one of the axis variables (usually as Y-axis in most cases), while the other plotted quantity on the other axis can be the amount of overall formed solid alloy phases (`NS` in mole-fraction or `BS` in mass-fraction), the amount of remaining liquid phase (`NL` in mole-fraction or `BL` in mass fraction), the heat of latent along the solidification process (`NH` in J/mol or `BH` in J/gram), among many other properties in the solidified alloy phases or in the whole alloy system.

T-zero (T)



See Console Mode example 41.

This advanced option allows a stepping calculation of the so-called T0 (T-zero) line in a diffusionless transformation (where two specific partially-equilibrated phases have the same Gibbs energy) along a composition variable which has already set as the stepping variable with SET_AXIS_VARIABLE.



The temperature condition cannot be set as the stepping variable if you want to make a STEP T-ZERO calculation.



Prior to performing the step T0 command sequence, and to ensure a successful calculation of T0 line between two specific phases after an initial equilibrium calculation in the current system, it is sometimes recommended to make a single T0 point calculation using ADVANCED_OPTIONS → T-ZERO.

Specify these prompts:

```
Name of first phase:  <Phase A>
Name of second phase: <Phase B>
```

The names of the target phases, for which the Gibbs energies equal to each other at each point on the T0 line, must be entered.

During the calculation, the T0 values are shown after the corresponding scanned conditions (of the stepping composition variable), e.g.

```
  Phase Region from   1.000000E-01 for:
       BCC_A2
       FCC_A1
     1.000000E-01         940.24
     9.250000E-02         941.20
     . . . . . .
     2.500000E-03         977.61
     7.500000E-09         979.34
  Phase Region from   1.000000E-01 for:
       BCC_A2
       FCC_A1
     1.000000E-01         940.24
     1.075000E-01         939.62
     . . . . . .
     2.950000E-01        1084.87
  3.000000E-01        1080.99
```

After a successful calculation, you can go to the POST module to plot the T0 line against the stepping composition variable or another varying axis, or to impose the calculated T0 line onto a normal phase diagram [normally plotted as a T-X isopleth].

Paraequilibrium (P)



See Console Mode examples 42 and 43.

This is an advanced option. Select `P` to calculate the paraequilibrium state between two specific phases (the *paraequilibrium lines*). It allows a stepping calculation of paraequilibrium lines where the chemical potential for one or more interstitial components (that are considered as back diffusion elements, such as C and N) but not for the other (s) in two partially equilibrated phases are equal.

More than one interstitial component can be treated as fast-diffusion species (such as C, N, O, S, etc., as individual or combined) in a paraequilibrium stepping calculation.



The composition condition for the interstitial components cannot be set as the stepping variable if you want to make this calculation.

To ensure a successful stepping calculation of paraequilibrium states between two specific phases in a defined alloy system, it is important to first make a starting-point equilibrium calculation with an initial overall composition in the current system. However, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable.

The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true where there is more than one interstitial component to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Always check if the chosen `phaseA` and `phaseB` have the exact same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).

Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and staring bulk composition for the system.

Always set the status of the chosen interstitial components as SPECIAL using the command:

```
CHANGE_STATUS COMPONENT <interstitial component> = SPECIAL
```

By doing this, you get a clear picture on u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from the paraequilibrium calculations are u-fraction related quantities.

Always make a single-point paraequilibrium calculation by the command-sequence of ADVANCED_OPTIONS → PARAEQUILIBRIUM, prior to performing this STEP → PARAEQUILIBRIUM command-sequence, although this might not be always necessary for some systems.

With this stepping calculation specify the following:

```
Name of first phase:  <Phase A>
Name of second phase: <Phase B>
```

The names of the two target phases `A` and `B`, between which the paraequilibrium states establish, must be typed at the above two prompts subsequently or on the same (first) line at once (separated by an empty space, e.g. `FCC BCC`, `FCC#2 M23C6`).



It is important to understand that this is the calculation of a paraequilibrium state between the two specified phases.

Particularly, there are these issues to consider:

1. Both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component(s) occupy.
2. The choice on the target phase pair must be reasonable for the defined system and specified initial overall composition.
3. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or
4. It is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

```
Fast diffusing component: /C/: <Interstitial component(s)>
Fast diffusing component: /None/: <Interstitial component(s)>
```

The name(s) of the fast-diffusing interstitial component(s) (`C` as the default single component) must be given either one by one at each of the above prompts subsequently or in a combination (separated by an empty space in between, e.g. `C N S`) at the same (first) prompt; otherwise, press <Enter> key to start the paraequilibrium line stepping-calculation.



Note the following:

Such specified fast-diffusing interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: These must be located on the interstitial/vacancy sublattices in both chosen phases.

If there is only one fast-diffusing component which is carbon, press <Enter> to accept the default value (`C`) at the first prompt; if the single fast-diffusing interstitial component is another element (e.g. N), appropriately type interstitial component the name at the first prompt;

If there are two or more fast-diffusing components (e.g. `C` and `N`), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as `C N`);

To finish the input of fast-diffusing elements, accept `NONE` at a repeated prompt;

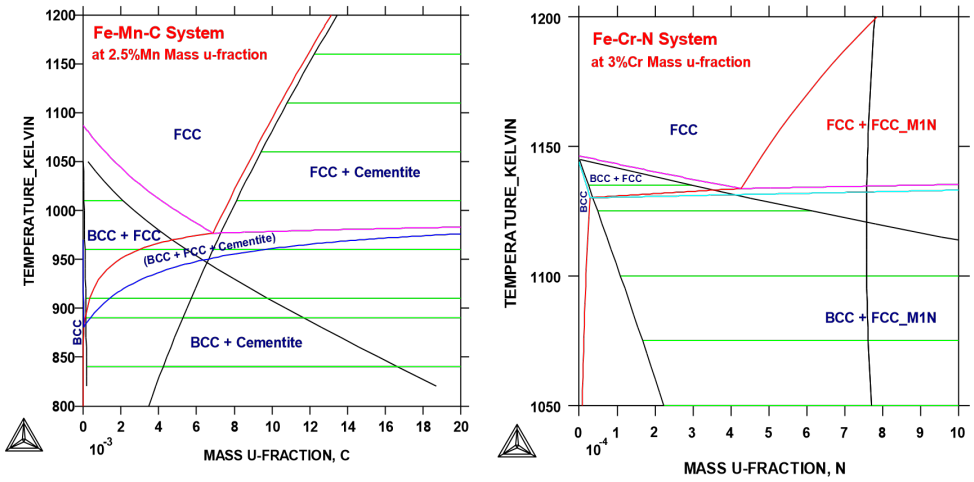
If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.

During the STEP → PARAEQUILIBRIUM calculation procedure, the calculated paraequilibrium states include the:

- corresponding stepping conditions (e.g. temperature in K, or the stepping composition variable of the matrix component or of one of substitutional components) which has already set as the stepping variable by the SET_AXIS_VAR command);
- amounts of the phase `A` in mole number [i.e. `NP(phaseA)`];
- amounts of the phase `B` in mole number [i.e. `NP(phaseB)`];
- contents of the interstitial component(s) in the phase `A` expressed in u-fractions [i.e. `u-f(phaseA,component(s))`];
- contents of the interstitial component(s) in the phase `B` expressed in u-fractions [i.e. `u-f(phaseB,component(s))`];
- `LNACR(component)` value(s) for the interstitial(s).

After a successful STEP → PARAEQUILIBRIUM calculation, you can go to the POST module to plot a paraequilibrium phase diagram, or to impose the calculated paraequilibrium states onto a normal phase diagram [normally plotted as a `T-X` isopleth with one of the considered interstitial component(s) as the x-axis variable].

However, the stepping calculation procedure for the currently specified paraequilibrium states between the two specified phases may find difficulties at some steps due to some possible numerical problems (normally regarding to the u-fractions of the interstitial components under some composition ranges), or it may completely fails. In the latter case, it implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s) and substitutional components. Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.



The figure shows the plot of a paraequilibrium calculation of isopleths: Formation of para-pearlite in two Fe-based alloys, with equilibrium results appended.

The calculated paraequilibrium phase boundaries (black lines) are shown with tie-lines (in green-colour). In the Fe-2.5Mn-C alloy system, C is considered as fast diffusing interstitial component in the BCC+FCC and FCC+Cementite paraequilibrium stepping calculations; while in the Fe-3Cr-N alloy system, N is treated as fast diffusing interstitial components in the BCC+FCC and FCC+FCC_ M1N (i.e. FCC#1+FCC#2) paraequilibrium stepping calculations.

During a STEP calculation, the value of the stepping axis variable for each calculated equilibrium is listed and also the set of stable phases.



You can terminate the mapping of a line by pressing a single <Ctrl-A> (Windows) or <Ctrl-C> (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by a STEP_WITH_OPTIONS command-sequence, this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30   to
hardware precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command SET_NUMERICAL_LIMITS to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Complex miscibility gaps of various solution phases are automatically detected during a stepping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a `Global Test Interval` value and confirming the `Automatically add initial equilibria` in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can now start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as `FCC_A1#2`, `FCC_A1#3`, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable.

Occasionally, it may be necessary to have a specified increment other than the default value for the defined stepping axis-variable, in order to calculate/plot a smoother property diagram.

To get a complete property diagram, sometimes (especially in some earlier Thermo-Calc versions) it may also be required to have more than one starting equilibrium-points (under another starting equilibrium condition), and repeat the stepping calculation over the same stepping axis-variable range (while without over-writing the same POLY3 workspaces via a SAVE_WORKSPACE command). However, using the current STEP procedure such a requirement become less necessary.

TABULATE



This command is available for a table entered in either the POLY or POST module.

For any entered table, this command gives a table of values from equilibria calculated with a STEP command.



Unlike the TAB module's command (also called TABULATE) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	`Name: <Name of a table entered in either POLY or POST>` Specify a table name that is entered in either the POLY or POST module.
	`Output on screen or file /Screen/:` Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

TOGGLE_ALTERNATE_MODE



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Toggle the ALTERNATE mode for experimental equilibrium calculation between DEFAULT, ALWAYS and NEVER, during data-assessments using the PARROT optimization.

```
Set alternate toggle to DEFAULT, ALWAYS, or NEVER?
Set global toggle to DEFAULT, ALWAYS, or NEVER?
```

- `DEFAULT`: the experiment points are calculated according to the Alternate Technique depending on the SET_ALTERNATE command.
- `ALWAYS`: the experiment points are always calculated according to the Alternate Technique even if the Alternate Mode is switched off in the PARROT module.
- `NEVER`: the experiment points are calculated as normal equilibria even if you SET_ ALTERNATE in the PARROT module.

T-ZERO_TEMPERATURE

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

This calculates the temperature when two specific phases have the same Gibbs energy, i.e. the so-called T0 temperature. You must calculate an equilibrium state at an estimated temperature before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium state in which either one or both of the target phases is stable.

The following prompts are shown.

```
Name of first phase:  <Phase A>
Name of second phase: <Phase B>
```

The names of phases A and B must be given, for which the T0 temperature (where the Gibbs energies are equal) is to be calculated.

If the T0 temperature between the two specified phases is successfully calculated, a message displays, e.g.

```
The T0 temperature is 840.82 K. Note: LIST-EQUILIBRIUM is not relevant
```

The first message shows the calculated T0 temperature between the two specified phases.

The second message indicates that after this option calculation with LIST_EQUILIBRIUM is irrelevant and does not list the equilibrium for the system at the T0-temperature.

Gibbs Energy System (GES) Commands

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Solution Models in the GIBBS (GES) Module

AMEND_PHASE_DESCRIPTION

The AMEND_PHASE_DESCRIPTION command is used to specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

This topic outlines the application of each option and includes important information about each command.

There are many solution models implemented in the GIBBS module (type `INFO MODELS` to see details about various thermodynamic models). However, these are switched on and handled differently via various GIBBS routines/commands:

- The first models the non-ideality as excess parts, i.e. by amending the phase's EXCESS_MODEL and/or TERNARY_EXTRAPOLAT models.
- The second models the non-ideality as ADDITIONAL parts, i.e. by amending the phase's other subjects in this command, e.g. MAGNETIC_ORDERING for the Magnetic Ordering Model, DISORDERED_PART for the CVM Approach in modelling chemical ordering/disordering phenomenon, QUASICHEM_IONIC for using a quasi-chemical entropy term for an ionic two-sublattice liquid solution phase, QUASICHEM_FACT00 or QUASICHEM_IRSID for describing a substitutional liquid solution phase, DEBYE_HUCKEL for the DHLL/SIT Model in describing a dilute aqueous solution phase, etc.
- The third implements the model entirely or partially into the GIBBS module and related database(s), such as for the electrostatic contribution in an AQUEOUS solution phase by the Complete Revised_HKF Model, the Murngham Model, Birch-Murngham Model or Generalized PVT Model for high-pressure/temperature volume contribution in a solid or liquid phase, the SUPERFLUID Model for the non-ideal EOS and non-ideal mixing in a gaseous mixture.

NEW_CONSTITUENT

Use this if you want to add a new constituent to a phase. It is illegal to add new constituents to an ionic two-sublattice liquid phase.

RENAME_PHASE

Use this to change the names of some specific phases. For example, a phase called *FE3O4_S* may be better named *Magnetite* to help identify it during the calculations and postprocessing. This is also a way to delete a phase by hiding it under a new name.

SITE_RATIOS

Use this to change the number of sites (i.e. the stoichiometric coefficients of various sublattices) in a sublattice phase.

COMPOSITION_SETS

Use this for solution phases that may have miscibility gap(s). However, this is less important today and often unnecessary to define additional composition set(s), since the implemented Global Minimization Technique can usually detect and add such composition set(s) in an automatic manner where it is really necessary during equilibrium calculations (of single-points, stepping or mapping).

MAJOR_CONSTITUENT

Use this to set major constituent(s) on each sublattice in each composition set for a solution phase. This is useful to make calculations converge faster because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set. The databases often set major constituents for several phases automatically when data are retrieved.

FRACTION_LIMITS

Use this to limit the application range (in terms of mole-fractions of all the involved elements) of a particular solution phase. This is useful to avoid automatic creations (enforced by the Global Minimization Technique) of additional composition sets for some solution phases (such as AQUEOUS solutions or dilute Fe-based liquid mixtures) of which the used models [e.g. the `SIT Model` or the `Complete Revised_HKF Model` for AQUEOUS

solution, or the modified dilute solution parameters (plus a quadratic term, according to Hillert (1986) based on the SigworthElliot Model (Sigworth and Elliot, 1974) for Fe-rich liquid mixture] cannot be appropriately applied on a full scale.

Globally set the composition limits (in terms of mole fractions of various elements) in a specific solution phase, so that whenever the program finds a potential phase composition or a new composition set of possible miscibility gap(s) but that is out of this globally-set composition range, the program automatically ignores such a phase composition in an equilibrium calculation. This can be done either permanently inside a database (by enforcing this option for amending the phase-description of the solution phase) or temporarily within the GIBBS module (by using this phase-description amendment option).

This is important for solution phases for which the thermodynamic models and assessed data for the phases are for specific composition ranges, for example, the FE_LIQUID phase in the SLAG database is only applicable for Fe-rich liquid mixture, and the AQUEOUS phase in the TCAQ/PAQ and AQS/PAQS databases is only applicable for H2O-dominant aqueous solution phase.

Specify the low and high mole-fraction limits for each of the elements possibly available within the considered phase (in the currently defined system, or in a certain database). Do this for all the possible elements (defined in the phase) in a single AMEND_PHASE_ DESCRIPTION FRACTION_LIMITS command-sequence, for example:

```
TYPE_DEFINITION R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
      Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
      Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
      Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
      B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
P  0 0.01  S  0 0.01  !
```

DISORDERED_PART

This command is needed for the special treatment of chemically-ordered phases where the contributions from the disordered state are described by a phase without ordering sublattices (the disordered phase name must be specified).

Several checks are made that the ordered and disordered phases are compatible (sublattices, sites and constituents). A link is then created between the phases, and the disordered phase is hidden from application programs. The Gibbs energy for the ordered phase also includes the Gibbs energy for the disordered phase.

Phases which can have an order/disorder transformation have parameters split on two phases and are referred to as the *two phase* description in the GIBBS module. One of them has sublattices for chemical ordering, the other one represents the disordered state. Normally, the ordered BCC and FCC or HCP phases may have either 2 or 4 substitutional sublattice (plus one additional interstitial site), that are handled by the Two Substitutional-Sublattice Ordering Model or Four Substitutional-Sublattice Ordering Model, respectively.

Two phase means that the *ordered* phase has parameters that describe the ordering. The *disordered* phase has all parameters for the reference state and those for describing the disordered phase. The ordered phase may occur only is some systems whereas the disordered phase may occur frequently, typical examples are the disordered FCC and BCC which may become ordered as L12 or B2 in certain systems. In order to treat multicomponent systems where some subsystems have ordering it would be necessary to transform all parameters of BCC into a B2 model.

The parameters describing the disordered phase are not changed but the Gibbs Energy system is informed that the Gibbs Energy for the two phases should be added.

The method used calculates the Gibbs Energy of a two phase model with two or four substitutional sublattices for ordering.

$$G_m = G_m^{ord}(y_i', y_i') + G_m^{dis}(x_i) - G_m^{ord}(y_i' = x_i, y_i'' = x_i)$$

The mole fractions *x*i are calculated from the site fractions *y*i. The last term means that the contribution from Gmord in a disordered state (same site fraction, equal to the mole fraction, on both sublattices) is subtracted. The effect of this is that the parameters in the ordered phase have no contribution to the disordered state.

MAGNETIC_ORDERING

Change the magnetic ordering parameter for a certain phase with magnetic ordering contribution, in terms of its anti-ferromagnetic factor. By default this is –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.). The fraction value of the total enthalpy (due to short-range ordering above the magnetic transition temperature) is by default 0.40 for BCC phase and 0.28 for all other phases (FCC, HCP, etc.).

EXCESS_MODEL

See example tcex52.

Use this to change the default Excess Model (for interaction energies) from the default (REDLICH-KISTER_MUGGIANU). The model handles the excess interaction energies in a solution phase is chosen from:

- REDLICH-KISTER_MUGGIANU: for binary (R-K) & ternary (R-K-M) interactions
- REDLICH-KISTER_KOHLER: for binary (R-K) & ternary (R-K-K) interactions
- FLORY-HUGGINS POLYMER MODEL: for interactions in a polymer mixture phase (F-H)
- MIXED-EXCESS-MODELS: (R-K default) for mixed binary excess model (R-K, Legendre & Polynom) of a substitutional solution phase
- HKF: for interaction in an AQUEOUS solution phase (HKF)
- PITZER: for interaction in an AQUEOUS solution phase (PIT)
- CENTRAL_ATOM_MODEL: for interaction in a liquid slag solution phase (C-A-M)

For extrapolations of excess energies from related binary systems to ternary or higher-order systems, the Redlich-Kister binary excess interaction parameters may be extrapolated with either a Muggianu extension (i.e. the default REDLICH-KISTER_MUGGIANU model) and a Kohler extension (i.e. the alternative REDLICH-KISTER_KOHLER model), where there is no ternary, quaternary or higher-order interaction parameter.



The REDLICHKISTER_KOHLER model is implemented only for ternary systems.

The MIXED-EXCESS-MODELS option works only for a substitutional phase with no sublattice (such as the metallic LIQUID phase) and it can be used to invoke asymmetrical simple or Legendre polynomial as binary excess energy models in addition to the default symmetrical Redlich-Kister model for the chosen pair of constituents in a substitutional phase with no sublattice. Asymmetrical here means that the power series depend only on one of the constituents, for example with expansions based on the [1-2*X(B)] term rather than [X(A)X (B)].



Binary interaction parameters for such a pair of constituents must be entered prior to turning on the non-default Legendre or Polynom models.

TERNARY_EXTRAPOLAT



See example tcex52.

Use this to change the extrapolation method from the default REDLICH-KISTER_MUGGIANU to another extrapolation model. This method extrapolates from binary to ternary (and higher-order) excess interaction parameters in a solution phase and is chosen from:

- MUGGIANU for Muggianu Extrapolation from R-K parameters
- TOOP-KOHLER for Toop-Kohler Extrapolation Model
- KOHLER-ALL for Kohler Extrapolation Model
- MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model



Only when all the relevant binary excess energies in the current solution phase are treated by the default Redlich-Kister Model (i.e. the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the RedlichKister_Kohler Model.

The default ternary extrapolation method MUGGIANU_RESTOR applies to a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Muggianu Model (in short as R-K-M), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such a default R-K-M Model is always used.

The KOHLER-ALL ternary extrapolation method can be turned on also for a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model.

REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Kohler Model (in short as R-K-K), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such an R-K-K Model is used.

The TOOP-KOHLER ternary extrapolation method is applied in a special way: for a specific ternary system (e.g. A-B-C) in a solution phase, specify which two constituents as the so-called Kohler constituents and the remaining constituent as the so-called Toop constituent on a given sublattice. If for the A-B-C ternary system you have specified A and B, or B and A, as the Kohler constituents (entered as the basis constituent and first interacting constituent) and C as the Toop constituent, only the A-B binary interaction parameters are used in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters involving the Toop species C (i.e. of A-C and B-C binaries) are used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions).

DEBYE_HUCKEL

To use the DHLL (Debye-Hückel Limiting Law) model and SIT (Specific Ionic Interaction Theory) model for a dilute AQUEOUS solution phase, switch the DEBYE_HUCKEL part on, and it removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS phase.

HKF_ELECTROSTATIC

To use the hypothetical electrostatic contribution for the chosen phase (it must be an aqueous solution phase using the Complete Revised_HKF Model). It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS solution phase.

QUASICHEM_IONIC

To use the Quasichemical-Ionic model for the chosen liquid phase, you must have already entered/retrieved a liquid phase as an ionic two-sublattice liquid solution phase (normally, that is the IONIC_LIQ phase), and then use this amending option to switch QUASICHEM_ IONIC on. It creates a completely new liquid solution phase [namely the QUAS_IONIC phase which uses the Quasichemical Model for the entropy, according to Mats Hillert (2001: *J of Alloys and Compounds*, 320, 161-176)], while the original IONIC_LIQ phase remains in the system and is not changed by this option.

QUASICHEM_FACT00

 See example tcex49.

To use the Quasichemical Model developed by Kongoli et al. [1998, Kongoli], you must have entered/retrieved a liquid phase using a normal substitutional liquid model with specified associates or species (on a single lattice site), and then turn on the option QUASICHEM_ FACT00. This removes the previously-set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

Reference

[1998, Kongoli] F. Kongoli, A. D. Pelton, Y. Dessureault, Thermodynamic modeling of liquid Fe-Ni-Cu-Co-S mattes. Metall. Mater. Trans. B. 29, 591–601 (1998).

QUASICHEM_IRSID

To use the Kapoor-Frohberg-Gaye Quasichemical Cell Model (i.e. the Quasichemical Model developed by ISRID, France) for a liquid SLAG solution phase, you can use a normal liquid model with specified associates or species.

GLASS_TRANSITION

To use the special model for glass transition of a liquid phase. It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

REMOVE_ADDITION

To remove all the selected ADDITIONAL part from the Gibbs energy description for the chosen phase. If preferred, set a specific phase-status bit for a phase, use the PHASE_BITS option as long you know the restrict meaning of each part of a phase- status bits.

DEFAULT_STABLE

Set phases as default-stable, which helps you to have a better guess of which phases that should be stable at the first calculation.

About the ENTER_PHASE Command

ENTER_PHASE

With the command ENTER_PHASE, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces.

About Phase Names

A thermochemical system must have at least one phase (which is a homogeneous part of the system with a uniform composition and structure). In the GIBBS module, any number of phases can be entered for a system and for each phase there must be a description of how its Gibbs energy varies with temperature, pressure and composition. A phase has a large amount of data connected to it, e.g. it starts with a phase name:

- It may be treated as a special phase-type;
- It may have structural information about sublattice(s), etc.,
- There must be a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase);
- There may be basic information on what kind of EXCESS_MODEL (polynomial expression) is used to describe the binary, ternary and/or higher-order interactions between constituents;
- There may be so-called Additional contributions to the Gibbs energy of the phase from special physical phenomena, e.g. magnetic ordering, hypothetical electrostatic interaction, and so forth;
- There must exist all the parameters required for the descriptions of thermochemical properties (i.e. `G` terms for standard Gibbs energies, and `L` terms for binary, ternary or higher-order interaction excess energies) and of some special physical properties (e.g. the Curie temperature `TC` and Bohr magneton number `BMAGN` (or `BM`) for magnetic ordering, `V0-VA-VC-VK` parameters for volume contributions, Born functions for hypothetical electrostatic interaction in an aqueous solution phase) stored in connection with the phase.

About Phase Type Code

A G phase (gaseous mixture) or an A phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and that an L phase (ordinary liquid solution) is normally (but not always) modeled as a substitutional phase without sublattice, too.

The F and B phase-types are useful for ordered FCC (or HCP) and BCC solution phases handled by the so-called Four Substitutional-Sublattice Ordering Model, which always requires that the solution phase must have four sublattices for substitutional ordering and can additionally have an interstitial sublattice.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices all of which are the nearest neighbours. A *Normal 4-Sublattice Model* requires that all the G parameters for each of end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically. To be more clarified: An A-B binary solution phase (with the element A locates on one sublattice site and B on three sublattice sites) treated by the Normal 4-Sublattice Model has to have 4 G parameters for 4 end-members, i.e. G(phase,A:B:B:B), G(phase,B:A:B:B), G(phase,B:B:A:B) and G(phase,B:B:B:A), because of that in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, these are identical and thus all G parameters of such end-members need be given only once, and the possible permutations are then automatically handled by the GIBBS module. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

There are restrictions on the excess parameters allowed with the phase-type option `F`. You can only have excess parameters of these types:

```
L(phase,A,B:*:*:*;0…9)
L(phase,A,B:C,D:*:*;0…9)
```

The asterisk * means that the interaction parameter is independent on the constituents on its corresponding sublattice. No ternary interaction parameters (i.e. with three elements on one sublattice site) are allowed. The reason for this restriction is that it would be too complicated to handle all possible permutations. In the current *Four Substitutional Sublattice Ordering Model*, the binary interaction between A and B atoms is thus independent of the constituents on the other sublattices, where there are many other parameters to model the composition-dependence of the Gibbs energy (both in the ordered and disordered parts of the phase). The model for these ordered phases are always partitioned in a disordered part (with a single substitutional sublattice) and an ordered part (with four substitutional sublattices for ordering).

For ordered BCC phases, the phase-type option B means the same thing but the situation is more complicated, as the 4-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase (with the element A locates on two sublattice site and B on other two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the G

(phase,A:A:B:B) term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the G(phase,A:B:A:B) term has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds



For detailed reference visit the Crystal Lattice Structure web page https://www.nrl.navy.mil/mstd/6390.

The first end-member (described by the G(phase,A:A:B:B) term) represents B2- ordering and the second (described by the G(phase,A:B:A:B) term) stands for B32-ordering. There are two permutations of the G(phase,A:A:B:B) term and four permutations of the G(phase,A:B:A:B) term, automatically conducted in the Four Substitutional-Sublattice Ordering Model. And there are also two kinds of reciprocal interaction parameters, i.e.

```
L(phase,A,B:C,D:*:*;0…9) L(phase,A,B:*:C,D:*;0…9)
```

An advanced feature with the phase-type options F and B is that a composition set that represents the solution phase has a suffix (indicating that it is really as an ordered or disordered phase) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams). Such suffix indications can be:

- `_L12` or `_L10` for ordered FCC
- `_A1` for disordered FCC
- `_B2`, `_B32`, `_D03` or `_L21` for ordered BCC
- `_A2` for disordered BCC
- `_D019` and `_B19` for ordered HCP
- `_A3` for disordered HCP

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
FCC PHASE	PHASE_A1	PHASE_L12
		PHASE_L10
BCC PHASE	PHASE_A2	PHASE_B2
		PHASE_B32
		PHASE_D03
		PHASE_L21

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
HCP PHASE	PHASE_A3	PHASE_D019
		PHASE_B19

ADD_COMMENT



This command is for the Gibbs Energy System (GES) module.

Use the ADD_COMMENT command to add a comment or make notes about parameters.

AMEND_ELEMENT_DATA

This command is for the Gibbs Energy System (GES) module.

The data for an element (in the SER, the Stable Element Reference, state) can be changed by this command. It should only be used for the elements that do not have any data in the database because the element data available in the database is set by the database-developer for the purpose of internal consistency. Except for the mass, the other values have no influence on the calculations.

Syntax	AMEND_ELEMENT_DATA
Prompts	`Element name: <Element name>` Specify the name of the element for which you want to change the data.
	`New stable element reference /ABCD/: <Name of ser>` Press <Enter> to accept the default `SER` or specify a new SER for the element. Important: The default name should not be changed if this data is retrieved from a database. This name is used when parameters for a phase are listed and the database assumes that the stable element reference is the same as in the database. Only if the element's data have not been fetched from a database, e.g. entered manually, can you enter a new SER.
	`New atomic mass /xx.xxxx/: <yyyyyy>` Press <Enter> to accept the default atomic mass or specify a new value for the element. The atomic mass of the element is given in g/mol.
	`New h(298.15)-h(0) /xxx.xxx/: <yyyyy>` Press <Enter> to accept the default H(298.15)-H(0) or specify a new value for the element. H(298.15)-H(0) is the enthalpy difference between 298.15 K and 0 K for the element in its SER state.
	`New s(298.15) /xx.xxxx/: <yyyyy>` Press <Enter> to accept the default S(298.15) or specify a new value for the element. S(298.15) is the absolute value of the entropy at 298.15 K for the element in its SER state.
	`Default element reference state symbol index /#/: <index>` The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data, you must set the index to get the correct symbol. Specify an index for the default listing parameters (symbol), or press <Enter> to accept the pre-set index. 0 is for `G`, 1 is for `H298` and 2 is for `H0`. The index is to define the symbol printed in parameter listings. The symbol can be: • `G` the data are referred to Gibbs energy at a variable temperature (also called *lattice stability*). • `H298` the data are referred to the enthalpy of the element at 298.15 K and 1 bar.

Syntax	AMEND_ELEMENT_DATA
	• `H0` is the same as `H298` but at the temperature 0 K.

AMEND_PARAMETER

This command is for the Gibbs Energy System (GES) module.

There is also a PARROT module command with the same name.

Use this command to interactively change/amend the temperature-pressure function of a parameter. This is useful to correct typing errors because the old function is made available on the terminal for interactive editing.

About the ENTER_PARAMETER Command

Syntax	AMEND_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct parameter name. If a parameter name is not acceptable or you only press <Enter>, the error message displays:
	`Error, please re-enter each part separately`
	The program prompts for separate input for each part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these legal identifiers as described for ENTER_PARAMETER.
	`Phase name (/ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name.
	`Interacting constituent (in sublattice # /xyz/): <Species name>` Specify the interacting constituent name: If there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /xyz/): <Species name>` If there are more than one interacting constituents, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>` Specify a numerical number as the degree of the phase parameter.

	After the parameter name is specified correctly, the program lists its current definition (either present in the database or defined by the ENTER_PARAMETER command), such as:
	`L(PHASE2,AL,MG;1)=`
	`298.15<T<2000.00: +5000`
	`2000.00<T<4500.00: +4500`
	`4500.00<T<6000.00: +4000`
	Then you are prompted to change the parameter definition, as shown below:
	`Do you want to change the number of ranges /No/:`

Syntax	AMEND_PARAMETER

	Enter Y if you want to change the number of ranges for the chosen function, or change some of the temperature limits in the definition. Then retype both the low/high temperature limits and functions.
	
	If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> to accept the default N, then the whole definition of the chosen parameter in all ranges (if any) is listed on screen, such as:
	
	`DIFFERENT FUNCTIONS IN THESE RANGES`
	`298.15<T<2000.00`
	`2000.00<T<4500.00`
	`4500.00<T<6000.00`
	
	The prompt is given:
	
	`Do you want to change range limits /No/:`
	
	If there is more than one range, this question is prompted press <Enter>.

	`Range number (0 to exit) /0/: <Range number>` If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any changes.

	`Function:`
	
	The previous function is available for editing. The editing is performed within the general subroutine FOOLED, as described in AMEND_SYMBOL. This routine prompts as follows:
	
	`1:+:>`
	
	The prompt consists of the current position in the string and the character at that position between colons, (::).
	
	Commands
	
	These commands can be given:
	
	• Help: `?`
	• Move CP to last or first character: `<+/-> A`
	• Delete characters from CP: `<+-#characters> D`
	• Exit: `E`
	• Find: `<#occurrences> F<string>@`
	• Insert: `I<string>@`
	• Move: `<+-#positions> M`
	• Restore string: `R`
	• Substitute: `S<OLD>@<NEW>@`
	• Type string: `T`
	
	Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.

Syntax	AMEND_PARAMETER
	 When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type E at the prompt.

AMEND_PHASE_DESCRIPTION

This command is for the Gibbs Energy System (GES) module.

Also see Solution Models in the GIBBS (GES) Module for detailed information about this command and its options.

Specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

Syntax	AMEND_PHASE_DESCRIPTION

Prompts	`Phase name: <Phase name>`
	Specify the name of the phase.
	`Amend what /Composition_Set/: <Subject>`
	Several subjects for the phase can be amended but most often this command is used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.
	Enter a question mark at the prompt to get a list of all possibly amended subjects for a phase.

There are no additional prompts for DEBYE_HUCKEL, HKF_ELECTROSTATIC, GLASS_TRANSITION, QUASICHEM_FACT00, QUASICHEM_ISRID, REMOVE_ADDITION, and DEFAULT_STABLE.	
`RENAME_PHASE`	`New phase name /ABCD/: <Phase name>` Give a new phase name for the chosen phase, or press <Enter> to keep the default shown.
`Site_ratios`	`Sites in first sublattice /XX/ : <YY> Sites in second sublattice /XX/ : <YY>` Specify the site numbers for each of the prompted sublattices for the current phase. Press <Enter> to accept the previous definitions.

`New_ constituent`	`Sublattice /#/: <Sublattice number>`
	Specify the sublattice where the new constituents are located.
	`Species: <Species name>`
	Give a valid species name.

`Composition_ sets`	`New highest set number /#/: <Set number n>` The default value (#) is usually one higher than the current value. All phases have initially one composition set. If a lower value (i.e. lower than the default one) is given, that specific composition sets are deleted. You cannot take away the first composition set.

Syntax	AMEND_PHASE_DESCRIPTION
	`Major constituent(s) for sublattice #: /AB/: <Major constituent(s)>` Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which was automatically set according to the specified composition set of the phase. This prompt is repeated for all available sublattices in the chosen phase. The major constituents in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

`Major_ constituent`	`Composition set /1/: <Composition set number>`
	
	Give the composition set (digit number) for the chosen phase, or press <Enter> if you want to set major constituents for the specified composition set.
	
	`Major constituent(s) for sublattice #: /AB/: <Major constituent(s)>`
	
	Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which is automatically set according to the specified composition set of the phase.
	
	This prompt is repeated for all available sublattices in the chosen phase for the specified composition set.
	
	The major constituents in each sublattice can be specified. This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). The databases often set major constituents for several phases automatically when data are retrieved.

`Fraction_ limits`	`Element : <el1>`
	`Low fraction limit /0/ :  <Appropriate low limit>`
	`High fraction limit /1/ : <Appropriate high limit >`
	`Element : <el2>`
	`Low fraction limit /0/ :  <Appropriate low limit>`
	`High fraction limit /1/ : <Appropriate high limit>`
	`Element : <eln>`
	`Low fraction limit /0/ :  <Appropriate low limit>`
	`High fraction limit /1/ : <Appropriate high limit >`

`Magnetic_ ordering`	`The antiferromagnetic factor /XX/: <YY>`
	
	Specify the anti-ferromagnetic factor for the chosen phase. This should be –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.).
	
	`Short range order fraction of the enthalpy /XX/: <YY>`
	
	The magnetic ordering is a second-order transformation and part of the enthalpy due to this transformation is due to short-range order. This value is the fraction of the total enthalpy that is due to short-range ordering above the magnetic transition temperature.
	
	The default value (xx) is 0.40 for BCC phase, and 0.28 for all other phases (FCC, HCP, etc.).

`Disordered_ part`	`Disordered phase name: <Phase name>` Give the disordered phase name for which there is no ordering sublattice.
`Excess_model`	`Model name /ABCDEFG/: <Model name>`

Syntax	AMEND_PHASE_DESCRIPTION

	The default model is the pre-set model for the solution phase, normally the REDLICH-KISTER_MUGGIANU model, or choose another model for the phase to be amended:
	• REDLICH-KISTER_MUGGIANU
	• REDLICH-KISTER_KOHLER
	• FLORY-HUGGINS POLYMER MODEL
	• MIXED-EXCESS-MODELS (R-K default)
	• HKF
	• PITZER
	• CENTRAL_ATOM_MODEL
	The MIXED-EXCESS-MODELS option has sub-options:
	`First (the independent) constituent: <Constituent name>`
	`Second (the dependent) constituent: <Constituent name>`
	Specify the binary pair of constituents in the current substitutional solution phase (the first one as the so-called independent constituent, and the second one as the dependent constituent), for which you wish to change the binary excess model from the default REDLICH-KISTER model to another model (LEGENDRE or POLYNOM).
	You are prompted with the first sub-option (i.e. `First (the independent) constituent` after you have specified the desired binary Excess model type. To make further changes of binary excess model for other specific binary pairs in the current substitutional solution phase, press <Enter> (implying that there are no more changes of binary excess model for all other possibly-remaining binary pairs that shall still use the default REDLICH-KISTER model).
	`Excess model type: /Legendre/: <Desired binary excess model type>`
	For the currently-specified binary pair, choose one the legal binary excess models: LEGENDRE, POLYNOM or REDLICH-KISTER. If the default binary excess model REDLICH-KISTER is used for a certain binary pair, you can either specify the model name (or in short as R-K) or press <Enter>. After this sub-option, it returns to the first sub-option *First (the independent) constituent:* either for further change(s) of binary excess model of any other binary pair(s) or for termination (by pressing <Enter>) in the MIXED-EXCESS-MODELS option.

`Ternary_ extrapolat`	`Extrapolation method: /Toop-Kohler/: <Ternary model>`
	Choose a ternary extrapolation model for the current solution phase:
	• TOOP-KOHLER for Toop-Kohler Extrapolation Model
	• KOHLER-ALL for Kohler Extrapolation Model
	• MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model
	The TOOP-KOHLER option further prompts:
	`Constituent in sublattice #: <Basis constituent name>`
	`First interaction constituent: <Interacting constituent name>`
	`Toop constituent: <Toop constituent name>`
	Specify the so-called Kohler constituents (entered as the basis constituent and first interacting constituent) and Toop constituent on a given sublattice in the current solution phase.

Syntax	AMEND_PHASE_DESCRIPTION
`Quasichem_ ionic`	To use the Quasichemical Model for the chosen liquid phase, you must first enter it as an ionic liquid phase, and then use this amending option. It creates a completely new phase, the original IONIC_LIQUID phase remains in the system and is not changed. `Number of bonds/atom /2/: <Number of bonds per atom>` Specify the Z value (number of bonds per atom).
`Status_bits`	Correct the phase status bits. It is important to fully understand this command before using it: `New status word (in hexadecimal) /04204000/: <New status bits>` LIST_STATUS Normally, these should never be changed in this way, because such phase status bits are automatically set on when all the phase descriptions (predefined in databases and amended in the GIBBS module) are defined properly. The only exceptions are for the Kapoor-Frohberg-Gaye cell model for liquid SLAG solution phase, which can be set only as 04208000; and for the complete Revised HKF AQUEOUS solution model, which can be set as `02084000`.

AMEND_SYMBOL

This command is for the Gibbs Energy System (GES) module.

The same command is also available for the PARROT module.

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered with ENTER_SYMBOL) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.

The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with LIST_STATUS. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL

Prompts	`Name: <Symbol name>`
	Specify the name of an entered symbol.
	For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the `Parameter` keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:
	`FUNCTION VALUE  2.52500000E+01`
	`TABLE VALUE  1.56000000E+02`
	For variables and functions (or parameters), there are additional prompts and depend on the symbol type.

	For a variable, its current value is displayed, and you can change it to a new value:
	`Value /Current value/: <New value>`
	For a function (or a parameter entered as a symbol):
	`Do you want to change the number of ranges /No/:`
	Enter Y to change the number of ranges for the function, or change some of the temperature limits

Syntax	AMEND_SYMBOL

	in the definition, then retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.
	
	If you do not want to change it, press <Enter>. The definition of the chosen function in all ranges (if any) is listed, for example:
	
	`DIFFERENT FUNCTIONS IN THESE RANGES`
	`298.15<T<2000.00`
	`2000.00<T<4500.00`
	`4500.00<T<6000.00`
	
	and this message displays:
	
	`Do you want to change range limits /No/:`
	
	If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

	`Range number (0 to exit) /0/: <Range number>`
	`Function:`
	
	The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:
	
	`1:+:>`
	
	The prompt consists of the current position in the string and the character at that position between colons (::).
	
	## *Commands*
	
	These commands can be given:
	
	• Help: `?`
	• Move CP to last or first character: `<+/-> A`
	• Delete characters from CP: `<+-#characters> D`
	• Exit: `E`
	• Find: `<#occurrences> F<string>@`
	• Insert: `I<string>@`
	• Move: `<+-#positions> M`
	• Restore string: `R`
	• Substitute: `S<OLD>@<NEW>@`
	• Type string: `T`
	
	Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.
	
	  When the string is typed the character at the current position is replaced by an underscore _.

Syntax	AMEND_SYMBOL
	To finish the editing of the current function, type `E` at the prompt.

CHANGE_STATUS



This command is for the Gibbs Energy System (GES) module.

The status of an element or species or phase can be either ENTERED or SUSPENDED. The suspended status can be either implicit or explicit. The implicitly suspended status can be set e.g. for a species if any of the elements in its chemical formula is explicitly suspended. A species that is implicitly suspended becomes entered automatically if all its elements are set entered. After this command, a message shows which elements/species/phases are suspended or restored (entered). Consequently, the status bits for the specified elements or species or phases are changed, as listed with LIST_STATUS.

Syntax	CHANGE_STATUS
Prompts	`For Element, Species or Phase /Species/: <Keyword>` Specify the keyword (element, species or phase).
	`Suspend /Y/:` By default the status is changed from ENTERED to SUSPENDED. If an element is suspended all species with this element become implicitly SUSPENDED too. A phase may become implicitly suspended if all its constituents or all constituents in a sublattice are suspended.
	`List of elements/species/phases: <Name of elements or species or phases>` Specify the names or indices of those elements or species or phases that shall become suspended or active. For names, these should be separated by a space and terminated with a semicolon (;) or an empty line. For indices it is possible to give a range by separating two numbers by a hyphen (-). The list should be terminated by a semicolon (;). Example: `5 1 7-12 FE;`

ENTER_ELEMENT

Specify a system interactively. The program searches the currently switched or preset database for data for the given elements. The data for the elements in the database are the:

- mass in g/mol
- name of the Selected Element Reference State (SER) which normally is the stable phase for the element at 298.15 K
- enthalpy difference for the element in the SER state at 298.15 K and zero K
- absolute entropy for the element in the SER state at 298.15 K.

The two predefined elements, i.e. electrons and vacancies, have the chemical symbols `/-` and `VA`, respectively. Initially, these are suspended but can be entered either by this command or CHANGE_STATUS.

If an aqueous solution phase is involved, in the GIBBS module you enter a special aqueous electron called, ZE. This is specially designed for appropriately calculating the standard electric potential in the aqueous solution system.

Syntax	ENTER_ELEMENT
Prompt	`Element name: <Element name>` Specify several elements on one line. The name of an element is its chemical symbol. The chemical symbols must be separated by spaces. Fictitious element names are legal but naturally no data are found in the database for them.
	 An element name (maximum 2 characters) can either have its first letter in upper and the second (if any) in lower case (i.e. Lower Case Mode) or both letters can be in upper or lower case (i.e. Upper Case Mode). The Upper or Lower Case Mode is selected by the command REINITIATE, which removes all data, and should be executed before any other command.

ENTER_FUNCTION

This command is available with the GES and TAB modules.

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

Syntax	ENTER_FUNCTION
Prompt	`Name: <Name>` `Function: <Definition>`
	A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, -(G-H)/T can be defined as a function which is identical to S for a substance or ΔS for a reaction, G+T*S-P*V can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction.
Options	`Name`of the function (maximum 8 characters) and `Definition` of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line.

Example

For the pure substance Fe (using the SSUB database), by entering a function as `G+T*S-P*V`, the following table is obtained by typing <Enter> in the prompt `Output file /Screen/:`, and the figure by typing `6` in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION
Name: InEnergy
Function: G+T*S-P*V;
TAB: TABULATE_SUBSTANCE
Substance (phase): Fe
Pressure /100000/: <Enter>
Low temperature limit /298.15/: <Enter>
High temperature limit /2000/: <Enter>
Step in temperature /100/: <Enter>
Output file /try1/: try2
Graphical output? /Y/: <Enter>
Plot column? /2/: 6
```

This gives the following output:

```
O U T P U T  F R O M  T H E R M O - C A L C

Column 6: InEnergy G+T*S-P*V

Phase : FE_S                        Pressure :      100000.00

Specie: FE

************************************************************

    T      Cp            H             S             G             InEnergy

   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)

************************************************************

  298.15   2.48446E+01   2.17972E-06   2.72800E+01  -8.13353E+03   2.17972E-06

  300.00   2.48905E+01   4.60049E+01   2.74338E+01  -8.18414E+03   4.60049E+01

  400.00   2.71299E+01   2.64957E+03   3.49085E+01  -1.13138E+04   2.64957E+03

  500.00   2.93561E+01   5.47211E+03   4.11976E+01  -1.51267E+04   5.47211E+03

  600.00   3.19293E+01   8.53245E+03   4.67701E+01  -1.95296E+04   8.53245E+03

  700.00   3.50985E+01   1.18777E+04   5.19207E+01  -2.44667E+04   1.18777E+04

  800.00   3.92042E+01   1.55830E+04   5.68623E+01  -2.99068E+04   1.55830E+04

  900.00   4.49645E+01   1.97726E+04   6.17903E+01  -3.58387E+04   1.97726E+04

1000.00   5.42147E+01   2.46891E+04   6.69619E+01  -4.22728E+04   2.46891E+04

1100.00   4.55851E+01   2.99025E+04   7.19412E+01  -4.92328E+04   2.99025E+04 $
Stable phase is FE_S2

1200.00   3.40840E+01   3.51037E+04   7.64466E+01  -5.66322E+04   3.51037E+04

1300.00   3.49398E+01   3.85549E+04   7.92086E+01  -6.44162E+04   3.85549E+04
1400.00   3.57994E+01   4.20918E+04   8.18293E+01  -7.24692E+04   4.20918E+04

1500.00   3.66636E+01   4.57149E+04   8.43287E+01  -8.07780E+04   4.57149E+04

1600.00   3.75330E+01   4.94247E+04   8.67226E+01  -8.93314E+04   4.94247E+04 $
Stable phase is FE_S3

1700.00   4.05217E+01   5.41173E+04   8.95609E+01  -9.81363E+04   5.41173E+04

1800.00   4.12595E+01   5.82055E+04   9.18975E+01  -1.07210E+05   5.82055E+04 $
Stable phase is FE_L

1900.00   4.60000E+01   7.74165E+04   1.02377E+02  -1.17099E+05   7.74165E+04
2000.00   4.60000E+01   8.20165E+04   1.04736E+02  -1.27456E+05   8.20165E+04
```

ENTER_PARAMETER

This command is for the Gibbs Energy System (GES) module.

There is also a PARROT module command with the same name.

About the ENTER_PARAMETER Command

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command AMEND_PARAMETER.

Syntax	ENTER_PARAMETER

Prompts	`Parameter: <Parameter name>`
	As explained in About the ENTER_PARAMETER Command, specify a correct and complete `Parameter Name`, which should contain all the necessary parts of the general form:
	`<Identifier>(<Phase>,<Constituent array>;<Digit>)`
	If a parameter name is not acceptable or <Enter>, is pressed, a message displays:
	`*** Error, please re-enter each part separately`
	and you are prompted for input for each required part for a parameter name.

Options	**Description or Information**
`Identifier`	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`Phase name`	`Phase name (/ABCD/): <Phase name>` Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.
`Constituent`	`Constituent (in sublattice # /ABC/): <Species name>` A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated. It is the species name, not the stoichiometric formula required here. If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.
`Interacting constituent`	For phases with several sublattices, the program asks for one constituent in each sublattice.

Syntax	ENTER_PARAMETER
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name.  To cancel the default value of the interacting constituent type `NONE` or the name of another constituent. This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.
`Degree`	`Degree /#/: <Degree>` Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0`, `VA`, `VC` or `VK`). For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index. For a standard `G` parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.

`Phase parameter`	After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`Function: <Definition for a function>`
	A TP-Function consists of terms in T and P.
	`& <Continuation of the definition for the current function>`
	Continuation of a TP-Function definition.
	`High temperature limit /6000/: <High temperature limit in K>`
	Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the *lowest limit* is entered as a negative number) for the current TP-Function.
	`Any more ranges? /N/:`
	Enter Y for more function(s) or N to end this command.

ENTER_PHASE

See About the ENTER_PHASE Command for details about the phase-type and other prompts.

With this command, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces. However, for the remaining parts of thermodynamic descriptions (i.e. thermochemical and physical parameters, excess model, and possibly additional contribution term) for the phase, the GIBBS commands ENTER_PARAMETER and AMEND_PHASE_DESCRIPTION, should be used sequentially.

Normally, data for a system are retrieved from the preset database after the elements and species are specified. This is automatically done through GET_DATA. In some cases, specify a phase interactively.

Syntax	ENTER_PHASE
Options	**Description and Information**

`Phase name`	`Name of phase: <Phase name>`
	The phase name is any string starting with a letter and containing only letters, digits or the underscore character. The phase name must be unique.
	`Type code: <Phase-type code>`
	The `Phase-type code` must be specified for the phase if it is not an ordinary solution phase. Press <Enter> if the phase is ordinary.

`Phase-type`	
`G`	Gaseous mixture phase. There may only exist one gas phase in a system.
`A`	Aqueous solution phase.
`L`	Liquid solution phase but not `A` (aqueous) or `Y` (ionic liquid)
`Y`	Ionic liquid solution phase (that is specially treated by the Ionic Two Sublattice Liquid Model).
`I`	A phase with charged species but not `G` (gaseous), `A` (aqueous) or `Y` (ionic liquid).
`F`	An ordered FCC or HCP solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).
`B`	An ordered BCC solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).
`Sublattice number`	`Number of sublattices /1/: <Sublattice number>`

Syntax	ENTER_PHASE
	Phases with stoichiometric constraints usually have two or more sublattices. On each sublattice one or more species can be entered as constituents. The number of sublattices must not exceed 10. Substitutional phases with no sublattices are treated as phases with one sublattice. `Number of sites on sublattice  # /1/: <Site number>` For phases with sublattices, the ratio of the sites on each sublattice (donated with #) must be given. The program asks for values for all sublattices (by repeating this question for each sublattice), but these may have a common factor extracted. It is recommended to use integer numbers as sites if possible. For substitutional phases with no sublattices, this question does not show up.

`Constituents`	`Name of constituent: <Constituent name(s)>`
	For each sublattice specify at least one species as constituent. Several constituents can be given consequently (on the repeated prompt) or on the same line separated by a space. This question is repeated till pressing <Enter> or giving a semi-colon (;), meaning that the list of constituents is terminated by (;) or an empty line.
	`Will you add constituents later /N/:`
	For Y add other constituents to the phase by specifying new components in e.g. an ENTER_ PARAMETER command.
	If illegal constituents are used, you get a message e.g. when parameters are entered.
	`Do you want a list of possible parameters /N/:`
	Enter Y for a list of all possible parameters up to the fifth interaction order for the entered phase.

ENTER_SPECIES

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. For each species, its name and chemical formula must be given.



All elements are automatically entered simultaneously as species. The constituents of a phase must be species, but there is no thermochemical data associated with the species except as constituents of a phase.

Syntax	ENTER_SPECIES

Prompt	`Species name: <Species name>`
	
	Enter a unique species name. This is usually its chemical formula but it can be any string which starts with a letter and contains only letters or digits. Parenthesis `()` and an underscore _ are permitted. The combination /- or /+ used to denote charge.
	
	Species Names Examples
	
	`NACL2, FE2O3, FEO3/2, FE1O1.5, CA.5MG.5SI1O3,`
	
	`AL1H1O1_Al(OH) , AL1H1O1_HAlO, C2H4O3_124TRIOXOLANE, NA+, SIO4-4, H1/+1, H1O1/-1, AGC2N2-1.`
	
	The species name can be used to separate isomers with the same stoichiometry, e.g. `C2H2Cl2, (CHCl)2_cis, (CHCl)2_trans, CH2_CCl2.`

	`Stoichiometry /Species name/: <Chemical formula>` The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis () nor an underscore _ is allowed in the chemical formula, while the special combination /- or /+ can be used. In upper case mode (see REINITIATE), the stoichiometric number unity can be excluded only if the element symbol consists of two letters. In lower case mode, the element must be typed with the first letter in UPPER case and the second in lower, and it is thus possible to distinguish CO (carbon monoxide) from Co (cobalt) without any stoichiometry number.  All elements in a species must be entered prior to entering the species.

ENTER_SYMBOL

This command is for the Gibbs Energy System (GES) module.

There are also a POLY and POST module commands with the same name. However, symbols entered in the GIBBS module are not the same symbols as defined in the POLY and POST modules.

In the GIBBS module, a symbol can be used to represent a numeric quantity (e.g. a *variable*), a *function*, or a *table*. The entered symbol (with a symbol name of maximum eight characters) can be used later when parameters are entered, and this is a flexible way to manipulate thermodynamic functions. Symbols are especially useful if the same function or table is used in several thermochemical parameters. A *parameter* symbol is used to assign the values of phase parameters (which are defined with the command ENTER_PARAMETER) to specific characterized symbols. If you want to define a constant quantity, enter it as a simple function with a constant value in all (temperature) ranges.

The symbols entered in the GIBBS module can also be listed and used in the PARROT module (for data optimization) where you can use the GIBBS-entered symbols (variables, functions or parameters) to define parameters that shall be optimized.

See example 44 for an example of using variables and functions.

Syntax	ENTER_SYMBOL

Prompt	`Variable, function, table or parameter? /Function/: <Keyword>`
	The keyword can be a variable, function, table or parameter.
	• `Variables` are similar to functions because these can also be expressions of state variables. It is possible to enter a variable with a new expression anytime.
	• `Functions` are expressions of state variables or other functions.
	• `Tables` are used for listing results. A table consists of a list of any number of state variables, functions or variables.
	• `Parameter` symbols are used to assign the values of phase parameters (which are defined by the command ENTER_PARAMETER) to specific characterized symbols. If the phase parameter is not defined yet, the parameter symbol is assigned zero or a symbol which is valued as zero. In this way it is easy to refer to entered phase parameters in further defining other phase parameters.
	`Name: <Name of the symbol>`
	Each symbol has a unique name that must start with a letter and can have maximum 8 characters.

Syntax	ENTER_SYMBOL
	The following prompts are based on the type of symbol.
`Variable` symbol	`Value: <Numeric value of a variable>` Only a constant numeric value, not an expression, is accepted.

`Function` symbol	Enter the lower-temperature limit, the expression, an upper-temperature limit and if there is another expression above this upper limit:
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest-temperature limit, below which its (first) expression is not applicable. The default lowest limit of all kinds of data is 298.15 K.
	If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this function; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function are also taken as pressure limit values (in Pascal).
	The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-FUNCTIONS valid in the nearest temperature/pressure range.
	`Function: <Definition for a TP-function>`
	A TP-Function consists of terms in T and P. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. An expression can be continued on more than one line. A PT-function must be terminated by a semicolon (;) or an empty line. No more than 78 characters can be written on a line. If this is not sufficient space on one line, press <Enter> and continue on the next line. The program prompts with an ampersand `&` when a continuation is expected.
	  A function can have several temperature ranges, and a different expression (i.e. a TP-Function) for each region; if required, a single function can have up to ten different temperature ranges (and thus have up to ten different TP-Functions).
	This question is repeated if the current function has more than one expression (TPFunction) in various temperature ranges [or pressure ranges; only if the *lowest limit* is entered as a negative number)].
	`& <Continuation of the definition for the current TP-Function>`
	This is for a continuation of the definition for the current TP-Function. The ampersand & means that you can continue to write the function on the new line if one line is not enough for the current TP-Function. If you are finished the current TP-Function, press <Enter> again.
	`High temperature limit /6000/: <High temperature limit in K>`
	For a TP-Function, specify the high-temperature limit, above which its current expression is not applicable. The default high-temperature limit for all kinds of data is always 6000 K.
	This question is repeated if the function has more than one expression (TPFunction) in various temperature ranges.

Syntax	ENTER_SYMBOL
	All the temperature limits for the presently-be-entered TP-Function MUST be in an increasing order; otherwise the whole function is given a single value of zero. If a negative number is given as the lowest-temperature limit, it is interpreted as the low-pressure limit (in Pascal), and the high-temperature limit is also taken as the high-pressure limit (in Pascal) for the current TP-Function. The high-temperature/pressure limit for the current applicable expression (TPFunction) is the low temperature/pressure limit for the next range if several ranges are needed to describe the temperature/pressure-dependence of this function. The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-Function valid in the nearest temperature/pressure range. `Any more ranges /N/: <Y or N>` Answer `N` to finish the definition of the current function. If `Y` the program asks for a new function valid above the last high temperature limit and below a new high temperature limit. The maximum number of temperature ranges is 10. Important note: Make sure that the function and its first derivatives are continuous across break points.

`Table` symbol	Specify the low and high temperature limits, temperature step and tabled value at each specified temperature:
	
	`Low temperature limit /298.15/: <Low temperature limit in K>`
	
	The lowest temperature where the table has a value.
	
	`High temperature limit /6000/: <High temperature limit in K>`
	
	The highest temperature where the table has a value.
	
	`Step in temperature /100/: <Temperature step>`
	
	The step in temperature between each value in the table. This step must be constant for the whole table. If a table cannot be described with a single step it must be divided into several tables for different temperature ranges. The upper and lower limits are truncated to give reasonable values where the table values must be specified.
	
	`Table value at  XX /YY/: <Table value>`
	
	The value of the table at the specified temperature (`xx`) must be given. The default value (`yy`) is the last value.

`Parameter` symbol	Input the correct name of a phase parameter (including its identifier, phase name, constituent and interacting constituent(s) in various sublattices (if exist), and degree of the parameter. Most of the settings are the same as in the ENTER_PARAMETER command or the Function symbol prompts above.
	
	`Parameter: <Parameter name>`
	
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form:
	
	`<Identifier>(<Phase>,<Constituent array>;<Digit>)`
	
	If a parameter name is not acceptable or <Enter> is pressed, this error message displays:

Syntax	ENTER_SYMBOL

	`*** Error, please re-enter each part separately`
	
	The program prompts for separate input for each required part for a parameter name.
	
	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>`
	
	Specify one of these types of legal identifiers.
	
	`Phase name (/abcd/): <Phase name>`
	
	Specify the phase name.
	
	`Constituent (in sublattice  # /abc/): <Species name>`
	
	Specify the constituent name on the specified sublattice site of the given phase.
	
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>`
	
	Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>`
	
	If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	
	`Degree /#/: <Degree>`
	
	Specify an integer number (a value from 0 through 9) as the degree for the phase parameter.
	
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	
	Specify the lowest-temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	
	`Function: <Definition for a function>`
	
	Specify the desired TP-Function for the current temperature range (or current pressure range; only if the *lowest limit* is entered as a negative number).
	
	`& <Continuation of the definition for the current TP-function>`
	
	Specify the desired TP-Function continuation for the current temperature range (or current pressure range; only if the lowest limit is entered as a negative number).
	
	`High temperature limit /6000/: <High temperature limit in K>`
	
	Specify the high-temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the lowest limit is entered as a negative number) for the current TP Function.
	
	`Any more ranges /N/:`

LIST_CONSTITUTION

This command is for the Gibbs Energy System (GES) module.

Syntax	LIST_CONSTITUTION
	List all the constitutions (as site-fractions) for all the phases in the defined system.
	This is mainly for software managers. There are no commands in the GIBBS monitor to set the constitution.

LIST_DATA

This command is for the Gibbs Energy System (GES) module.

Use the LIST_DATA command to retrieve and then list the data included with a database in the DATA module or directly entered in the GIBBS module. All data for the current system that is defined within the current GIBBS workspace is written in a readable manner in the output file. If no output file is specified, by default the data displays on screen. The behavior of this command differs slightly based on whether you are using GES6 (the default) or GES5.

For encrypted commercial databases you may not be able to use this command to list any retrieved data. However, it can be used to list some basic definitions (such as phase models and phase-constituents) retrieved from an encrypted database, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Command Prompts

After entering the command in the console, the following prompt options are available.

Syntax	LIST_DATA
Prompts	`Output to screen or file /Screen/: <File name>` Specify the name of a file in which the data shall be written in a readable manner. The default value is the screen (by pressing <Enter>).
	`Options?: <Option(s)>` Choose one or several of the following options for output.  See the section about the differences between GES5 and GES6 output for these options. • `N` the output is written as a user database format. For GES6, and only for an unencrypted database, this option has a subcommand that allows filtering of phase parameters with respect to the property type e.g., to include only volume parameters and/or viscosity parameters in the output. • The subprompt is `Property type /All/`. Choose `All` or enter the property type. The valid alternatives (when available) are: V0, VA, VB, VC, VK, TC, TN, BM, MQ, MF, DQ, DF, OQ, VS, G, L, THCD, ELRS, ESPD, VISC, GD, SIGM or XI • `P` the output is written as a macro file for future input. This is useful for creating `*SETUP` files for data assessments. • `S` the symbols are suppressed.

Syntax	LIST_DATA
	• R the references for the parameters are listed (only for some databases in which references are available) • L the output is written suitable for a LaTeX preprocessor.

Output Differences: GES5 vs GES6

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features.

As required you can set Thermo-Calc to use GES5 instead of the default with the SET_GES_VERSION command. The application may also automatically and temporarily switch to GES5 when a database is being used that is not compatible with GES6.

For both GES5 and GES6 and when you enter P, S, R, or L, the output data consists of a list of all elements and the data followed by a list of all phases and the data associated with each phase. The thermochemical parameters listed for each phase are always in SI units.

For GES6, and only when option N is entered, the output data consists of a list of all elements and the data followed by a list of all phase definitions and the data associated with the phases, sorted by system. In this mode, and only for unencrypted databases, there is a subcommand that allows filtering of phase parameters with respect to the property type e.g., to include only volume parameters and/or viscosity parameters in the output.

Other differences between the GES5 and GES6 output are related to the output as shown below.

Output	GES5	GES6
Parameters	Includes implicitly defined zero-valued thermodynamic parameters	Only contains parameters that are actually defined in the database
Automatically suspended phases	Does not include	Includes
References	Contains references of functions and parameters with generic names, such as "REF123"	Retains the original reference names that are used in the database

LIST_PARAMETER

This command is for the Gibbs Energy System (GES) module.

There is also a PARROT module command with the same name.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

```
The parameter name: <Identifier>(<Phase>,<Constituent array>;<Digit>)
```

For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)
	
	See About the ENTER_PARAMETER Command to learn how to define the parameter name.
	
	If a parameter name is not acceptable or <Enter> is pressed, an error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these types of legal identifiers.
	`Phase name (/ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name on the specified sublattice site of the given phase.
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>` Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>`

Syntax	LIST_PARAMETER
	Specify a numerical number as the degree for the phase parameter.

LIST_PHASE_DATA



This command is for the Gibbs Energy System (GES) module.

All data for a specific phase are written in a readable manner on screen. The thermochemical parameters listed for the phase are always in SI units.



For encrypted commercial databases you may not be able to use this command to list any phase data. However, this command can be used for listing some basic definitions (such as phase model and phase-constituents) for the specified phase, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Syntax	LIST_PHASE_DATA
Prompt	`Phase name: <Phase name>` Specify a phase name (if abbreviated, it should be unique).

LIST_STATUS

This command is for the Gibbs Energy System (GES) module.

Syntax	LIST_STATUS
	List the entered elements, phases and species with the status word. The command is included for system managers. Each element, species, phase and symbol has a set of status bits. The values of these bits are listed with this command. The bits are listed as hexadecimal, i.e. four bits are written as a hexadecimal number. Two hexadecimal numbers make a byte. In hexadecimal, 0 to 9 mean normal digits. A to F means values 10 to 15. The number `E4000000` has thus bit 1, 2, 3 and 6 equal to one. The bits are numbered starting with 1 for the most significant (leftmost) bit.

Element Status Word

Set the element status word (*Bit. Meaning*) if:

1. Element cannot be deleted (only vacancy and electron)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (cannot occur for an element)

Species Status Word

Set species status word (*Bit. Meaning*) if:

1. Species record for an element (each element has a species record)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if a species element is suspended)
5. Charged (inclusive OR of bit 6 and 7)
6. Negative charge

7. Positive charge
8. Vacancy
9. Component (by default the elements are the components)

Phase Status Word

Set phase status word (*Bit. Meaning*) if:

1. Ideal (no sublattices and no excess parameters)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if all constituents suspended)
5. Gas phase
6. Liquid phase
7. Solution phase
8. Only one constituent (in each sublattice)
9. Ions (inclusive OR of bit 10 and 12)
10. New ionic liquid model (charge balance handled internally)
11. Constituents cannot be added
12. External charge balance needed
13. Aqueous model
14. Charged species (ions)
15. Dilute entropy
16. Last calculation exceeded temperature range for any parameter
17. Kapoor-Frohberg-Gaye cell model
18. Turbo calculation used
19. Turbo calculation impossible
20. Turbo calculation illegal
21. Phase is not ideal
22. Current site fractions saved
23. This phase is the ordered part
24. This phase is the disordered part (bit 2 and 3 also set)

25. Shadow phase with diffusion data
26. Error in ionic model
27. Sometimes
28. CVM-SRO (short-range ordering) entropy expression
29. CVM initialization is made
30. Used to test quasi-chemical ordering model
31. Major constituents check even if no miscibility gap (ordering)
32. Hoch-Arpshofen model

Symbol Status Word

Set symbol status word (*Bit meaning*) if:

1. Constant
2. Variable
3. Function
4. Table
5. Value must not be amended
6. Undefined

LIST_SYMBOL

This command is for the Gibbs Energy System (GES) module.

List the symbols available in the current GIBBS workspace, which are defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) and used in TP-functions for the entered model parameters for various phases in the defined system.

For encrypted commercial databases you may not be able to use this command to list any retrieved symbol.

Syntax	LIST_SYMBOL
Prompts	`Name: <Symbol name>` Specify a symbol name (either as the full name of a defined symbol, or as the first few common characters of several symbols which have names starting with such common characters). Only those symbols that match this name are listed. Or press <Enter> for a list of all the symbols defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) for the current system, which are available in the current GIBBS workspace.
	`Output to screen or file /Screen/: <File name>` Specify the name of a simple-textual file in which the entered symbols shall be written in a readable manner (such a basic textual file can later on be opened and edited by any text editor). The default value is the screen (by pressing <Enter>).

READ_GES_WORKSPACE

This command is for the Gibbs Energy System (GES) module.

Workspace Files

The data saved into a `*.GES5` with SAVE_GES_WORKSPACE can be read back into the GIBBS workspace.

Syntax	READ_GES_WORKSPACE
	Enter a **File name** and specify the working directory where to save the file in the **Look in** field. Normally the default file-type in the **Files of type** field is the correct one for the GES workspace format. The saved *.GES5 files are unique for each CPU type, and therefore a file saved on one CPU type cannot be read and used on another CPU type.

READ_WORKSPACES



This command is used in both the POLY and GES (GIBBS) modules.

Workspace Files

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with SAVE_WORKSPACES. Such a *.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	`File name` is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3, otherwise type the whole POLY-file name.  A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters. A window opens so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. POLY3) cannot be changed. Click **Open** to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.
	When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type `READ,,` or `READ_WORKSPACE ,,`

RECOVER_START_VALUES

Syntax	RECOVER_START_VALUES
	Recovers the start values in equilibrium calculations.

REINITIATE

This command is for the Gibbs Energy System (GES) module.

All data in the stored GIBBS workspace are erased, and all variables are initiated to their default values.

Syntax	REINITIATE
Prompts	`Upper case only /Y/:` Press <Enter> to keep the default where the name of elements and species is in only UPPER case. Or choose N to have the elements with two letter names with the first letter in Upper case and the second in lower case. In upper case mode all input in lower case is automatically converted to upper case.
	`Lower temperature limit /298.15/: <Lowest T in K>` This value is used as the lower temperature limit when data are entered interactively.
	`Upper temperature limit /6000/: <Highest T in K>` This value is used as the upper temperature limit when data are entered interactively.
	`Default element reference state symbol index /1/: <1 or 2 or 3>` Specify a proper index for the default listing parameters (symbol), or press <Enter> to accept the preset index 1. The *index* is for defining the symbol printed in listings of parameters. The symbol can be: • `G`: the data are referred to Gibbs energy at a variable temperature (also called *Lattice Stability*). • `H298`: the data are referred to the enthalpy of the element at 298.15 K and 1 bar. • `H0` is the same as H298 but at the temperature 0 K. The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data must you set the index to get the correct symbol. Set the index value to 0 to get the symbol `G`, to 1 to get the symbol `H298` and to 2 to get `H0`.

SAVE_GES_WORKSPACE

This command is for the Gibbs Energy System (GES) module.

Workspace Files

The data used by the GES workspace can be saved in a file with a default extension `*.GES5`. The default file name is `RESULT.GES5` or equal to the one used in a previous READ_GES_WORKSPACE command.

Syntax	SAVE_GES_WORKSPACE
	Enter a **File name** and specify the working directory where to save the file in the **Save in** field. Normally the default file-type in the **Files of type** field is the correct one for the GIBBS workspace format. The output is not formatted and cannot be printed.

SAVE_WORKSPACES



This command is available for both the POLY and GES (GIBBS) modules.

Workspace Files

You can save the current status and workspaces, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on a *.POLY3 file. The workspaces are saved to a file with this command. This is useful so you have access to the workspace for later use or when you need to terminate the current Console Mode session.

- In the Gibbs (GES) module workspace, all thermochemical data are stored.
- In the POLY module workspace, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GES workspace.
- When you are in a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings are saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called `POT.POLY3` ; the POURBAIX module saves a file called `POURBAIX.POLY3` and so forth.



After a SAVE_WORKSPACES command, you can always come back to exactly the state you had when you issued the command by giving a READ_WORKSPACE command. For example, after saving the POLY and GIBBS workspaces to a file, you can leave the program and at a later time READ the file and continue from the saved state.

Important Information About Map and Step Commands



A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Syntax	SAVE_WORKSPACES
Options	A `file name` must be specified. The default extension of the POLY workspace file is *.POLY3 but you can have any other file extension.  Linux and Mac are case sensitive so ensure you enter `.POLY3`. A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** cannot be changed. If there is already a file with the same file name under the directory a warning message displays. Click **OK** to overwrite the current POLY or GIBBS workspace onto the existing file. Click **Cancel** to return to the module. You can use the SAVE command with an unspecified name (i.e. through `SAVE , , ,` command-sequence) to save the POLY or GIBBS workspace.  When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Console Mode session or in a previous run (which is READ into the current POLY3 workspace), you can type `SAVE, , Y` or `SAVE_WORKSPACE , , y`. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.

SET_R_AND_P_NORM

The value of the gas constant (R) is used to define the energy units that are used for input of data. On output, all data are in SI units. The value of the pressure 1 atm is used to interpret values of the pressure given by application programs.

Syntax	SET_R_AND_P_NORM
Prompts	`Value of gas constant in your energy units /8.31451/: <New value>` The default value of the gas constant is in SI units (i.e. 8.31451). If you change this value, it only affects the interpretation of energy data given interactively from the terminal, e.g. if the value is set to 1.98717 you can give values in Calories.
	`Value of one bar in your presure units /100000/: <New value>` The value of the pressure given in application programs is divided by this value and then multiplied with the value of one bar expressed in Pascal before it is used inside the GIBBS module.

SCHEIL Module Commands

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BCC_TO_FCC_TRANSFORMATION

This command is for the SCHEIL module.

Use this command to allow transformations in the solidified part of the alloy caused by each of the components specified to be fast diffuser.

It is recommended that you only select this for steels.

Syntax	BCC_TO_FCC_TRANSFORMATION
Prompt	`Allow bcc → fcc ? /N/` Enter Y to allow transformations.

EVALUATE_SEGREGATION_PROFILE

This command is for the SCHEIL module.

Use this command in order to evaluate a segregation profile while performing the Scheil calculation. The Scheil calculation itself does not contain a spatial dimension. However, if it is assumed that the molar volume is constant and equal for all elements, and if a length is provided over which solidification occurs (for example the secondary dendrite arm spacing) then the generated profile corresponds to the segregation that would be obtained under the assumptions of a Scheil calculation. The grid is then equidistant and can be used as input for a DICTRAsimulation.

The generated text file contains, on each line, the mole fractions of all elements in alphabetical order at a certain grid point. If the composition is the same on several consecutive lines it means that the composition of the then remaining liquid has reached a state in which there are no degrees of freedom.

Syntax	EVALUATE_SEGRATION_PROFILE
Prompt	`Evaluate segregation profile? /N/` If the answer is Y, a segregation profile will be evaluated and saved to disc. Note that this feature is not supported with back diffusion; if back diffusion is enabled no segregation profile will be generated.
	`Number of grid points /100/` Enter the number of grid points for the segregation profile. A file dialogue window opens and allows you to specify the name of the file in which the segregation profile is written. In a macro file it is possible to enter all arguments on a single line, e.g. `EVALUATE_SEGREGATION_PROFILE Y 100 XF.TXT`, meaning that the segregation profile is evaluated over 100 grid points and saved to a file (XF.TXT) in the current working directory.

GLOBAL_MINIMIZATION

This command is for the SCHEIL module.

ADVANCED_OPTIONS for information about that GLOBAL_MINIMIZATION command.

Syntax	GLOBAL_MINIMIZATION
Prompt	`Use global minimization? /N/` The default (N) does not use global minimization. If you choose Y, the global minimization is done when possible (depending on the conditions setting), and a global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

LIQUID_PHASE_NAME



This command is for the SCHEIL module.

Use this command to use the liquid phase name from the database definitions or enter another phase name.

Syntax	LIQUID_PHASE_NAME
Prompt	`Liquid phase name /Default/` Default selects the liquid phase from the database definitions, otherwise enter a phase name.

SAVE_FILE_NAME



This command is for the SCHEIL module.

Use this command to save the file. The files get the console number added to this name, e.g. `005.->Scheil_006.POLY3 and Scheil_segregation_profile.txt`).

Syntax	SAVE_FILE_NAME
Prompt	Name of files to be saved, POLY and segregation profiles.  Linux and Mac are case sensitive so ensure you enter `.POLY3`.

SET_NUMERICAL_LIMITS



This command is available for the POLY, Scheil and ED-EXP modules.

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`Maximum number of iterations /500/:` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`Required accuracy /1E-6/:` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`Smallest fraction /1E-12/:` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is `1E-12` for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30` (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system).
	`Approximate driving force calculation for metastable phases /Y/:` Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. By default, the metastable phases are included in all iterations but these may not have reached their most favorable composition and thus their driving forces may be only approximate.

Syntax	SET_NUMERICAL_LIMITS
	If it is important that these driving forces are correct, choose N to force the calculation to converge for the metastable phases. This may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.

SOLUTE_TRAPPING

This command is for the SCHEIL module.

About the Scheil-Gulliver Solidification Simulations

The SOLUTE_TRAPPING command enables solute trapping. Once enabled, there are additional prompts and settings that are included and described with the START_WIZARD command.

Syntax	SOLUTE_TRAPPING
Prompt	`Consider solute trapping in primary phase? /N/` The default (N) does not use solute trapping. If you choose Y, then solute trapping is used. When the USE_BACK_DIFFUSION command is enabled, the SOLUTE TRAPPING command is automatically disabled (set to N).

START_WIZARD

This command is for the SCHEIL module.

About the Scheil-Gulliver Solidification Simulations

Use this command to use the START_WIZARD with step-by-step prompts to create a Scheil simulation.

You are prompted for settings including the major element or alloy, composition input in mass (weight) percent, the alloying elements, the temperature, fast diffusing components, and whether any phase should have a miscibility gap check. There are additional prompts included in the Start Wizard if USE BACK DIFFUSION or SOLUTE TRAPPING commands are set to `Yes` to enable back diffusion and solute trapping, respectively.

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

Use the other commands to make changes to settings that are not included in this wizard.

- BCC_TO_FCC_TRANSFORMATION
- EVALUATE_SEGREGATION_PROFILE
- GLOBAL_MINIMIZATION
- LIQUID_PHASE_NAME
- SAVE_FILE_NAME
- STORED_COMPOSITION_TYPE
- TEMPERATURE_STEP
- TERMINATION_CRITERIA

If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command INPUT_SCHEIL_PROFILE. Press F1 to search the online help.

Syntax	START_WIZARD
Prompt	The following is a list of the prompts. Press <Enter> to accept the defaults that are shown between the forward slashes (*/default/*). `Database /<Default>/:` The available thermodynamic database and its version are available to enter (based on license). Enter `?` for a list.

Syntax	START_WIZARD

`Major element or alloy:`

The major element in the system, e.g. Fe for a steel.

`Composition input in mass (weight) percent? /Y/:`

Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Enter `Y` for mass percent and `N` for mole percent.

`1st alloying element:`



You can specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element. For example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

You can directly specify mass or mole percent after the name (for example, enter `Cr 5`). If this is not specified, then you are prompted to enter it separately.

`Mass (weight) percent /1/`

`2nd alloying element:`

Specify the other alloying elements in the same way as you specify the first (for example, `c 1`).

`Mass (weight) percent /1/`

`Next alloying element:`

After you have specified your last alloying element, press <Enter> when requested to specify the next element. This ends the process of defining the bulk composition of the alloy system.

`Temperature (C) /2000/:`

Enter a value for the temperature in degrees C (Celsius) . This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

Decide which phases (if any) to reject at the `Reject phase(s)` prompt. Enter the name of the phases to reject or press <Enter> for `NONE`.

Decide whether to `Restore phase(s)`. You may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press <Enter> for `NONE`.

Then you are asked to confirm whether these phases should be retained in this system:

`OK? /Y/:`

Press <Enter> to accept the default `Y` or type `N` and press <Enter>. Thermodynamic data about the alloy system you defined is retrieved from the database.

`Should any phase have a miscibility gap check? /N/:`

If you answer `Y`, you are prompted to specify the `Phase with miscibility gap`. Answer with a solution phase name(s) (e.g. `FCC`) as well as the `Major constituents for sublattice` (for each sublattice site) (for this example, `Cr` is entered for sublattice 1 and `C` for sublattice 2).

Press Enter to specify another phase.

`Fast diffusing components: /None/:`

Enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.

Back Diffusion and Solute Trapping Settings

The following prompts are included with the Start Wizard at various points in the set up if the:

- USE_BACK_DIFFUSION command is set to `Y` to enable back diffusion
- SOLUTE_TRAPPING command is set to `Y` to enable solute trapping

Syntax	START_WIZARD

Back Diffusion settings	`Mobility Database /<Default>/:`
	
	The available mobility database and its version are available to enter (based on license). Enter `?` for a list.
	
	You then are shown a list of what phases are available for the database and the defined system and have the opportunity to reject or restore phases at the next prompts.
	
	`Reject phase(s) /NONE/:`
	
	`Restore phase(s): /NONE/:`
	
	Then you are asked to confirm whether these phases should be retained in this system:
	
	`OK? /Y/:`
	
	Press <Enter> to accept the default `Y` or type `N` and press <Enter>.
	
	`Temperature time dependence /LINEAR/:`
	
	Specify the type of temperature time dependence. Press <Enter> to accept this default.
	
	An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.
	
	  LINEAR is the only option and it corresponds to a constant cooling rate.
	
	`Cooling rate (K/s) /.1/:`
	
	Specify the cooling rate in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.
	
	`Expression for secondary dendrite arm spacing /CONSTANT/:`
	
	Secondary dendrite arm spacing is the distance in meters (m) between two secondary dendrite arms. Specify the type of secondary dendrite arm spacing by entering `CONSTANT` (the default) or `POWER_LAW`.
	
	An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation. Use
	
	• `CONSTANT` for a constant dendrite arm spacing. If you choose this, then enter a value for the `Secondary dendrite arm spacing (m) /5E-05/:` prompt.
	• `POWER_LAW` in the form `c*(cooling rate)^-n` where `c` and `n` are entered in the next prompts. If you choose this, then enter a value for the `Exponent n /.33/:` and `Scaling factor c /5E-05/:`
	
	`Primary phase /AUTOMATIC/:`
	
	The primary phase is the phase where the back diffusion takes place.
	
	If `Automatic` is selected (or kept as the default), the program tries to find the phase which gives

Syntax	START_WIZARD
	the most back diffusion. To override this setting, choose a specific primary phase from the list. For back diffusion, only phases with diffusion data can be used as primary phases.

Solute Trapping settings	`Expression for solidification speed /SCANNING_SPEED_AND_ANGLE/:`
	SCANNING_SPEED_AND_ANGLE is currently the only available option. It is calculated as scanning speed * cos(alpha) where scanning speed and the angle alpha are given by the user.
	Decreasing the value moves the result toward a Scheil-Gulliver calculation.
	`Scanning speed (m/s) /1/:`
	Enter the Scanning speed to calculate the solidification speed, Vs = $V_{scanning}$ * cos(α) m/s, where $V_{scanning}$ is the user specified scanning speed.
	`Alpha (degrees) /45/:`
	Enter an Alpha value in degrees, which is the alpha angle, α, between the solid/liquid boundary and scanning direction.
	`Primary phase /AUTOMATIC/:`
	If `Automatic` is selected (or kept as the default), the program tries to find the phase which gives the most solute trapping. To override this setting, choose a specific primary phase from the list. For solute trapping, only phases that dissolve all elements in the system can be used as primary phases.

TEMPERATURE_STEP



This command is for the SCHEIL module.

Use this command to define a temperature step.

Syntax	TEMPERATURE_STEP
Prompt	`Set temperature step (C) /1/`

TERMINATION_CRITERIA



This command is for the SCHEIL module.

Use this command to define the termination criteria for the fraction of liquid or temperature.

Syntax	TERMINATION_CRITERIA
Prompts	`Fraction of liquid or Temperature (F or T)? /F/`
	`Fraction of liquid /.01/`

USE_BACK_DIFFUSION

This command is for the SCHEIL module.

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

About the Scheil-Gulliver Solidification Simulations

The USE_BACK_DIFFUSION command enables back diffusion in the solid primary phase. Once enabled, there are additional prompts and settings that are included and described with the START_WIZARD command.

Syntax	USE_BACK_DIFFUSION
Prompt	`Use back diffusion? /N/` The default (`N`) does not use back diffusion. If you choose `Y`, then back diffusion is used. When the SOLUTE TRAPPING command is enabled, the USE_BACK_DIFFUSIONcommand is automatically disabled (set to `N`).

PARROT Module Commands

The PARROT Module in the *Data Optimization User Guide*.

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About the ENTER_PARAMETER Command



For the PARROT Module, this command is the same and is described here. See ENTER_PARAMETER for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered (see Gibbs Energy System (GES) Commands). The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

How to Define a Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy>
<keyword Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;
- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;

- <xxx> and <yyy> are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- <keyword Y or N> is the indicator on if there is continuation for the parameter expression or not;
- <zzz> is the reference index/number for the assessment of this parameter;
- The exclamation point ! is used to indicate that the current parameter definition is ended.

Parameter Name

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- G(GAS,C1O2): The Gibbs energy of formation of a CO_2 molecule in gas.
- G(FCC,FE:VA): The Gibbs energy of formation of fcc Fe with interstitials.
- L(LIQ,Fe,Cr;0: The regular solution parameter for Fe and Cr in liquid.
- L(LIQ,Fe,Cr;1): The sub-regular solution parameter.
- TC(BCC,Fe:Va): The Curie temperature of bcc Fe.
- BMAGN(BCC,Fe:Va): The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- G: Standard energy parameter (Gibbs energy of formation) or for interaction parameters;
- L: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;
- TC: Curie temperature for magnetic ordering;
- BMAGN or BM: Bohr magneton number for magnetic ordering (or Born function ωPr,Tr for aqueous solute species).
- VO: Molar volume at 298.15 K and 1 bar (a numeric value only);

- VA: Integrated thermal expansivity; $\int_{298.15}^{T} \alpha(T)\mathrm{dT}$
- VC: High-pressure fitting parameter;
- VK: Isothermal compressibility.



For more information about the high pressure volume, see X.-G. Lu, M. Selleby, B. Sundman, "Implementation of a new model for pressure dependence of condensed phases in Thermo-Calc", Calphad. 29, 49–55 (2005).



When necessary quantities as H (enthalpy), S (entropy), V (Volume), F (Helmholtz energy), etc., can be calculated from the Gibbs energy.

Phase Name

Specifying the PHASE NAME in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognizes uppercase phase names. It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, LIQUID:L,SLAG:L, IONIC-LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name when ENTER_PARAMETER is executed.

Constituent Array

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).



Solution phases with sublattices can have interacting constituents in each sublattice.

Interaction Parameter

An interaction parameter, which is used to describe the excess term of a quantity, must have two or more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands LIST_PARAMETER or LIST_PHASE_DATA). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12,AL,NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the `FCC_L12` solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk * is calculated with the term of [1∑y(specified constituents)], which implies that in an A-B binary system these `L` parameters are identical (but in higher-order systems, these are different):

- `L(phase,A,B)` is multiplied with X(A)*X(B)
- `L(phase,A,*)` is multiplied with X(A)*(1-X(A))
- `L(phase,B,*)` is multiplied with X(B)*(1-X(B))

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

AMEND_PARAMETER

This command is for the PARROT module.

There is also a Gibbs (GES) module command with the same name.

Interactively modify the TP-function(s) for a specific parameter for a phase with this command. This is useful in order to correct typing errors because the old function is made available for interactive editing on the terminal.

Syntax	AMEND_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct parameter name. If a parameter name is not acceptable or <Enter> is pressed, the error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these types of legal identifiers ▶ ENTER_PARAMETER
	`Phase name (ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name.
	`Interacting constituent (In sublattice # /XYZ/): <Species name>` Specify the interacting constituent name; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If there is more than one interacting constituent, specify these; otherwise press <Enter>.
	`Degree /#/: <Degree>` Specify a numerical number as the degree of the phase parameter.

	After the parameter name is specified correctly, the program lists its current definition (either preset in database or defined by the ENTER_PARAMETER command), such as:
	`L(PHASE2,AL,MG;1)=`
	`298.15<T<2000.00: +5000`
	`2000.00<T<4500.00: +4500`
	`4500.00<T<6000.00: +4000`
	You are prompted to change the parameter definition:
	`Do you want to change the number of ranges /No/:`

Syntax	AMEND_PARAMETER

	Enter Y to change the number of ranges for the chosen function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions
	
	If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> and the whole definition of the chosen parameter in all ranges (if any) is listed such as:
	
	`DIFFERENT FUNCTIONS IN THESE RANGES`
	`298.15<T<2000.00`
	`2000.00<T<4500.00`
	`4500.00<T<6000.00`
	
	This message prompts:
	
	`Do you want to change range limits /No/:`
	
	If there is more than one range, this question is prompted. Press <Enter>.

	`Range number (0 to exit) /0/: <Range number>` If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

	`Function`
	
	The previous function is available for editing. The editing is performed within the general subroutine `FOOLED`, as described in AMEND_SYMBOL. This routine prompts as follows:
	
	`1:+:>`
	
	The prompt consists of the current position in the string and the character at that position between colons, (::).
	
	Commands
	
	These commands can be given:
	
	• Help: `?`
	• Move CP to last or first character: `<+/-> A`
	• Delete characters from CP: `<+-#characters> D`
	• Exit: `E`
	• Find: `<#occurrences> F<string>@`
	• Insert: `I<string>@`
	• Move: `<+-#positions> M`
	• Restore string: `R`
	• Substitute: `S<OLD>@<NEW>@`
	• Type string: `T`
	
	Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.

Syntax	AMEND_PARAMETER
	 When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type `E` at the prompt.
	`Range number (0 to exit) /0/: <Range number>` Give a range number to edit that function, or press <Enter> or type `0` to exit this command.

AMEND_SYMBOL

This command is for the PARROT module.

The same command is also available for the Gibbs (GES) module.

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered with ENTER_SYMBOL) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.

The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with LIST_STATUS. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL

Prompts	`Name: <Symbol name>`
	Specify the name of an entered symbol.
	For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the `Parameter` keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:
	`FUNCTION VALUE  2.52500000E+01`
	`TABLE VALUE  1.56000000E+02`
	For variables and functions (or parameters), there are additional prompts and depend on the symbol type.

	For a variable, its current value is displayed, and you can change it to a new value:
	`Value /Current value/: <New value>`
	For a function (or a parameter entered as a symbol):
	`Do you want to change the number of ranges /No/:`
	Enter Y to change the number of ranges for the function, or change some of the temperature limits

Syntax	AMEND_SYMBOL

	in the definition, then retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.
	
	If you do not want to change it, press <Enter>. The definition of the chosen function in all ranges (if any) is listed, for example:
	
	`DIFFERENT FUNCTIONS IN THESE RANGES`
	`298.15<T<2000.00`
	`2000.00<T<4500.00`
	`4500.00<T<6000.00`
	
	and this message displays:
	
	`Do you want to change range limits /No/:`
	
	If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

	`Range number (0 to exit) /0/: <Range number>`
	`Function:`
	
	The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:
	
	`1:+:>`
	
	The prompt consists of the current position in the string and the character at that position between colons (::).
	
	## *Commands*
	
	These commands can be given:
	
	• Help: `?`
	• Move CP to last or first character: `<+/-> A`
	• Delete characters from CP: `<+-#characters> D`
	• Exit: `E`
	• Find: `<#occurrences> F<string>@`
	• Insert: `I<string>@`
	• Move: `<+-#positions> M`
	• Restore string: `R`
	• Substitute: `S<OLD>@<NEW>@`
	• Type string: `T`
	
	Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.
	
	  When the string is typed the character at the current position is replaced by an underscore _.

Syntax	AMEND_SYMBOL
	To finish the editing of the current function, type `E` at the prompt.

COMPILE_EXPERIMENTS

The descriptions of the experimental equilibria saved on a textual *.POP file, given as commands in the POLY and ED_EXP syntax, is compiled by this command into the PARROT structured data, i.e. stored into the current work *.PAR file which is created with CREATE_NEW_STORE_FILE, set by SET_STORE_FILE , or opened with READ_PARROT_WORKSPACES, all done before COMPILE_EXPERIMENTS.

This command also lists the compilation details on screen or onto a listing file (*.TXT).



If a syntax error in the commands is detected, the compilation is terminated. You need to correct the error in the *.POP file (using a textual editor) and recompile it with the *.PAR work (store) file.

After a successful compilation, the program translates all the experimental data points in the *.POP file into a graphical experimental data file (*.EXP) in the DATAPLOT syntax, which can be further edited and used as a graphical experimental data file (*.EXP) for the purposes of imposing onto calculated/plotted phase diagrams and/or property diagrams for comparisons during the assessment process.

- *DATAPLOT User Guide* included with this documentation set.

Syntax	COMPILE_EXPERIMENTS
	A window displays to open the original experimental data file (*.POP). Enter a *.POP **File name** box, and specify the working directory in the **Look in** box. Normally the default file-type in the **Files of type** field is the correct one for the experimental data format (i.e. *.POP file). Click **Open** or **Cancel** button as applicable.
Prompts	`Output to screen or file /Screen/: <*.pop file name>` A list of the source code in the *.POP file and error messages during compilation is written on screen (by pressing <Enter>) or on a list *.TXT file under a specific file name which can later on be opened and edited by any basic textual editor.
	`Initiate store file /Y/:` After a successful compilation, the data in the POLY workspace is stored as a new block of equilibria on the current work (store) file. By default the store file is initiated before compilation and only the compiled block is stored on the current work file (consequently, the *.PAR file is updated). A window displays to generate/store the graphical experimental data file (*.EXP) in the DATAPLOT syntax. Enter a *.EXP file name in the **File name** field and specify the working directory when opening the *.EXP file in the **Look in** field. Normally the default file type in the **Files of type** field is the correct one for the graphical experimental data format (i.e. *.EXP file). Click **Open** or **Cancel** as applicable. To keep the current work file, enter N.

CONTINUE_OPTIMIZATION



This command is for the PARROT module.

This command continues the optimization using the same Hessian matrix.



In some cases it is not possible to attempt continuation. For example, if the optimization has already converged or if the optimizing parameters or the set of experimental equilibria used in the current optimization runs are changed. The program gives a warning message if you try to continue when you make these changes.

Syntax	CONTINUE_OPTIMIZATION

Prompts	`Are you sure? /N/: <N or Y>`
	
	Prior to this question, a message displays to confirm if it is OK to continue:
	
	`It is safe to CONTINUE only after TOO MANY ITERATIONS and no change in variables and experiments ...`
	
	You can accept the default (N) in order to cancel this special attempt.

	`Number of iterations /N/: <Integral number of iteration>` Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT program tries this exact number of different sets of values of the optimizing variables without stopping the optimization even it would have converged earlier or should give up earlier.

CREATE_NEW_STORE_FILE



This file is hardware dependent and cannot be read by any text editor.

Create a binary file to be used as a *work file* (also called *store file*) before any optimization can be done. The workspace used by the GIBBS, POLY and PARROT modules is stored automatically on the work file but not any experimental information. The binary work file has a default extension of `PAR` under MS-Windows or `par` under Linux/UNIX.

A work file that is created at a previous run can be used in the PARROT module with the other command SET-STORE-FILE.

Syntax	CREATE_NEW_STORE_FILE
Prompt	<*.par file name> A **Save** window displays. Enter a **File name** and specify the working directory in the **Save in** field. Normally the default file-type in the **Files of type** field is the correct one for the PARROT workspace format (i.e. PAR file). Click **Save** or **Cancel** as applicable.

EDIT_EXPERIMENTS

Initialize and make available the sub-module for editing experimental equilibria, i.e. the ED_EXP module. All experimental equilibria compiled from the *.POP file can be accessed in the ED_EXP module.

The ED_EXP module is similar to the normal POLY module, but some commands are special and some POLY commands are not available. In the ED_EXP module, you can calculate each equilibrium separately or together, provide start values for equilibria which failed to converge, set weights, and modify the values of experiments or conditions.

Syntax	EDIT_EXPERIMENTS
	You are now in this submodule and can start using the commands.

- The first required command after entering the ED_EXP module for the first time (from the PARROT module GOTO MODULE ED-EXP) should always be READ_BLOCK in order to load the experimental data block from the current work *PAR-file for editing.
- The READ_BLOCK command must also be used prior to any other ED_EXP command if the module is reinitiated, or if no experimental data block is not previously read from a work file compiled with a proper experimental data .POP file, or if you want to change to another data block for editing.
- If any change is made in the ED_EXP module remember to use the command SAVE_WORKSPACE before going BACK to the PARROT module.



Although the TABLE_HEAD, COMMENT and FLUSH_BUFFER commands are visible in the ED_EXP module, these cannot be used here as these only work in a *.POP file (or *.DOP file for DICTRA).

ENTER_PARAMETER

This command is for the PARROT module.

There is also a Gibbs (GES) module command with the same name.

About the ENTER_PARAMETER Command

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command AMEND_PARAMETER.

Syntax	ENTER_PARAMETER

Prompts	`Parameter: <Parameter name>`
	As explained in About the ENTER_PARAMETER Command, specify a correct and complete `Parameter Name`, which should contain all the necessary parts of the general form:
	`<Identifier>(<Phase>,<Constituent array>;<Digit>)`
	If a parameter name is not acceptable or <Enter>, is pressed, a message displays:
	`*** Error, please re-enter each part separately`
	and you are prompted for input for each required part for a parameter name.

Options	**Description or Information**
`Identifier`	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`Phase name`	`Phase name (/ABCD/): <Phase name>` Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.
`Constituent`	`Constituent (in sublattice # /ABC/): <Species name>` A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated. It is the species name, not the stoichiometric formula required here. If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.
`Interacting constituent`	For phases with several sublattices, the program asks for one constituent in each sublattice.

Syntax	ENTER_PARAMETER
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name.  To cancel the default value of the interacting constituent type `NONE` or the name of another constituent. This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.
`Degree`	`Degree /#/: <Degree>` Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0`, `VA`, `VC` or `VK`). For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index. For a standard `G` parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.

`Phase parameter`	After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`Function: <Definition for a function>`
	A TP-Function consists of terms in T and P.
	`& <Continuation of the definition for the current function>`
	Continuation of a TP-Function definition.
	`High temperature limit /6000/: <High temperature limit in K>`
	Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the *lowest limit* is entered as a negative number) for the current TP-Function.
	`Any more ranges? /N/:`
	Enter Y for more function(s) or N to end this command.

LIST_ALL_VARIABLES



This command is for the PARROT module.

Create a list of the values and status of all variables in the PARROT workspace on screen or in a text file. After an optimization some statistical information is also written. The correlation matrix is written if that option is chosen.

- SET_OUTPUT_LEVELS.

Syntax	LIST_ALL_VARIABLES
Prompt	`Output to screen or file /Screen/: <File name>` A list of the current values and status, as well statistical information (if after optimization) and the correlation matrix (optionally), for all variables is written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.

Example

The following is the listed variables for the example TCEX36, after the first optimization when having set all variables available for optimization.

```
== OPTIMIZING VARIABLES ==
AVAILABLE VARIABLES ARE V1  TO V00
VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      2.03729090E+04    2.03688352E+04    2.03688352E+04    3.41524152E+00
V2     -2.94286372E+01   -2.94286372E+01   -2.94286372E+01    2.37944771E+00
V11    -2.17373936E+04   -2.18095983E+04   -2.18095983E+04    3.97086303E-02
V12     1.52107184E+01    1.51660547E+01    1.51660547E+01    5.84552327E-02
V15     2.42082351E+04    2.45139169E+04    2.45139169E+04    5.00914471E+00
V16    -8.38723972E+00   -8.83460472E+00   -8.83460472E+00    1.60961318E+01
V17     3.08916533E+03    3.15802558E+03    3.15802558E+03    9.63738108E+00
V19     2.20292586E+04    2.21385673E+04    2.21385673E+04    4.14274011E+01  V20    -
7.04217974E+00   -7.22424882E+00   -7.22424882E+00    1.00561540E+02
NUMBER OF OPTIMIZING VARIABLES :   9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   8.00002729E+04 TO   8.00002719E+04
DEGREES OF FREEDOM   45.  REDUCED SUM OF SQUARES   1.77778382E+03
```

LIST_CONDITIONS



This command is for the PARROT module.

Use this command to generate a list of the current values of optimization conditions, as well the current status of listing, either on screen or in a basic text file which can be opened and edited by a text editor.

Syntax	LIST_CONDITIONS
Prompt	`Output to screen or file /Screen/: <File name>` Press <Enter> to output to screen or on the list file under a specific file name.

LIST_PARAMETER

This command is for the PARROT module.

There is also a Gibbs (GES) module command with the same name.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

```
The parameter name: <Identifier>(<Phase>,<Constituent array>;<Digit>)
```

For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)
	
	See About the ENTER_PARAMETER Command to learn how to define the parameter name.
	
	If a parameter name is not acceptable or <Enter> is pressed, an error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these types of legal identifiers.
	`Phase name (/ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name on the specified sublattice site of the given phase.
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>` Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>`

Syntax	LIST_PARAMETER
	Specify a numerical number as the degree for the phase parameter.

LIST_PHASE_DATA



This command is for the PARROT module.

List all the phase from the Gibbs (GES) module for a specific phase. These are displayed on screen. The thermochemical parameters listed for each phase are always in SI units.

Syntax	LIST_PHASE_DATA
Prompt	`Phase name: <Phase name>` Specify a phase name.

LIST_RESULT



This command is for the PARROT module.

List the result of the current optimization run on screen or in a specified file. The level of detail listed can be prescribed by the command SET_OUTPUT_LEVELS.

The LIST_RESULT command has an option `G` for creation of an experimental data file with two columns, one for the experimental value and the other for the calculated value. It allows plotting a diagram and visualizing the fitting results. The plot is automatically plotted and you can scale it giving commands in the POST module. The option `D` lists all experiments, including those with fulfilled inequalities which are suppressed with the default option `C`.

Syntax	LIST_RESULT
Prompt	`Full, Condensed, Detailed or Graphic format: /C/: <C or D or F or G>`
	Choose a format. • The `F` (full) format is obsolete but retained for backward compatibility. • `C` (condensed) is the default. • `D` (detailed) lists all experiments, including those with fulfilled inequalities (not included with the default condensed file). • The `G` (graphical) format creates an experimental data file containing two columns, one with the experimental value and the other with the calculated value. This allows plotting of a diagram where all symbols should be on the diagonal if the fit is perfect. The plot is automatically plotted and you can scale it giving commands in the POST module. `Output to screen or file /Screen/: <File name>` A list of the current optimization results are written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.
	The output normally consists of these parts: • A title showing the data of the action; • A message on successful optimization with the iteration number in the last optimization; • A paragraph describing the optimization condition; • A list of the latest set of optimized and fixed variables; • A paragraph describing the optimization quality (some statistical information); • A correlation matrix for all optimizing variables (optionally shown, pre-set by the SET_ OUTPUT_LEVELS command); • A list of all parameters (including their symbol names, status and current values or function expressions), and all phase descriptions (including phase name, model names, constituents, and phase's `G/L/TC/BM` expressions) predefined for each phase in the system (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A paragraph describing the alternate equilibria (and possible error during optimization);

Syntax	LIST_RESULT
	• A detailed list on all the equilibrium points used in the current optimization. If the alternate-mode is used in the optimization, only an error value is shown. For normal-mode calculations, a list is shown for the experimental equilibrium numbers (first column) and corresponding original experimental data (second column, in the form `quantity = value`) which are used in optimization (i.e. non-zero weighted points). Such experimental data are by each point compared by the calculated value (third column) after the last optimization. Also listed are the experimental error (column 4), the difference between the calculated value and original experimental data (column 5), and the contribution to the sum of least square (column 6).

Example

The following is the listed result after the first optimization based on the prescribed definitions in the TCEX36a.TCM and TCEX36b.TCM, but having set all variables available for optimization.

```
=====================================================

           OUTPUT FROM P A R R O T.

*** SUCCESSFUL OPTIMIZATION. ***      NUMBER OF ITERATIONS:  10

== OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N

   MINIMUM SAVE ON FILE: Y

   ERROR FOR INEQUALITIES =  1.00000000E+00

   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04

ARGUMENTS FOR SUBROUTINE VA05AD (HSL)

   MAXFUN =   1   DMAX =  1.00000000E+02   H =  1.00000000E-04    ACC = (INITIAL
SUM OF SQUARES) *  1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV

V1      2.03749463E+04    2.03729090E+04    2.03729090E+04    3.41455863E+00

V2     -2.94286372E+01   -2.94286372E+01   -2.94286372E+01    2.37944774E+00

V11    -2.17395673E+04   -2.17373936E+04   -2.17373936E+04    3.98405298E-02

V12     1.52107184E+01    1.52107184E+01    1.52107184E+01    5.82861832E-02

V15     2.42106560E+04    2.42082351E+04    2.42082351E+04    5.07239609E+00

V16    -8.38723972E+00   -8.38723972E+00   -8.38723972E+00    1.69546796E+01

V17     3.08947424E+03    3.08916533E+03    3.08916533E+03    9.85220694E+00
```

```
V19     2.20314615E+04    2.20292586E+04    2.20292586E+04    4.16329629E+01  V20
-7.04217974E+00   -7.04217974E+00   -7.04217974E+00    1.03161466E+02

NUMBER OF OPTIMIZING VARIABLES :   9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM   8.00002719E+04 TO   8.00002709E+04

DEGREES OF FREEDOM   45.  REDUCED SUM OF SQUARES   1.77778380E+03

Number of alternate equilibria           14

SYMBOL        STATUS   VALUE/FUNCTION

R         80000000  8.3145100E+00

RTLNP     20000000 +R*T*LN(1E-05*P)

V1        48000000  2.0374946E+04

V2        48000000 -2.9428637E+01

V11       48000000 -2.1739567E+04

V12       48000000  1.5210718E+01

V15       48000000  2.4210656E+04

V16       48000000 -8.3872397E+00

V17       48000000  3.0894742E+03

  21 V19       48000000  2.2031462E+04   22 V20       48000000 -7.0421797E+00

LIQUID

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T

      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T

      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T       L(LIQUID,A,B;1) =
500.00<T< 2000.00: +V13+V14*T

A2B

  2 SUBLATTICES, SITES  2:  1     CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =

             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

BCC

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 0.0

      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: 0.0

      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T

      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T

FCC
```

```
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B
      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T
======  BLOCK NUMBER  1
DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
Alternate equilibrium calculation                  0.4183
Alternate equilibrium calculation                  0.1932
Alternate equilibrium calculation                  0.1016
Alternate equilibrium calculation                  1.4354E-03
Alternate equilibrium calculation                  2.5063E-02
Alternate equilibrium calculation                  8.3929E-03
Alternate equilibrium calculation                   141.4
Alternate equilibrium calculation                   141.4
Alternate equilibrium calculation                   141.4
Alternate equilibrium calculation                   141.4
Alternate equilibrium calculation                  1.2532E-03
Alternate equilibrium calculation                  5.4781E-04
Alternate equilibrium calculation                  1.5404E-03
Alternate equilibrium calculation                  1.2702E-03
ACR(B)=9.4E-1               0.9397      2.85E-02 -2.7745E-04 -9.7472E-03
ACR(B)=8.4E-1               0.8395      2.82E-02 -4.9038E-04 -1.7396E-02
ACR(B)=7.4E-1               0.7407      2.81E-02  7.3804E-04  2.6305E-02
ACR(B)=6.4E-1               0.6424      2.81E-02  2.3935E-03  8.5272E-02
ACR(B)=5.4E-1               0.5434      2.82E-02  3.4449E-03  0.1220
ACR(B)=4.4E-1               0.4428      2.85E-02  2.8265E-03  9.9024E-02
ACR(B)=3.4E-1               0.3394      2.90E-02 -5.8174E-04 -2.0040E-02
ACR(B)=2.3E-1               0.2320      2.97E-02  2.0260E-03  6.8208E-02
ACR(B)=1.2E-1               0.1194      3.06E-02 -6.4192E-04 -2.0981E-02
HMR(LIQUID)=-1964           -1957.      5.00E+02   7.439      1.4878E-02
HMR(LIQUID)=-3500           -3478.      5.00E+02   21.67      4.3338E-02
```

HMR(LIQUID)=-4588	-4565.	5.00E+02	22.69	4.5382E-02	
HMR(LIQUID)=-5239	-5217.	5.00E+02	21.50	4.3008E-02	
HMR(LIQUID)=-5454	-5435.	5.00E+02	19.11	3.8216E-02	
HMR(LIQUID)=-5233	-5217.	5.00E+02	15.50	3.1008E-02	
HMR(LIQUID)=-4575	-4565.	5.00E+02	9.691	1.9382E-02	
HMR(LIQUID)=-3481	-3478.	5.00E+02	2.669	5.3385E-03	118
HMR(LIQUID)=-1950	-1957.	5.00E+02	-6.561	-1.3122E-02	

LIST_STORE_FILE



This command is for the PARROT module.

Use the LIST_STORE_FILE command to display the name of the store file and its full path.

LIST_SYMBOL_IN_GES

This command is for the PARROT module.

Lists TP-function(s) for the entered model parameters for phases in the system on screen. In many cases, the optimizing variables are parts of the TP-functions which in turn are entered in model parameters for various phases in the GIBBS workspace.

This command is a way to find out how the functions depend on the optimizing variables. In the PARROT module the list is only shown on screen, not written to any file (which the LIST_SYMBOL command in the GIBBS module does).

Syntax	LIST_SYMBOL_IN_GES
Prompt	`Name: <Symbol name>` Specify a symbol name. Only those symbols that match this name are listed. Or press <Enter> for a list of all available symbols entered in the system.

OPTIMIZE_VARIABLES

This command is for the PARROT module.

Perform variable optimization. All system-definition data needed for the optimization is read from the current work file (*.PAR). The result of the optimization is automatically stored in the current work file.

Syntax	OPTIMIZE_VARIABLES
Prompt	`Number of iteration /N/: <Integral number of iteration>` Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT module tries this number of different sets of values of the optimizing variables unless it has converged earlier, or has given up earlier.
	It initially takes a small step in each variable to find the steepest slope. You can give zero iteration to calculate the error in all selected experiments, and then use LIST_RESULT to check how good (bad) the current fit is.

READ_PARROT_WORKSPACES

This command is for the PARROT module.

Workspace Files

Read the previous PARROT/GIBBS/POLY workspaces back to replace the current PARROT/GIBBS/POLY workspaces. It is useful if late changes made through various PARROT/GIBBS/POLY commands are not satisfactory.

Syntax	READ_PARROT_WORKSPACES
	The previous PARROT/GIBBS/POLY workspaces are always associated with the latest action to either open a work file by SET_STORE_FILE, or to create a work file by CREATE_NEW_STORE_FILE (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file), or to update the work file by SAVE_PARROT_WORKSPACES.
	Unlike the READ commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to read a previously opened/created/updated PARROT/GIBBS/POLY workspaces, for the reason described above.
	You cannot use this command if there is no work file opened or created already.

RECOVER_VARIABLES

The RECOVER_VARIABLES command is used to set back the values of all variable to the start values.

REINITIATE



This command should not be used unless you want to destroy the current PARROT workspace. However, this PARROT command does not reinitiate the GIBBS/POLY3 workspaces.



This command is for the PARROT module.

The REINITIATE command is used to reinitiate the workspace used by PARROT. All output and optimizing conditions are given their default values. All variables are set fixed with their value equal to zero.

RESCALE_VARIABLES

When using the RESCALE_VARIABLES command, the current values of all the parameters are copied to their start values and the scaling factors for further optimization. Thus it should be done now and again, in particular if you think the optimization results are improved after the previous run(s), or if any variable changes more than a factor of 10.

SAVE_PARROT_WORKSPACES

This command is for the PARROT module.

If the latest changes made through various PARROT/GIBBS/POLY commands are as required, use this command to save the current workspace (i.e. data area) used by the PARROT program (also including the current GIBBS and POLY workspaces), onto the present work *.PAR file which has already been opened by SET_STORE_FILE or been created by CREATE_NEW_STORE_FILE (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file).

The PARROT/GIBBS/POLY workspaces are updated after each PARROT/GIBBS/POLY command. This means the current PARROT/GIBBS/POLY workspaces are always updated onto the latest work *.PAR file that is associated with the latest SET_STORE_FILE or CREATE_NEW_STORE_FILE command.

Workspace Files

Syntax	SAVE_PARROT_WORKSPACE
	Unlike the SAVE commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to save the current PARROT/GIBBS/POLY workspaces, for the reason described above. You cannot use this command if there is no work *.PAR file opened or created already.

SET_ALTERNATE_MODE

Turn the alternate mode on or off.

With the ALTERNATE mode is possible to include functions to be evaluated together with an alternate calculation and to select ALTERNATE mode for each experimental equilibrium.



The alternate mode is described in About Alternate Mode. It should be used only to optimize start values of the model parameters in the beginning of the assessment.

Syntax	SET_ALTERNATE_MODE
Prompt	`On /Y/:` By default alternate mode is ON.

SET_EXTERNAL_PARAMETER

This command is for the PARROT module.

Optimize model parameters of the so-called external models, which may not be as fully-implemented/integrated parts inside the GIBBS system and thus are independently defined within user-specified/written source codes. This command makes links between the PARROT optimizing variables and external model parameters.

In order to be able to build the specified external model and to use this SET_EXTERNAL_PARAMETER command, it requires you to first write codes for a preferred external model (as it is not within the standard GIBBS system of the Thermo-Calc software) and then provide it to a consultant at Thermo-Calc Software AB for the purpose of including the external model in a separate DLL that is interactively connected to the software. For more information, see theConsultancy page on our website.

Syntax	SET_EXTERNAL_PARAMETER
Prompt	`External name: <Parameter name in the external model>` Correctly specify the parameter name defined within a specified/written external model.

	`As optimizing variable number: <n>`
	Give the number of the PARROT optimizing variable, which should have a unique link to the specified parameter name of the external model.
	For example, @@ Link PARROT variables to CAM parameters:
	`SET-EXTER-PAR GT(SLAG_A,O-2,SI+4,CA+2) 1`
	`SET-EXTER-PAR ET(SLAG_A,O-2,SI+4,CA+2) 2`
	`SET-EXTER-PAR EXT(SLAG_A,O-2,SI+4,CA+2) 3`

SET_FIX_VARIABLE

Prescribe a fixed value to a variable. The variable is considered as a constant at the optimization, usually after successful optimization runs for some specific variables (for some of the phases in the system). Such fixed variables can also be set back for further optimization run by using SET_OPTIMIZING_VARIABLE.

Syntax	SET_FIX_VARIABLE
Prompts	`Variable number: <Variable number(s)>` Specify the number of the variable. It is possible to give a range by giving two numbers with a hyphen in between (no spaces allowed), e.g. `1`. The parameters within the limits are set fixed to their current values (no question of values).
	`Start value /xxxx.xxxxx/: <A value to be fixed>` Specify a numerical value to be fixed for the selected variable (only when one variable number is specified at the previous prompt). The current value for the selected variable is shown as default. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values are used as fixed values.

SET_OPTIMIZING_CONDITION

This command is for the PARROT module.

Specify the conditions for the optimization. The default values are chosen automatically by the PARROT program, and in most cases these should not be changed.

The optimization stops when the sum of errors decreases by this value, even though it might be possible to increase it further with a new OPTIMIZE command.

Syntax	SET_OPTIMIZING_CONDITION
	`Relative standard deviation for experiments? /N/:` By default the standard deviation of the experimental determinations are absolute values. Enter Y if these are used as relative weighting factors. The estimated standard deviations of the optimized variables might be different for the two cases.
Prompt	`Min save on file? /Y/:` Specify whether the program should minimize the transfer of data to and from the current work file during the optimization: • If the default (N) is kept, the workspaces are stored on the current work file after every iteration in the optimization procedure. • Enter Y to speed up the optimization. After optimization use the SAVE_PARROT_WORKSPACES command to update the progress onto the current work file.
	`Relative step for calculation of derivatives: /1e-04/: <xxx>` In the calculation of the correlation matrix for equilibria with inaccuracy in the independent state variables, some numerical derivatives might have to be calculated. Specify the relative step (`xxx`) for the calculation of these derivatives.
	`Maxfun (va05ad): /100/: <n>` The maximum number of iterations in the optimization. The same value set by the OPTIMIZE command.
	`Dmax (va05ad): /100/: <n>` An estimate of the maximum distance between the start and the final values of the variables. A smaller value makes the program vary the parameters with smaller factors.
	`H (va05ad): /1e-04/: <xxx>` The step used in the scaled variables for calculating numerical derivatives during the optimization.
	`Acc/(initial sum of squares) (va05ad): /.001/: <xxx>` The break condition for the optimization. The accepted value is the difference between the true

Syntax	SET_OPTIMIZING_CONDITION
	minimum and the calculated one.

SET_OPTIMIZING_VARIABLE



This command is for the PARROT module.

Specify which variable value should be estimated at the optimization. Such a variable can have a value of zero or another start value, or is fixed by SET_FIX_VARIABLE prior to the previous optimization run.

For a good reference prior to this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as pre-entered in the *SETUP.TCM file or interactively entered in the GIBBS module) are obtained by using LIST_ALL_VARIABLES.

Syntax	SET_OPTIMIZING_VARIABLE
Prompts	`Variable number: <Variable number(s)>` Specify the number(s) for the variable(s) to be set. Any non-zero parameter within the range is allowed to be optimized. A parameter with a current value equal to zero must be specified explicitly here in order to be optimized. Specify a range by giving two numbers connected by a hyphen (no space allowed!), e.g. `2-8`. Under this circumstance, no question of start values are asked.
	`Start value /xxxx.xxxxx/: <A guess value>` Specify a start guess of the optimum value (only when one variable number is specified at the previous prompt). The current numerical value for the selected variable is shown as default.  This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values (as start values) are not changed.

SET_OUTPUT_LEVELS



This command is for the PARROT module.

Choose the type of information the PARROT module gives during the optimization procedure and when listing results.

Syntax	SET_OUTPUT_LEVELS
Prompts	`List increment /1/: <Increment in iteration number>` Specify the increment in iteration number for which information is listed on screen during the optimization. By giving a larger number it shortens the list.
	`List sum of squares: /Y/:` Choose whether the sum of squares is listed on screen during the optimization procedure.
	`List scaled variables: /Y/:` Choose whether the scaled variable values are listed on the terminal during the optimization procedure.
	`List weighted residuals: /N/:` Choose whether the weighted residuals are listed on the terminal during the optimization procedure.
	`List all parameters: /N/:` Choose whether all parameters in the models are listed in LIST_RESULT.
	`List correlation matrix: /N/:` Choose whether the correlation matrix of the variables are listed with the commands LIST_RESULT and LIST_ALL_VARIABLES.

SET_SCALED_VARIABLE

This command is similar to SET_OPTIMIZING_VARIABLE in that it specifies start values for optimizing variables. The difference being it is functional for only one optimizing variable at one time. It also prescribes a minimum and maximum value for the variable. During the optimization runs, the variable value is limited within this min-max range.

Such a variable may have a value of zero or another start value, or may be fixed by SET_FIX_VARIABLE prior to the previous optimization run. For a good reference prior to using this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as entered in the *SETUP.TCM file or interactively entered in the GIBBS module) is obtained by using LIST_ALL_VARIABLES.

Syntax	SET_SCALED_VARIABLE
Prompts	`Variable number: <Variable number(s)>` Specify the number for an optimizing variable to be set. Any non-zero parameter is allowed to be optimized, and a parameter with a current value equal to zero must be specified explicitly here in order to be optimized.
	`Start value /xxxx.xxxxx/: <A guess value>` Specify a start guess of the optimum value. The current numerical value for the selected variable is shown as default.  This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria.
	`Min value /xxxx.xxxxx/: <A guess value>` Specify a minimum guess of the optimum value. It should be smaller than, at least equal to, the current start value for the selected variable.
	`Max value /xxxx.xxxxx/: <A guess value>` Specify a maximum guess of the optimum value. It should be larger than, at least equal to, the current start value for the selected variable.

SET_STORE_FILE



This command is for the PARROT module.

Specify a store file (work file) to be used for compilation and optimization. The *.PAR work file must be created (CREATE_NEW_STORE_FILE) as a store file. The GIBBS, POLY and PARROT workspaces are read from the specified store file (with a default extension of PAR).

Syntax	SET_STORE_FILE
Prompt	Enter a `*.PAR file name` in the **File name** field and specify the working directory in the **Look in** field. Normally the default file-type in the **Files of type** field is the correct one for the PARROT workspace format (i.e. *.PAR file). Click **Open** or **Cancel** as applicable.

EDIT_EXPERIMENTS (ED_EXP) Submodule Commands



EDIT_EXPERIMENTS (ED-EXP) is a submodule of PARROT.

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ADVANCED_OPTIONS



This command is available with the POLY and ED-EXP modules.

ADVANCED_OPTIONS described for the POLY module.

Syntax	ADVANCED_OPTIONS
Prompt	`Which option? /Step_and_Map/:  <Option>`

CHANGE_STATUS

This command is available with the POLY and ED-EXP modules.

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the SUSPENDED or DORMANT phase-status. Another important applications is to calculate paraequilibria by setting some components to the SPECIAL component-status.

For a component and for a species, the status can be one of the following:

- `ENTERED`: the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED`: the component(s) or species are not considered in the calculation.
- `SPECIAL`: the specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).

Only component(s) can have the status SPECIAL, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_ STATUS command.

Syntax	CHANGE_STATUS
Prompts	`For phases, species or components? /Phases/: <Keyword>` *Keyword* = phase or species or components
	`Phase name(s): <Name(s) of the phase(s)>` For `phase` as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be assigned to the phases can also be given on the same line if preceded with an equal sign (=).

Syntax	CHANGE_STATUS
	An asterisk, *, can be used to denote all phases. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended phases. In the same way, *D means all dormant phases, and *E means all entered phases.
	Name(s): <Name(s) of the Species or Component(s)> For species or components as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of phase as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =. An asterisk, *, can be used to denote all species or components. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended species or components. In the same way, *E means all entered species or components.
	Status /Entered/: <New status> The new status to be assigned must be given. For species, the values ENTERED or SUSPENDED can be used. For the POLY module, using the Entered or Suspended status here has the same result as using the commands MAKE_COMPONENT_ENTERED and MAKE_COMPONENT_SUSPENDED. The exception is that any existing conditions that depend on a suspended component are removed when using the MAKE_COMPONENT_SUSPENDED command. For components, the status ENTERED, SUSPENDED or SPECIAL can be given. SPECIAL means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the *ufractions* or other normalized fractions of system components. For phases, the status ENTERED, SUSPENDED, DORMANT or FIXED can be given. DORMANT means the same as suspended but the driving force is calculated. FIXED means that it is a condition that the phase is stable at a certain amount. For example, for the ufractions, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status SPECIAL. This is assigned by the CHANGE_STATUS command: Change_Status comp C=special.
	Start value, number of mole formula units /0/: <Initial amount> For ENTERED phases, an initial amount of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.
	Number of mole formula units /0/: <Equilibrium amount> For FIXED phases, the equilibrium amount of the phase [always using an initial estimation being the NPF(phase) value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.

Syntax	CHANGE_STATUS

Note when specifying a FIXED phase status

Special attention should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below.

The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the CHANGE_STATUS command to set a relevant condition, e.g. `CHANGE_STATUS phase <phase>=fix <amount>` where the fixed <amount> is roughly the same as the F-suffixed quantity `NPF(phase)`.

The `NPF(phase)` quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other `F`-suffixed state variables [e.g. GF(phase), HF(phase) and DGF(phase)] cannot be directly applied in any POLY command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: `NPFabc = NP(abc)/NA` or `NPFabc = NPM(abc)/NA*N`. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1 NA = 1
FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1 NA = 1
BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3 NA = 1
SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18 NA = 30
```

If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modeled by the Two-Sublattice Ionic Liquid Model, i.e.:

```
IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q,7
```

then the evaluation of its NA value becomes even more complicated:

```
NA = p + q*yC2 + q*yN2 + q*yO2 + q*yFeO2 3/ 2
```

where the stoichiometric coefficients *p* and *q* are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

There is no strange thing when using a zero value [i.e. `0`] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.

However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations.

Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a

Syntax	CHANGE_STATUS
	liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. N=1). When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [NA>1; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF(phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper `NPF(ION_LIQ)` value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of N/[$p + q^{*}y$C2 + $q^{*}y_N$2 + $q^{*}y_O$22 + $q^{*}y_{FeO}$2 3/ 2].

Examples

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_Status comp C=special
```

The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statues:

- `ENTERED`: the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.
- `SUSPENDED`: the phase(s) are not considered in the equilibrium calculations.
- `DORMANT`: the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.

- `FIXED`: it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMMENT



This command is for the ED-EXP module.

The COMMENT command is only used in the *.POP/*.DOP files (so can be included with experimental data files) to write brief comments or descriptive information on a newly created equilibrium (experimental) data point or a set of points given in a table.

A comment can have a maximum of about 60 characters written on the same line.

COMPUTE_ALL_EQUILIBRIA

This command is for the ED-EXP module.

In ED_EXP and PARROT modules, each experiment is treated as an individual equilibrium with some measured values. These are created with CREATE_NEW_EQUILIBRIUM, and stored in an experimental data *.POP file and then compiled and saved in the POLY workspace of a PARROT work *.PAR file.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

With COMPUTE-ALL-EQUILIBRIA, all equilibria from the current to the last experimental points are calculated. If an equilibrium calculation fails, the calculation is stopped at that equilibrium. Equilibria with weight zero is skipped.

A current or present experimental point means the latest selected or calculated one. Once used the current point turns to the last point in the data block; in such a case you first use SELECT_EQUILIBRIUM so that the current point is switched to a desired one.

For this command there is always a list output on screen, which consists of six columns for all experimental points available in the current data block:

- The first column is the *equilibrium identifier* (a number) assigned by this command,
- the second the *data label* assigned with LABEL_DATA,
- the third the *number of iterations*,
- the fourth the *current weight*, and
- the fifth the *current temperature*.
- In the sixth column the *fixed stable phases* are listed together with any *comment text* given after a COMMENT in the *.POP or *.DOP file.

If the weight is zero for an equilibrium columns 3-5 are replaced by the text *<unused>*. If the alternate mode is used for some experimental points, the listing is slightly different for such points. The 3-4 columns are displayed with *alt*, instead. If an alternate calculation is failed at one experimental point, the point is automatically assigned with a zero weight, and a warning message is shown above the data line (with all six columns).

CREATE_NEW_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

During data-assessments using the ED_EXP module (a submodule of PARROT), you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

Syntax	CREATE_NEW_EQUILIBRIUM
Prompts	`Equilibrium number /2/: <A new equilibrium number>` Each equilibrium in the POLY workspace is identified by a unique integer number. Such an equilibrium number can be recalled with SELECT_EQUILIBRIUM.
	`Initiation code /2/:` When an equilibrium is created, you can choose to `ENTER` all components and phases (initiation code 2), `ENTER` the components only (initiation code 1) or `SUSPEND` everything (initiation code 0). No other values are legal. The entered components and phases can later be changed with CHANGE_STATUS.

DEFINE_COMPONENTS

This command is available with the POLY and ED-EXP modules.

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.

This implies a command REINITIATE_MODULE and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	`Give all new components / existing components/: <New components>` The `new components` must be specified all on one line. These replace the existing component definitions. The number of components cannot be changed with this command. Use CHANGE_STATUS instead.
	To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements. The new components do not have to be present as species.

DELETE_SYMBOL



This command is available with the POLY and ED-EXP modules.

Use the DELETE_SYMBOL command to remove symbols i.e. constants, variables, functions or tables.

Syntax	DELETE_SYMBOL
Prompt	`Name: <Name of a symbol>` Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.

ENTER_SYMBOL

This command is for the ED-EXP module.

The GES, POLY and POST modules also have a command with the same name.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Syntax	ENTER_SYMBOL
Prompt	`Constant, Variable, Function or Table? /Function/: <Keyword>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION` or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER_CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST. There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`Name: <Name of the symbol>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.

Syntax	ENTER_SYMBOL
	For different types of symbol (constant, function, variable or table), the questions have different prompts.

	`Function: <Definition for a function or variable>`
	
	Functions and *variables* are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).
	
	Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS` and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).
	
	Examples of function expressions:
	
	• `GM(LIQUID)`: The Gibbs energy of liquid per mole component
	• `H.T/4.184`: The heat capacity of the system in calories
	• `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
	• `T-273.15`: The temperature in Celsius
	
	`&: <Continuation of the definition for the symbol>`
	
	The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.

	`Value: <Value for a constant>` A *constant* can only be assigned a numeric value once.
	`Value or expression: <Value of expression for a variable>` A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

	`Variable(s): <Variable(s) in a table>`
	
	A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.
	
	Example:
	
	`ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)`
	
	Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.
	
	To show the temperature in Celsius in a table, give the command ENTER_FUNCTION `TC=T-273`; and then use the symbol `TC` in the table.
	
	`& <Continuation of the definition for the table>`
	
	The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press `<Enter>` again.

EVALUATE_FUNCTIONS

This command is available with the POLY and ED-EXP modules.

The value of one or more or all entered functions or variables are evaluated and listed.

Syntax	EVALUATE_FUNCTIONS
Prompt	`Name(s): <Name(s) of defined function(s)>` The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated. Variables are evaluated only if these are explicitly named.

EXPERIMENT

This command is for the ED-EXP module.

This command is used in original experimental data files (*.POP or *.DOP), but can also be given interactively inside the ED-EXP module, to change the value or uncertainty of an experiment or to add more experimental information.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

An experiment usually consists of two parts with a colon (:) separating them:

- as a quantity relation, and
- as the uncertainty of the value for the quantity,

The quantity relation can be a normal POLY module condition or an inequality (which is similar to condition but the relation between the quantity and given value is not in equality, i.e. < or >). The uncertainty can be expressed as an absolute value or relative to the value (x%).

An experiment that uses an inequality gives zero contribution to the sum of errors in the optimization procedure of PARROT if the value is on the right side. If the value is on the wrong side, the value after the colon determines how steeply the error increases with the value.

Syntax	EXPERIMENT
	The experiment must be typed after the command. Several experiments can be given on the same line. The syntax of EXPERIMENT is similar to a CONDITION. Usually, a state variable set equal to a value with a given uncertainty is specified after the colon (:). For example, `T=1273.15:5`. An inequality, < or >, can also be used. For example: `ACR(C)<-0.01:0.001, W(BCC,AG)>0.05:10%`

Additional Information About the Experment Command

A typical experiment added interactively specifies that a phase should not be stable in a certain experiment, because a phase may appear in a range of composition or of temperature where it has never been observed during the optimization. A phase is unstable if its driving force is negative, and you can add experimental information to enforce that. For example, you can suppress the HCP phase in an existing experimental point:

```
CHANGE-STATUS HCP=DORMANT
EXPERIMENT DGM(HCP)<-.001:.0001
```



DGM is the POLY variable for the driving force that is already divided by `RT`, and it is dimensionless. Only dormant phases can have driving forces larger than zero, as this indicates that these would be stable if allowed to form. The experiment in the above case tries to modify the model parameters to make the HCP phase unstable.

More general examples of experiment definitions:

```
EXPERIMENT X(LIQ,PB)=.10:.01 X(FCC,PB)=0.02:.01
EXPERIMENT ACR(PB)=0.8:5%
EXPERIMENT T=700:5
```

The first experiment above describes a tie-line where the experimentally measured mole fraction of Pb is 0.1 in the liquid phase and 0.02 in the FCC phase, and its uncertainty is 0.01 for both measurements. The second experiment is that the activity of Pb should be 0.8 with an uncertainty of 5 percent.



The reference state of the component Pb must be set with the command SET_REFERENCE_STATE. The final one is that the temperature should be 700 K with an uncertainty of 5 degrees.

Experiments that are functions of states variable(s) must be described as the defined functions. For example:

```
ENTER_FUNCTION HTR=HM(LIQUID)-HM(FCC);
EXPERIMENT HTR=7000:1000
```

EXPORT

This command is for the ED-EXP module.

Transfer/export a calculated value from an equilibrium to an optimizing variable in the PARROT workspace. Thus the value can be used, for example, in the Gibbs energy description of a phase. This variable should not be optimized (i.e. it should be set as a fixed variable in PARROT).

Syntax	EXPORT
Prompt	`Function name: <Function name>#<n>` Specify the name of the function, the value of which should be transferred to a `V` variable. The number (n) of the `V` variable must be given after the function name, separated by hash character #. The function name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.

	Example
	`Enter_function strngy=gm(fcc).x(cu);`
	`Export strngy#6`
	This transfers the value of the partial derivative of the Gibbs energy of the FCC phase with respect to the mole fraction of Cu to the optimizing variable 6 (i.e. `V6`).

FLUSH_BUFFER



This command is for the ED-EXP module.

This command is only used in the *.POP file (i.e. it can also be used in the experimental data files). It is needed if the number of experiments require more space than can be fitted into one buffer.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

When the PARROT program compiles experiments, it informs if any FLUSH commands are needed. FLUSH_BUFFER terminates the current block, saves it to the work file and starts a new block. With the READ command in the EDIT-EXP module, you can select the block to edit.

Syntax	FLUSH_BUFFER
	After a FLUSH_BUFFER command, the workspace is reinitiated and all functions or constants must be entered again in the *.POP file. You can take advantage of this; for example, you can use the FLUSH command to have blocks with different components in one *.POP file.

GRAPHICS_PLOT

This command is for the ED-EXP module.

This command can help create a experimental data file from the *.POP file. Several data sets and different symbols are allowed.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

Syntax	GRAPHICS_PLOT
	`<Dataset#> <X value> <Y value> <Symbol index>`

IMPORT

This command is for the ED-EXP module.

Transfer/import the value of one of the optimizing variables to a constant. Normally, it is directly used inside an experimental data (*.POP) file. It is the opposite of the EXPORT command.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

The IMPORT command is useful if several experiments are done at the same activity of a component, but this activity is not known. The activity should then be optimized and all equilibria with the same activity should use the same value. In this case the variable must be set as an optimizing variable, and an initial guess of the activity should be given. During the optimization, the PARROT program tries to find the activity that gives the best fit.

If an approximate value of the activity is known, it can be supplied as an experiment.

Syntax	IMPORT
Prompt	`Constant name: <Constant name>#<n>` The value of the `V` variable must be assigned a symbolic constant. The number (`n`) of the `V` variable must be given after the constant name, separated by hash character `#`. The constant name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.

	Example
	`Enter_constant acu=0.1`
	`Import acu#2`
	This transfers the value of the optimizing variable 2 (i.e. `V2`) to the constant `ACU`.

LABEL_DATA



This command is for the ED-EXP module.

Add a label to the experimental equilibrium point, either as a single point or several points given individually or in a table. The label is maximum four characters and must start with the letter A. Normally, it is directly used inside an experimental data file (*.POP).



In the DICTRA module, you work with a .DOP file instead of a .POP file.

Several experimental equilibria can be given the same label, and the label can be used with SET_WEIGHT to assign the same weight to all equilibria with the same label.

Syntax	LABEL_DATA
Prompt	`Label? /A1/: a<bcd>` Specify a textual label (as maximum characters and must start with the letter A) for the current experimental equilibrium point(s).

LIST_ALL_EQUILIBRIA



This command is for the ED-EXP module.

Syntax	LIST_ALL_EQUILIBRIA
	List all the details (including equilibrium indicators, labels, iteration numbers, weight, and fixed phases or comments) of all equilibrium points from the current one to the last one on screen. You can always use SELECT_EQUILIBRIUM to select a specific point as the current equilibrium point for such a list.

LIST_CONDITIONS



This command is available with the POLY and ED-EXP modules.

All the conditions that are set by the SET_CONDITION command and the command-sequence CHANGE_STATUS PHASE =FIXED <0 or 1 or alike>, are listed. The current conditions are also listed by the LIST_EQUILIBRIUM command. The degree of freedom in the defined system is also shown.

- If this is zero, you can perform a COMPUTE_EQUILIBRIUM command.
- If it is larger than zero, some more conditions are required, and you must further set additional ones, using SET_CONDITION or CHANGE_STATUS.
- If it is negative, then too many conditions are defined and the unnecessary ones conditions need to be removed using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or the CHANGE_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

Syntax	LIST_CONDITIONS
Example	P=100000, T=800, N(NI)=1E-1, N=1 FIXED PHASES FCC_A1=1 LIQUID=0 DEGREE OF FREEDO 0

LIST_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a text file.

You can also execute this command if no calculation is made or if the calculation fails. Make sure to interpret the results accordingly.

Syntax	LIST_EQUILIBRIUM
Prompt	`Output to screen or file /Screen/: <File name>` The name of the text file where the list of the calculation results shall be written.
	`Options /VWCS/: <Option(s)>` Select the output units and formats by optionally specifying a combination of these letters. • *Fraction order:* `V` means VALUE ORDER; `A` means ALPHABETICAL ORDER. • *Fraction type*: `W` means MASS FRACTION; `X` means MOLE FRACTION. • *Composition*: `C` means only COMPOSITION; `N` means CONSTITUTION and COMPOSITION. • *Phase*: `S` means including only STABLE PHASES; `P` means including ALL NON-SUSPENDED PHASES.
	Default options are `VWCS`. If the output fraction type should be in mole fraction (rather than mass fraction), then give `VXCS` or type `X` (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase). If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type `L_E,,,` or `LIST_EQUILIBRIUM ,,,` LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See CHANGE_LEGEND for details.

LIST_STATUS

This command is for the ED-EXP module.

There is also a POLY module command with the same name.

List the status of components, species or phases.

Syntax	LIST_STATUS
Prompt	Specify what to list: `Option /CPS/:`*<keyword(s)>* keyword = C or P or S, or any combination • `C`: list component status • `P`: list phase status • `S`: list species status • `CS`: list both components and species Default is `CPS`.
	The results depend on the key word specified in the options for CHANGE_STATUS, a table with the current status of phases or species or components, or the combinations, is shown: • For components, the statuses and reference states are listed. • For species, only the status is listed. • For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed.
	The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.

LIST_SYMBOLS



This command is for the ED-EXP module.



There are also POLY and POST module commands with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

MAKE_POP_FILE



This command is for the ED-EXP module.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

Use this command to make interactive changes and additions to the original experimental data file (the *.POP or *.DOP file). For example, to document or transfer the current or final experimental data to a *.POP file, this command will write it to a new *.POP file or overwrite previous versions.



Check the output carefully for errors. Tables in original *.POP files are written as individual experimental points. The output can be shown on screen or be saved as a new *.POP file where to write or overwrite the edited experimental information in a simple text format.

Syntax	MAKE_POP_FILE
Prompt	`Output to screen or file /Screen/: <POP/DOP-file name>` Specify a name of the new *.POP file where to write or overwrite the edited experimental information in a simple text format. If an existing *.POP file name is specified, it is overwritten.

READ_WORKSPACES

This command must be given each time the ED_EXP module is entered, unless it is already given once in ED_EXP and does not use LIST_RESULT or OPTIMIZE_VARIABLES in PARROT in between.

Syntax	READ_WORKSPACES
Prompt	`Block number /#/: <n>` The number of a data block that should be edited must be given. If there is no FLUSH_BUFFER command in the original POP file, then there is only one data block with the number 1.
	READ_WORKSPACE = READ This command is equivalent to READ_WORKSPACES in the POLY module, but it only reads the POLY workspace from the work file set by SET_STORE_FILE in the PARROT module.

REINITIATE_MODULE



This command is for the ED-EXP module.

The REINITIATE_MODULE command makes sure that the entire ED-EXP module is reinitiated to the original state.

Syntax	REINITIATE_MODULE
	All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.

RESTORE_ALL_WEIGHTS



This command is for the ED-EXP module.

Restore a specific weight-set (previously saved by STORE_ALL_WEIGHTS) and assign all the different experimental points in the current data block with the previously-set weights in the sequential assessments.

Syntax	RESTORE_ALL_WEIGHTS
Prompt	`Set number (0 for list) /0/: <weight-set number>` The default value 0 is for a list on screen.

SAVE_WORKSPACES

This command is for the ED-EXP module.

In the PARROT workspace this command saves the current status of the ED_EXP submodule before you switch back to the PARROT module. This is required when you want to save equilibria changes, including changes to conditions, experimental data, and/or computed equilibria results, as well as any newly added equilibria.

With this command all the changes made in the ED_EXP submodule are saved in the PARROT workspace. This means you do not need to execute SAVE_PARROT_WORKSPACES in the PARROT module.

However, when in the PARROT module, additional changes can only be saved with the SAVE_PARROT_WORKSPACES command even if they have been made prior to executing SAVE_WORKSPACES in ED_EXP.

When you exit the ED_EXP (or Thermo-Calc), the next time the file is opened it is in the same state as when you executed the SAVE_WORKSPACES command. However, if you use OPTIMIZE_VARIABLES the computed results are automatically updated.

Syntax	SAVE_WORKSPACES
Prompt	`<File name>` Sometimes good starting values (SET_START_VALUE) are required to successfully get or compute an equilibrium correctly. In this case, it is important to save the computed equilibrium in the PARROT workspace. It is important to remember that the computed results can be ruined by improper optimizations. For this reason, it is suggested you save the .PAR file with a different name to back up the PARROT workspace.

SELECT_EQUILIBRIUM



This command is available with the POLY and ED-EXP modules.

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.

Syntax	SELECT_EQUILIBRIUM
Prompt	`Number /Next/: <Choice on equilibrium>` Options: `FIRST`, `LAST`, `NEXT`, `PREVIOUS` or `PRESENT`. Most commands affect only the `PRESENT` equilibrium. However, the REINITIATE_MODULE and DEFINE_COMPONENTS commands remove all the stored equilibria.

SET_ALL_START_VALUES

This command is available for the POLY and ED-EXP modules.

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

Syntax	SET_ALL_START_VALUES
	`T /XXXX/: <Temperature in K>` If the temperature is not a condition, supply a guess of its final value (in K).
	`P /100000/: <Pressure in Pa>` If the pressure is not a condition supply a guess of its final value (in Pa).
Prompts	`Automatic start values for phase constitutions? /N/: <Y, N or F>` • For N, enter an initial amount of each entered phase and the major constituents or site fraction of each constituent. • For Y, the program automatically sets the start values for phase constitutions in all possible phases. • `F` is for force. In some cases the calculation fails because impossible conditions are set, e.g. `W(C)=1.5` `[W(C)` is mass fraction and must thus be less than unity. The program tries to fulfill this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set `W(C) to 0.015`, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, choose `F`.
	`Should <phase> be stable /N/: <Y/1 or N/2>` A guess if this phase should be stable or not is requested. All entered phases are prompted for this question and next two. You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No). The `phase` name may have a hash sign # followed by a digit, e.g. `BCC_A2#2`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.
	`Major constituent(s): <Name of major constituent(s) in the phase>` The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving $ the constituent is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.

Syntax	SET_ALL_START_VALUES
	`Y(<phase>,<constituent>) /.XXXXXXXXXX/: <.YYYYY>` The current value (`.XXXXXXXXXX`) is default. You can accept the default by pressing <Enter> or give a new value (`.YYYYY`). The phase name or constituent name may have a hash sign # followed by a digit, e.g. `Y(BCC_A2#2,FE), Y(BCC_A2#2,C#2)`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.

SET_ALTERNATE_CONDITION

This command is for the ED-EXP module.

A special command used in the experimental data *.POP file but also possible in the ED_EXP module. It is used only when you have specified that the alternate mode is set in the PARROT module.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

The command syntax is almost the same as for the POLY command SET_CONDITION while the uncertainty should also be specified.

The alternate condition (including the normally POLY module condition plus uncertainly; see below) must be given explicitly, but can be given on the same line or on separate lines with each one started with the command.

Syntax	SET_ALTERNATE_CONDITION
Prompt	`State variable expression: <State variable name or linear expression>` Give either a state variable or a linear expression of state variables.
Options	**Description and Information**
State variables	Some of the state variables that can be used in conditions are: • `T`: temperature in the system (in K) • `P`: pressure in the system (in Pascal) • `N`: system size (mole number in moles) • `B`: system size (mass in grams) • `N(<component>)`: mole number of a component in the system • `X(<component>)`: mole fraction of a component in the system • `W(<component>)`: weight fraction of a component in the system • For the SET_CONDITION command this is `ACR(<component>)`: activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `ACR(<phase>,<component>)` (activity of a component in a phase) • For the SET_CONDITION command this is `MUR(<component>)`: chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `MUR(<phase>,<component>)` (chemical potential of a component in a phase) • `X(<phase>,<component>)`: mole fraction of a component in a phase

Syntax	SET_ALTERNATE_CONDITION
	• W(<phase>,<component>): weight fraction of a component in a phase • ACR(<species>,<phase>): activity of a species referred to a phase • MUR(<species>,<phase>): chemical potential of a species referred to a phase • H: enthalpy in the system (in J) • HM(<phase>): enthalpy of a phase (in J/mol)
Additional prompts	Factor: <A factor for the state variable, or a continuation> This question means that the previous question was not answered. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is: 2*MUR(FE)+3*MUR(O)=-35000 This means that it should be a condition that two times the chemical potential of FE plus three times the chemical potential of O should be -35000 J/mol.
	State variable: <A specified state variable, or a continuation> This question is prompted if a single state variable name has not given in either the prompt State variable expression or Factor, or a state variable expression is given but the expression is incomplete, for example, T- or 2*MUR(FE)+, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	Value /X/: <A numeric value, a constant or a variable> The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value NONE means that the condition is removed.
	Uncertainty /None/: <Uncertainty of the condition> The uncertainty of the condition. This can be a numeric value, a constant or a variable. The default value NONE means that the uncertainty for the value specified above is zero. The uncertainty can either be expressed as an absolute value or relative to the value of the condition in percent (x%).
Notes	There are more state variables that can be used in conditions. For more information, type an INFO STATE_VARIABLES command in the POLY module. A condition is normally a value of a single state variable with its value. ***Example*** T=1273.15 P=1E5 X(C)=.002 W(CR)=1.5 ACR(CR)=0.85 X(FCC,C)=.001 H=-250000 HM(BCC)=-225000

Syntax	SET_ALTERNATE_CONDITION
	A condition can also be a value of a linear expression involving more than one state variable. ***Example*** `X(LIQ,S)-X(PYRR,S)=0` This means that it is a condition that the mole fraction of `S` should be the same in the LIQUID and PYRRHOTITE phases. In practice that should be the congruent melting point.  After the equal sign only a numeric value is allowed.

SET_CONDITION

This command is available with the POLY and ED-EXP modules.

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the M/W/V/F-suffixed state variables (for normalization) and R-suffixed state variables (with respect to chosen reference states), can be used as conditions. In addition to temperature and pressure conditions, a multicomponent system can have mixed types of conditions. You should repeat this command for a multicomponent system until the degree of freedom in the defined system becomes zero. When a FIXED phase status is used on a specific phase (use CHANGE_STATUS), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax	SET_CONDITION

	Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.
	
	Example
	`SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2`
	or
	`SET_COND T=1273, P=1E5`
	`SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2`
	In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.

Prompt	`State variable expression: <State variable name or linear expression> or a linear expression of state variables.` Some of the state variables that can be used in conditions are: • T: temperature in the system (in K) • P: pressure in the system (in Pascal) • N: system size (mole number in moles) • B: system size (mass in grams) • N(<component>): mole number of a component in the system • X(<component>): mole fraction of a component in the system • W(<component>): weight fraction of a component in the system • For the SET_CONDITION command this is ACR(<component>): activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is ACR(<phase>,<component>) (activity of a component in a phase) • For the SET_CONDITION command this is MUR(<component>): chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is MUR (<phase>,<component>) (chemical potential of a component in a phase)

Syntax	SET_CONDITION

- `X(<phase>,<component>)`: mole fraction of a component in a phase
- `W(<phase>,<component>)`: weight fraction of a component in a phase
- `ACR(<species>,<phase>)`: activity of a species referred to a phase
- `MUR(<species>,<phase>)`: chemical potential of a species referred to a phase
- `H`: enthalpy in the system (in J)
- `HM(<phase>)`: enthalpy of a phase (in J/mol)

There are many state variables that can be used in conditions. For more information, enter an `INFO STATE_VARIABLES` command. A condition is normally a value of a single state variable with its value.

Example

```
T=1273.15  P=1E5
X(C)=.002
W(CR)=0.5
ACR(CR)=0.85
X(FCC,C)=.001
H=-250000
HM(BCC)=-225000
```

A condition can also be a value of a linear expression involving more than one state variable. For example,

```
X(LIQ,S)-X(PYRR,S)=0
```

This means that it is a condition that the mole fraction of `S` component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.

After the equal sign only a numeric value is allowed in the expression.

`Factor: <A factor for the state variable, or a continuation>`

This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:

```
2*MUR(FE)+3*MUR(O)=-35000
```

This means that it should be a condition that two times the chemical potential of `FE` plus three times the chemical potential of `O` should be -35000 J/mol.

`State variable: <A specified state variable, or a continuation>`

This question is prompted if a single state variable name has not given in either the prompt `State variable expression` or `Factor`, or a state variable expression is given but the expression is incomplete, for example, `T-` or `2*MUR(FE)+`, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).

Syntax	SET_CONDITION
	`Value /X/: <A numeric value, a constant or a variable>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed; for example `T=NONE` takes away the temperature condition.

SET_NUMERICAL_LIMITS



This command is available for the POLY, Scheil and ED-EXP modules.

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`Maximum number of iterations /500/:` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`Required accuracy /1E-6/:` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`Smallest fraction /1E-12/:` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is `1E-12` for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30` (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system).
	`Approximate driving force calculation for metastable phases /Y/:` Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. By default, the metastable phases are included in all iterations but these may not have reached their most favorable composition and thus their driving forces may be only approximate.

Syntax	SET_NUMERICAL_LIMITS
	 If it is important that these driving forces are correct, choose N to force the calculation to converge for the metastable phases. This may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.

SET_REFERENCE_STATE

This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials, and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature, and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials, and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC (O2,GAS), LNACR(O2,GAS).

For the POST module, and after calculating with the STEP_WITH_OPTIONS or MAP commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. MUR(comp), MUR (comp,ph), ACR(comp), ACR(comp,ph) or the common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`Component: <Name of the component>` The name of the component must be given.
	`Reference phase: <Name of a phase used as the new reference state>`

Syntax	SET_REFERENCE_STATE
	Enter the `Name of a phase` for the system. For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed. If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy. The following are example using temperature. Pressure is used in the same way: • In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C. • If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1. • Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state.
	`Temperature /*/: <Temperature for the reference state>` Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation. The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.
	`Pressure /1E5/: <Pressure for the reference state>` Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.

	Examples
	
	`S-R-S Fe SER`
	`S-R-S Cr FCC * 100000`
	`S-R-S H2O AQUEOUS * 100000`
	`S-R-S ZE REF_ELECTRODE * 100000`

SET_START_CONSTITUTION



This command is available with the POLY and ED-EXP modules.

This command is similar to SET_ALL_START_VALUES, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
Prompts	`Phase name: <Name of a phase, and possible major constituent(s)>` Specify the name of a phase for which the constitution shall be set. If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A $ means keeping the same constitution, and `NONE` means to give individual site-fractions.
	`Y(<Phase>#<Composition_set>,<Constituent>#<Sublattice>) /xxx/: <SF>` The site fraction (`SF`) of the constituent shall be given. The default value `xxx` is the last calculated one.

SET_START_VALUE

This command is available with the POLY and ED-EXP modules.

This command is not often required as the automatic start values can be handled for most problems.

Set a start value of an individual variable.

Syntax	SET_START_VALUE
Prompts	`State variable: <Name of a state variable>` The state variable must be given.
	`Value` Specify the value to be assigned the state variable as start value.

SET_WEIGHT

This command is for the ED-EXP module.

Each experimental value has an uncertainty associated with it, specified by the value after the colon (:) with the command EXPERIMENT. During an optimization the absolute difference between the experimental and calculated values gives a contribution to the sum of error.

With the SET_WEIGHT command, you can change the scale of such a contribution (the uncertainty) for a single experimental point, or the contributions (all uncertainties) for a set of equilibria. The default weight is always unity. A value smaller than one means that the experiments should have less weight. A value larger than one that these should have higher weight. The special value zero means that the set of equilibria should be ignored in editing in ED_EXP (as is given) and in OPTIMIZE_VARIABLES in PARROT.

The weight may be needed to obtain a balance between different kinds of experiments. For example, if there are only five experimental values of the composition of a phase diagram but 500 experimental values of activities or enthalpies, then the five composition points may have to be given higher weight than unity, otherwise these are not well described by the optimizing procedure.

Syntax	SET_WEIGHT
Prompts	`Value /1/: <Weight value>` Specify a weight of the experiments in the specified equilibria (asked in the next prompt). The contribution to the sum of errors of these experiments are multiplied by this weight. The weight is squared, thus use 0.7 to make the error half (0.49) as big, and 1.4 to make it twice (1.96) as large.
	`Equilibria (range) or label(s) /Present/:<Selection>` Define the equilibria. These are available in the read data block from the current work file and are given the above-defined weight. The selection may be given as a range but the equilibrium numbers must then be separated only by a minus sign. The start and end equilibrium numbers must be available in the read data block read from the current work file. For example, `5-101`, means that all equilibria starting from the identifier 5 until the identifier `101`. Some of numbers between these two identifiers may not exist in the data block. The selection may also be given as one or more labels (which should be separated only by a space). All equilibria with the specified label(s) in the read data block are given the above-defined weight.

Syntax	SET_WEIGHT
	By pressing <Enter> to accept the default value `present`, the above defined weight is only assigned to the current or present experimental point (which is selected by the POLY SELECT_EQUILIBRIUM command).  If is used but no specific equilibrium point is selected afterwards, the last point in the read data block remains the `present` point.

SHOW_VALUE

This command is available for the POLY and ED-EXP modules.

Show the current value of any state variable, function or variable.

Syntax	SHOW_VALUE
Prompt	`State variable or symbol: <Name(s) of state variable(s) or symbol(s)>` A single or several state variables or symbols (entered functions or variables) can be specified.
	The wildcard * can be used to denote all phases or all components. You can use the dollar-sign `$` to denote all stable phases. Thus, the command SHOW W(*,*)lists the mass fraction of all phases, whereas `SHOW W($,*)` lists the mass fraction of all stable phases. If you `SHOW` a function, all functions are evaluated using the current values of the state variables. But if you `SHOW` a variable, it retains its value from the time it was `ENTERED` or last `EVALUATED`. Therefore to save a value from one calculation to another, `ENTER` it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.

STORE_ALL_WEIGHTS

Store a new weight-set that is the current situation of specified weights for all the different experimental points read from the currently-selected experimental data block in an assessment. This is useful when you want to try various weight-settings for some experimental points or for all the points, and then compare the assessment results from different weight-sets. Such a saved weight-set can be recalled and restored for all experimental data point with RESTORE_ALL_WEIGHTS sequentially.

Syntax	STORE_ALL_WEIGHTS
Prompt	`Command line: <Weight-set name>` Give a weight-set name (comment line texts) for the current weight set for all experimental points.

TABLE_HEAD, TABLE_VALUES and TABLE_END

These commands are used only in the *.POP file. It represents a convenient way to enter many experimental measurements of the same type in a table format.



In the DICTRA module, you work with a .DOP file instead of a .POP file.



These commands should always be used together and in a sequence, meaning that a table should always start with the TABLE-HEAD command, then TABLE-VALUES, and finish with TABLE-END. Between TABLE_HEAD and TABLE-VALUES also add definition lines (e.g. on phase status, reference states, conditions, experiments, labels, etc.) for the experimental measurements of the current information type.

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END
Prompt	
	After the TABLE-HEAD command, there must be an equilibrium description similar to a single experimental equilibrium but with some special notation. Then, there is always a TABLE-VALUES command, after which the actual data is given in columns. At the end of each table, there must be a TABLE-END command. The TABLE-HEAD command must be followed by a numeric value. This is used to generate unique numeric identifiers for all the equilibria in the table. The numeric identifier is incremented by one for each experimental (equilibrium) point in the table.

	Example
	An example of the use of a table for enthalpy measurements in the liquid is given here. Much more elaborate tables can be used
	`$ Enthalpies of mixing, Topor and Kleppa, Met Trans 1984 TABLE-HEAD 1`
	`CREATE-NEW @@ 1`
	`CHANGE-STATUS PHASE LIQ=FIX 1`
	`SET-REFERENCE-STATE AU LIQ * 1E5`
	`SET-REFERENCE-STATE CU LIQ * 1E5`
	`SET-CONDITION P=1E5 T=1379 X(LIQ,AU)=@1`
	`LABEL ALH`
	`EXPER HMR=@2:5%`
	`TABLE-VALUES`
	`0.0115 -322`

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END
	0.0563 -1520 0.8499 -2976 0.9002 -2114 TABLE_END
	The equilibrium description between TABLE-HEAD and TABLE-VALUES is similar as for a single experiment, except for these details: • @@ Used to automatically generate a series of identifying numbers instead of creating only one with the command CREATE_NEW_EQUILIBRIUM. The program automatically generates the identifying numbers starting after the number given after the TABLE-HEAD command (in this case it is 1). • @1 values in the table are specified by an @ sign followed by a column number. In the above case, the mole fraction of Au in the liquid is in column 1 (see the line for SET_ CONDITION). The columns may have other information than values, and you can use phase names or any text. If the text contains spaces or special characters, it must be surrounded by double quotes in the table, e.g. "ABC DEF&ghi". • For the *syntax checker* all commands describing the equilibrium must be in UPPER case after the TABLE_HEAD command. • After the TABLE-VALUES command, there should be one line for each experimental measurement of the same type giving the values or texts that should be copied into the places of the condition or experiment defined by @1, t, etc. You can have columns that are not used but there must be exactly the same number of columns of each line, otherwise the syntax checker gives an error message in the PARROT module.

TRANSFER_START_VALUES



This command is for the ED-EXP module.

In the ED_EXP module it is time consuming to calculate all equilibria when the optimization is sensitive to start values of the composition of the phases. Usually in one data block there are several experimental points with the same kind of equilibrium and each must have its start value set. When you manage to calculate equilibriums of such experimental points, this command is useful to transfer the site fractions from a successfully-calculated equilibria to the present experimental point.

Syntax	TRANSFER_START_VALUES
Prompt	`From equilibrium /Previous/: <Equilibrium number>` The equilibrium number is the numeric identifier for the equilibrium from which the start values should be copied to the present experimental point. `Previous` is the default if you press <Enter>.

Tabulation Reaction (TAB) Commands

In this section:

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ENTER_FUNCTION

This command is available with the GES and TAB modules.

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

Syntax	ENTER_FUNCTION
Prompt	`Name: <Name>` `Function: <Definition>`
	A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, -(G-H)/T can be defined as a function which is identical to S for a substance or ΔS for a reaction, G+T*S-P*V can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction.
Options	`Name`of the function (maximum 8 characters) and `Definition` of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line.

Example

For the pure substance Fe (using the SSUB database), by entering a function as `G+T*S-P*V`, the following table is obtained by typing <Enter> in the prompt `Output file /Screen/:`, and the figure by typing `6` in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION
Name: InEnergy
Function: G+T*S-P*V;
TAB: TABULATE_SUBSTANCE
Substance (phase): Fe
Pressure /100000/: <Enter>
Low temperature limit /298.15/: <Enter>
High temperature limit /2000/: <Enter>
Step in temperature /100/: <Enter>
Output file /try1/: try2
Graphical output? /Y/: <Enter>
Plot column? /2/: 6
```

This gives the following output:

```
O U T P U T  F R O M  T H E R M O - C A L C

Column 6: InEnergy G+T*S-P*V

Phase : FE_S                        Pressure :      100000.00

Specie: FE

************************************************************

    T      Cp            H             S             G             InEnergy

   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)

************************************************************

  298.15   2.48446E+01   2.17972E-06   2.72800E+01  -8.13353E+03   2.17972E-06

  300.00   2.48905E+01   4.60049E+01   2.74338E+01  -8.18414E+03   4.60049E+01

  400.00   2.71299E+01   2.64957E+03   3.49085E+01  -1.13138E+04   2.64957E+03

  500.00   2.93561E+01   5.47211E+03   4.11976E+01  -1.51267E+04   5.47211E+03

  600.00   3.19293E+01   8.53245E+03   4.67701E+01  -1.95296E+04   8.53245E+03

  700.00   3.50985E+01   1.18777E+04   5.19207E+01  -2.44667E+04   1.18777E+04

  800.00   3.92042E+01   1.55830E+04   5.68623E+01  -2.99068E+04   1.55830E+04

  900.00   4.49645E+01   1.97726E+04   6.17903E+01  -3.58387E+04   1.97726E+04

1000.00   5.42147E+01   2.46891E+04   6.69619E+01  -4.22728E+04   2.46891E+04

1100.00   4.55851E+01   2.99025E+04   7.19412E+01  -4.92328E+04   2.99025E+04 $
Stable phase is FE_S2

1200.00   3.40840E+01   3.51037E+04   7.64466E+01  -5.66322E+04   3.51037E+04

1300.00   3.49398E+01   3.85549E+04   7.92086E+01  -6.44162E+04   3.85549E+04
1400.00   3.57994E+01   4.20918E+04   8.18293E+01  -7.24692E+04   4.20918E+04

1500.00   3.66636E+01   4.57149E+04   8.43287E+01  -8.07780E+04   4.57149E+04

1600.00   3.75330E+01   4.94247E+04   8.67226E+01  -8.93314E+04   4.94247E+04 $
Stable phase is FE_S3

1700.00   4.05217E+01   5.41173E+04   8.95609E+01  -9.81363E+04   5.41173E+04

1800.00   4.12595E+01   5.82055E+04   9.18975E+01  -1.07210E+05   5.82055E+04 $
Stable phase is FE_L

1900.00   4.60000E+01   7.74165E+04   1.02377E+02  -1.17099E+05   7.74165E+04
2000.00   4.60000E+01   8.20165E+04   1.04736E+02  -1.27456E+05   8.20165E+04
```

ENTER_REACTION

This command is for the TABULATE_REACTION (TAB) module.

This is the same as TABULATE_REACTION in that both the chemical reaction can be specified and the thermodynamic property changes for the reaction can be generated as a table, and plotted as a graph or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB database (by default), or the current database set by SWITCH_DATABASE (thus there is no need to use the TDB module before this command). You can select any other database by using the SWITCH_DATABASE command in the TAB module. The rules to specify a reaction are the same as TABULATE_ REACTION.

Syntax	ENTER_REACTION
Prompts	`Same reaction? /Y/:` This displays if there is at least one reaction already defined either by ENTER_REACTION or TABULATE_ REACTION. For `Y` the next prompt for defining reaction is not asked.

	`Reaction: <Chemical reaction equation> & <RA+RB=PC+PD>`
	A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (`;`) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.:
	`Pressure /100000/: <Pressure of interest, in pa>`
	`Low temperature limit /298.15/: <T-low, in K>`
	`High temperature limit /2000/: <T-high, in K> Step in temperature /100/: <T-step>`

	`Output file /Screen: <Return for screen, or type a file name>` If you type `Return for screen` a list of thermodynamic property changes for the defined/chosen reaction is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is displayed and saved as an *.EXP or an *.TAB file. Then prompts:
	`Graphical output /Y/:` For `N` a table is output to the screen and this table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. By default a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file). You are also prompted for the plot column.
	`Plot column? /2/: <1 or 2 or 3 or 4 or 5 or 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the

Syntax	ENTER_REACTION
	screen, followed by a POST prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST prompt always takes you back to the TAB module.

LIST_SUBSTANCES

This command is for the TABULATE_REACTION (TAB) module.

List all species in the current database with a certain set of elements. This is useful to specify species as pure substances in the command TABULATE_SUBSTANCE.

Syntax	LIST_SUBSTANCES
Prompts	`With elements /*/ <* or a set of elements>` The elements building up various species must be specified. The wildcard * means all elements in the current database. If some elements are specified, it also prompts for how to list species with such elements.
	`Exclusively with those elements /Y/:` All species (not phases) in the current database are searched. Keep the default (Y) if you do not want other elements included in the search except for those specified. Enter N to list all species containing at least one of the specified elements.

Example

For the SSOL database, there are different lists, as shown below:

```
TAB: l-sub
With elements /*/: <Enter>
VA                       AG                       AL
AM                       AS                       AU
B                        BA                      BE BI  BR C
CA                       CD                       CE
CL                       CO                       CR
CS                       CU                       DY
ER                       EU                       F
FE                       GA                       GD
GE                       H                        HF
HG                       HO                       I
IN                       IR                       K
LA                       LI                       LU
MG                       MN                       MO
NA                       NB
```

```
ND                    NI                    NP
OS                    P
PA                    PB                    PD
PR                    PT                    PU
RB                    RE                    RH
RU                    S                     SB
SC                    SE                    SI
SM                    SN                    SR
TA                    TB                    TC
TE                    TH                    TI
TL                    TM                    U
V                     W                     Y
YB                    ZN                    ZR
C1                    C2                    C3
C4                    C5                    C6
C7                    N2                    O2
P1                    P2                    P4
NA/+1                 K/+1                  CL/-1
H2O                   H1/+                  LI1/+
CS1/+                 RB1/+                 O1H1/-
F1/-                  BR1/-                 I1/-
H1/+1                 H1O1/-1               SI1O2 CA1O1 TAB:
TAB: l-sub
With elements /*/: fe cr ni c n o
Exclusively with those elements? /Y/: <Enter>
C               CR                    FE
N               NI                    O
C               C2                    C3
C          C5                    C6
C               N2                    O2
TAB:l-sub fe cr ni c n o
Exclusively with those elements? /Y/: n
C               CR                    FE N   NI O
C1              C2                    C3
C4              C5                    C6
C7              N2                    O2
```

```
H2O             O1H1/-              H1O1/-1 SI1O2 CA1O1 TAB:
```

SET_ENERGY_UNIT

Set the energy unit as calories or Joule, in all the subsequent outputs (tables, graphs, and files) in the current calculation operation.

Syntax	SET_ENERGY_UNIT
Prompt	`Energy unit (C=Cal, J=Joule) /J/: <Unit>`

SET_PLOT_FORMAT



This command is for the TABULATE_REACTION (TAB) module.

Set the plotting format while the result is plotted on screen or the file is saved as EXP file [using DATAPLOT graphical format] and TAB file (as a basic text file and as displayed on screen).



This command is different from SET_PLOT_FORMAT in the POST module, but is identical to SET_PLOT_ENVIRONMENT in the SYS (system utility) monitor.

Syntax	SET_PLOT_FORMAT
Options	The default set `Unit`is `1` (Windows) or `9` (Linux) for graphical presentation on screen, or all other units for outputs as *.EXP and *.TAB files. Also set the format of the graphical output to different graphical devices. The default unit 22 (1 for legacy Windows, and 9 for legacy Linux) may be altered with SET_PLOT_ENVIRONMENT in the SYS monitor or by the TC.INI file.

SWITCH_DATABASE



This command is for the TABULATE_REACTION (TAB) module.

By default, the TAB module always automatically retrieves thermodynamic data for substances or reactant/product substances in a defined reaction, or for pure phases or ideal solution phases, from the SSUB Substances database. However, you can select thermodynamic data for complex non-ideal solution phases from another database, which is possible with this command.

Syntax	SWITCH_DATABASE
Prompt	`Database /XYZ/: <new database name>` Specify a `New database name`. `XYZ` stands for the default SSUB database or the current database which is switched on. If an appropriate database name is not given and the `USER` option is not used, a list displays of available databases. Use one of these databases: • PURE = SGTE Pure Elements Database • SSUB = SGTE Substances Database • USER = user defined database

This command switches (or changes) from the current database to a new one, and reinitializes the entire TAB module for defining a substance or reaction and the GIBBS workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file `tc_initd.tdb` are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument USER and then the database name and, if it is not located in the current working directory, its correct path.

This command (when required to use another database for subsequent tabulations) must be used before executing the TAB commands TABULATE_SUBSTANCE for substances, and ENTER_REACTION or TABULATE_REACTION for reactions.

When a predefined database or an appropriate USER database is switched on, the DATA command GET_DATA is automatically executed.

DATABASE NAME: The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. For convenience when switching/appending databases you can add them to the predefined database list in the database initiation file `tc_initd.tdb` of your installed software.

When this command is used in a macro (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the user database, and its correct path, must be provided.

If a USER database name or its path is not given on the same line of the SWITCH_DATABASE command, or if it is incomplete or incorrect, an Open window displays to specify the filename of the database setup file name (*setup.TDB) of the to-be-switched USER database.



Unlike in the TDB module, if a user database is chosen, the Gibbs energy system is also reinitialized and only data from the user databases are retrieved for tabulations.

After this command, those commands to define systems (in terms of either elements or species), to reject/restore phases or species, retrieve data, as well as to append data from additional database(s), can be done.

TABULATE



This command is for the TABULATE_REACTION (TAB) module.

Gives the values of an already-defined table (with various properties varied with the stepping axis variable) from equilibria calculated with a STEP command. You can tabulate a table even if the table is entered after the step calculation.

Syntax	TABULATE
Prompts	`Name: <Name of a defined table>` The name of the table must be given. The table must be entered.
	`Output to Screen or file /Screen/: <File name>` The table can be listed on the screen (by pressing <Enter>), on a file (the file name must be specified here).

TABULATE_DERIVATIVES

This command is for the TABULATE_REACTION (TAB) module.

This command is mainly for system debugging purposes and for experienced users. It automatically calculates all partial derivatives for a pure phase or solution phase at a given composition.

This is not the same as the chemical potential.

Before using this command, the system must be defined and thermodynamic data retrieved from an appropriate solution database in the TDB module. The phase name can be given in either upper, lower or mixed cases, and can be abbreviated until it is unique, e.g. fcc, BCC, cem, Liq, etc. as the SSOL database is used for the tabulations, or GAS, FE-S, wustite, Fe2O3-hem, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, thermodynamic properties can be tabulated for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Syntax	TABULATE_DERIVATIVES
Prompts	`Phase name /XXXX/: <Name of the phase>` Specify the phase name of a pure phase or a solution phase. `XXXX` is the last phase the TAB module accounted for. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase. For a pure phase (such as `Fe-S`, `Wustite`, and `Fe2O3-Hematite`), no further composition definition is needed. For a solution phase with one sublattice (such as `AQUEOUS` solution, `GAS` mixture and `SLAG` solution), it requests *n*-1 site-fraction inputs for the phase constituents (if there are *n* species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the *n*th species is automatically assigned as the rest. The sum of input site fractions must not exceed unity.

Syntax	TABULATE_DERIVATIVES

	### *Example Prompts*
	For example, these prompts and inputs can be seen for a `LIQUID` solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted `Ni` species are assigned as the rest):
	`FRACTION OF CONSTITUENT (RETURN FOR PROMPT): <RETURN> C /1/: .05`
	`CR /1/: .1`
	`FE /1/: < RETURN>`
	`SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER`
	`FE /1/: .8`
	`N /1/: .005`
	For a solution phase with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (of course, this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice n-1 times if there are n species on such a sublattice in the defined phase; the nth species on each of the sublattices is automatically assigned as the rest. For example, the following prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted O species on its sublattice 1 and VA on its sublattice 2 are assigned as the rest):
	`SPECIFY SUBLATTICE (0 FOR ALL) /0/: <RETURN>`
	`FRACTIONS IN SUBLATTICE 1`
	`CR /1/: .1`
	`FE /1/: .8`
	`NI /1/: .0995`
	`FRACTIONS IN SUBLATTICE 2`
	`C /1/: .05`
	`N /1/: .05`

	`Temperature /2000/: <Temperature of interest, in K>` Specify the temperature of interest in K.
	`Pressure /100000/: <Pressure of interest, in pa>` Specify the pressure of interest in Pa.

Example Output

For the FCC phase in the Fe-Cr-Ni-C-N-O system (using the SSOL database), the following table is obtained at a specified composition:

```
TAB: TAB_DER
```

```
Phase name /BCC/: FCC

SPECIFY SUBLATTICE (0 FOR ALL) /0/: <Enter>

FRACTIONS IN SUBLATTICE 1

CR /1/: .1

FE /1/: .8

NI /1/: .3

SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER

NI /0/: .0995

FRACTIONS IN SUBLATTICE 2

C /1/: .05

N /1/: .05

Temperature /1800/: <Enter>

Pressure /100000/: <Enter>

Gibbs energy: ..................... -1.27432533E+05

Helmholz energy: .................. -1.27433205E+05

Enthalpy: .........................  5.95773994E+04

Internal energy: ..................  5.95767279E+04

Entropy: ..........................  1.03894407E+02

Molar volume: .....................  6.71473258E-06

Thermal expansivity: ..............  7.63886416E-05

Isothermal compressibility: .......  6.02925387E-12

Heat capacity at constant pressure:  4.33555074E+01

First partial derivative with respect to CR in sublattice  1     of Gibbs energy:
.................. -1.26034739E+05     of enthalpy: .....................
4.63000206E+04     of entropy: ......................  9.57415334E+01     of
volume: ......................  6.87203263E-06

Second partial derivative of Gibbs energy with respect to also

  CR                       in  1:  1.54392858E+05

  FE                       in  1: -1.53353158E+04

  NI                       in  1: -1.71750366E+04

  O                        in  1:  0.00000000E+00

  C                        in  2: -1.82016870E+05

in  2: -3.73062665E+05

  VA                       in  2: -9.36260878E+04

irst partial derivative with respect to FE in sublattice  1     of Gibbs energy:
.................. -1.02869265E+05
```

```
    of enthalpy: .....................  6.11738912E+04     of entropy:
..................... 9.11350866E+01     of volume: ......................
7.53441165E-06

Second partial derivative of Gibbs energy with respect to also

FE                      in  1:  1.82508696E+04

NI                      in  1: -3.07043434E+03

in  1:  0.00000000E+00

C                       in  2: -1.36027071E+05

in  2: -2.13007485E+05

VA                      in  2: -1.11741180E+05

First partial derivative with respect to NI in sublattice  1     of Gibbs energy:
................. -1.32427029E+05     of enthalpy: .....................
5.21563580E+04     of entropy: ......................  1.02546326E+02     of
volume: ......................  0.00000000E+00

    Second partial derivative of Gibbs energy with respect to also

  NI                      in  1:  1.48390257E+05

in  1:  0.00000000E+00

  C                       in  2: -7.70620431E+04

in  2: -1.61551726E+05

VA                      in  2: -1.12772206E+05

First partial derivative with respect to O in sublattice  1     of Gibbs energy:
................. -2.62929308E+05     of enthalpy: .....................
5.02555370E+04     of entropy: ......................  1.73991581E+02     of
volume: ......................  0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

in  1:  2.99322360E+07

C                       in  2:  0.00000000E+00

N                       in  2:  0.00000000E+00

VA                      in  2: -1.82377137E+05

First partial derivative with respect to C in sublattice  2     of Gibbs energy:
................. -1.59508417E+05     of enthalpy: .....................
1.21269096E+05     of entropy: ......................  1.55987507E+02     of
volume: ......................  1.06885187E-05

Second partial derivative of Gibbs energy with respect to also

C                       in  2:  2.99322360E+05

N                       in  2: -1.90144000E+04

VA                      in  2: -2.78465070E+04

First partial derivative with respect to N in sublattice  2     of Gibbs energy:
................. -2.39671400E+05     of enthalpy: .....................
4.04456947E+04     of entropy: ......................  1.55620608E+02     of
volume: ......................  0.00000000E+00
```

```
Second partial derivative of Gibbs energy with respect to also

N                         in  2:  2.99322360E+05

VA                        in  2: -3.30383665E+04

First partial derivative with respect to VA in sublattice  2     of Gibbs energy:
................ -9.52042686E+04     of enthalpy: ....................
5.37142294E+04     of entropy: ......................  8.27324989E+01     of
volume: ......................  6.86700739E-06

Second partial derivative of Gibbs energy with respect to also

VA                        in  2:  1.66290200E+04
```

TABULATE_REACTION



This command is for the TABULATE_REACTION (TAB) module.

Tabulate thermodynamic property changes for a chemical reaction as a table, or variation of one chosen property can be plotted against temperature as a graph, or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by the SWITCH_DATABASE command (thus there is no need to use the DATA module before this command). You can select any other database by using SWITCH_DATABASE.

It is important to remember the rules to specify a reaction:

- The reaction is specified, by giving the reactants and products, such as `Ga+S=GaS`, `5Al+2Fe=Al5Fe2`.
- Under Linux environments, the notation for a chemical formula treats upper and lower cases as the same (such as `ga+s=GaS`, `5Al+2Fe=al5fe2`); but under Windows, the TAB module only accepts upper cases, e.g. `GA+S=GAS`, `5AL+2FE=AL5FE2`.
- Elements with a single letter symbol must be followed by a stoichiometry factor, even if it is 1; thus, the symbol `CO` is taken as cobalt, carbon monoxide must be given as `C1O1` (or `O1C1`).
- All the reactants and products must be defined as species-stoichiometries in the currently-used database; in other words, the reaction definition only accepts already-defined species-stoichiometries as reactants and products. For example, if a database does not have a species defined with a stoichiometry of Al5Fe2 {e.g. the Al and Fe (but not Al5Fe2) may be defined as species, and the Al5Fe2 phase may be defined as a two-sublattice stoichiometric phase [Al]5[Fe]2, rather than a single sublattice stoichiometric phase [Al5Fe2]}, then the reaction 5Al+2Fe=Al5Fe2 cannot be tabulated.
- Make sure that the Gibbs free energy expression for a stoichiometric phase is really corresponding to the species-stoichiometry. For example, if a database has a definition of Function GAL5FE2 for 1/7 of the AL5FE2 formula, then the relation G(Al5Fe2)=7*GAL5FE2 must be defined; otherwise, the tabulated thermodynamic properties for the reaction 5Al+2Fe=Al5Fe2 is wrong.

Syntax	TABULATE_REACTION
Prompts	`Same reaction? /Y/:` This prompt displays if there is at least one reaction already defined either with the commands ENTER_REACTION or TABULATE_REACTION. The following prompts only display if `N` is entered.
	`Reaction: <Chemical reaction equation> & <RA+RB=PC+PD>`

Syntax	TABULATE_REACTION

	A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.
	`Pressure /100000/: <pressure of interest, in pa>`
	`Low temperature limit /298.15/: <T-low, in K> Specify the starting temperature K.`
	`High temperature limit /298.15/: <T-high, in K> Specify the ending temperature K. Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.`

	`Output file /Screen/: <Return for screen, or type a file name>` If you type `Return for screen`, a list of thermodynamic property changes for the defined/chosen reaction is shown as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program prompts:
	`Graphical output /Y/:` • For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. • For Y a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also asks which column is to be plotted on the resulting graph:
	`Plot column? /2/: <1 or 2 or 3 or 4 or 5 or 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module automatically opens, and all types of the POST module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the `POST:` prompt always takes you back to the TAB module.

Example

For the reaction Ga+S=GaS (using the SSUB database), the following table is obtained by typing <Enter> in the prompt Output file /SCREEN/, and the figure by typing `2` in the prompt `Plot column /2/:`

```
    O U T P U T   F R O M   T H E R M O - C A L C

     Reaction:  S+GA=GA1S1

  stable as S_S

  GA stable as GA_S
```

```
GA1S1 stable as GA1S1_S
Delta-Cp      Delta-H       Delta-S       Delta-G
(K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
************************************************************
298.15  -2.79489E+00  -2.09200E+05  -1.50580E+01  -2.04710E+05
300.00  -2.87516E+00  -2.09205E+05  -1.50755E+01  -2.04683E+05
302.   ---- GA becomes GA_L ,delta-H =   5589.80
367.   ---- S becomes S_S2 ,delta-H =    401.00
389.   ---- S becomes S_L ,delta-H =   1721.00
400.00  -1.22278E+01  -2.17521E+05  -4.07488E+01  -2.01222E+05
500.00  -1.57686E+01  -2.19323E+05  -4.47280E+01  -1.96959E+05
600.00  -1.02518E+01  -2.20583E+05  -4.70410E+01  -1.92359E+05
700.00  -6.58954E+00  -2.21430E+05  -4.83534E+01  -1.87583E+05
800.00  -4.46246E+00  -2.21963E+05  -4.90686E+01  -1.82709E+05
900.00  -2.82671E+00  -2.22328E+05  -4.94995E+01  -1.77778E+05
1000.00  -1.21787E+00  -2.22530E+05  -4.97138E+01  -1.72816E+05
1100.00   3.71702E-01  -2.22572E+05  -4.97552E+01  -1.67841E+05
```

TABULATE_SUBSTANCE



This command is for the TABULATE_REACTION (TAB) module.

Tabulate thermodynamic properties of a substance (with a given chemical formula but it is not certain in which phase/state it may form) or a pure stoichiometric phase (getting data from a specific substance database such as SSUB, or from a specific solution database such as SSOL and TCFE), or of a solution phase with a fixed composition (getting data from a specific solution database such as SSOL and TCFE), under a constant pressure and various temperatures.

In case of a pure stoichiometric phase or a solution phase with a fixed composition, you must already define the system and get thermodynamic data from an appropriate solution database in the TDB module before using this TAB command. The phase name can be given either upper or lower or mixed cases, and can be abbreviated until it is unique, e.g. `fcc`, `BCC`, `Liq`, `cem`, `Al5Fe2`, etc. as the SSOL database is used for the tabulations, or `GAS`, `FE-S`, `wustite`, `Fe2O3-hem`, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, you can tabulate thermodynamic properties for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Moreover, the variation for one of the tabulated properties for a substance, a pure stoichiometric phase, or a solution phase with a fixed composition can be plotted against temperature as a graph or saved as an experimental file (with an extension of .EXP).

Syntax	TABULATE_SUBSTANCE
Prompt	`Substance (phase): <Name of the species or phase>` In case of a substance, give its chemical formula, e.g. Fe, H2, C1H6, FeC1, CaC1O3, MgSiO3, etc. When the TABULATE_SUBSTANCE <SUBSTANCE> command sequence is used for the first time in the TAB module, it always uses the SSUB Substances database as the default. If SSUB is not available and a specific database has not been switched on yet, it may prompt to specify an appropriate substance or solution database (e.g. typing `SSUB<version number>`; `SSOL<version number>`; `TCFE<version number>` etc.). Prior to this command, you can also use SWITCH_DATABASE to set the current database. If a solution database is set as the current database, only the neutral species that are valid substance standing by themselves as phases can be tabulated.

Syntax	TABULATE_SUBSTANCE
	Before other prompts, a list of the used database, defined elements, getting-data sequence, references, etc. is displayed on screen. From such information, you know what the TAB module is performing. In case of a pure stoichiometric phase or a solution phase, give its phase name, e.g. FCC, CEMENTITE, LIQUID, SLAG, AQUEOUS, GAS, Al5Fe2, Fe-S, Wustite, Fe2O3-Hematite, etc. REMEMBER: It is important that you have already defined the system and gotten thermodynamic data from an appropriate solution database in the TDB module before using this TAB_SUB command. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase. For a pure stoichiometric phase defined with one single sublattice (such as Fe-S, Wustite, and Fe2O3-Hematite), no further composition definition is needed. For a solution phase defined with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests n-1 site-fraction inputs for the phase constituents (if there are *n* species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the *n*th species is automatically assigned as the rest. The sum of input site fractions must not exceed unity. For example, the following prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species is assigned as the rest):

	`Fraction of constituent (return for prompt): <Return>`
	`C /1/: .05`
	`CR /1/: .1`
	`FE /1/: <RETURN>`

	`Sum of fractions exceed unity, please reenter`
	`FE /1/: .8`
	`N /1/: .005`
	
	For a pure stoichiometric phase defined with two or more sublattices (such as Al5Fe2 inter-metallic stoichiometric phase) and for a solution phase defined with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution, Al5Fe4 inter-metallic solution phase), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice *n*-1 times if there are n species on such a sublattice in the defined phase; the *n*th species on each of the sublattices are automatically assigned as the rest. For example, these prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted `O` species on its sublattice `1` and `VA` on its sublattice `2` is assigned as the rest):

Syntax	TABULATE_SUBSTANCE

	`Specify sublattice (0 for all) /0/:`
	`FRACTIONS IN SUBLATTICE 1`
	`CR /1/: .1`
	`FE /1/: .8`
	`NI /1/: .0995`
	`FRACTIONS IN SUBLATTICE 2`
	`C /1/: .05`
	`N /1/: .05`

	`Pressure /100000/: <Pressure of interest, in pa>` Specify the constant pressure condition in Pa.
	`Low temperature limit /298.15/: <T-low, in K>` Specify the starting temperature K.
	`High temperature limit /298.15/: <T-high, in K>` Specify the ending temperature K.
	`Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.`
	`Output file /Screen/: <Return for screen, or type a file name>` If you type `Return for screen` a list of basic thermodynamic functions for the chosen substance or for the specified pure or solution phase with the fixed composition is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program further prompts:
	`Graphical output /Y/:` • For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. • For Y a table is created with all the thermodynamic functions as normal (which is displayed on screen) as well as generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also ask which column is to be plotted on the resulting graph:
	`Plot column ? /2/: <1 or 2 or 3 or 4 or 5 or 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.

Example 1

For the FCC alloy phase as a non-ideal solution with a fixed composition

```
[Fe0.80,Cr0.10,Ni0.0995,O0.005][C0.05,N0.05,VA0.90]
```

The following table is obtained by typing `Return for screen` at the prompt `Output file /SCREEN/`:

```
O U T P U T  F R O M  T H E R M O - C A L C
Phase : FCC                        Pressure :      100000.00
Specie: CR1/--2
************************************************************
    T      Cp            H             S             G
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
************************************************************
298.15   2.70517E+01   6.23824E+03   4.40241E+01  -6.88755E+03
300.00   2.70889E+01   6.28832E+03   4.41916E+01  -6.96915E+03
400.00   2.87304E+01   9.08420E+03   5.22235E+01  -1.18052E+04
500.00   2.99904E+01   1.20222E+04   5.87742E+01  -1.73649E+04
600.00   3.10889E+01   1.50770E+04   6.43408E+01  -2.35275E+04
700.00   3.21116E+01   1.82375E+04   6.92106E+01  -3.02100E+04
800.00   3.30994E+01   2.14982E+04   7.35633E+01  -3.73524E+04
900.00   3.40742E+01   2.48569E+04   7.75182E+01  -4.49094E+04
1000.00   3.50483E+01   2.83130E+04   8.11586E+01  -5.28456E+04
1100.00   3.60268E+01   3.18667E+04   8.45449E+01  -6.11327E+04
1200.00   3.70143E+01   3.55187E+04   8.77219E+01  -6.97476E+04
1300.00   3.80149E+01   3.92700E+04   9.07241E+01  -7.86713E+04
1400.00   3.90311E+01   4.31222E+04   9.35784E+01  -8.78875E+04
1500.00   4.00649E+01   4.70768E+04   9.63064E+01  -9.73827E+04
1600.00   4.11174E+01   5.11358E+04   9.89256E+01  -1.07145E+05
1700.00   4.21896E+01   5.53010E+04   1.01450E+02  -1.17165E+05
1800.00   4.33555E+01   5.95774E+04   1.03894E+02  -1.27433E+05
1900.00   4.58528E+01   6.40379E+04   1.06306E+02  -1.37943E+05
2000.00   4.75402E+01   6.87138E+04   1.08704E+02  -1.48694E+05
```

Example 2

For a phase, as either an end-member or real solution, the listed species name is irrelevant.

For the H2 species as a pure substance (using the SSUB5 database), the following table is obtained by typing `Return for screen` at the prompt `Output file /SCREEN/`, whilst the figure is generated by typing 5 at the prompt Plot column /2/:

```
          O U T P U T F R O M T H E R M O - C A L C

  Phase : GAS                         Pressure :      100000.00

Specie: H2

************************************************************    T      Cp
H             S             G

   (K)     (Joule/K)       (Joule)       (Joule/K)       (Joule)

************************************************************  298.15
2.88369E+01   3.17684E-06   1.30680E+02  -3.89622E+04

300.00   2.88473E+01   5.33580E+01   1.30858E+02  -3.92042E+04

400.00   2.91591E+01   2.95686E+03   1.39209E+02  -5.27268E+04

500.00   2.92650E+01   5.87874E+03   1.45729E+02  -6.69856E+04

600.00   2.93441E+01   8.80908E+03   1.51071E+02  -8.18336E+04

700.00   2.94579E+01   1.17488E+04   1.55602E+02  -9.71730E+04

800.00   2.96320E+01   1.47027E+04   1.59547E+02  -1.12935E+05

900.00   2.98786E+01   1.76776E+04   1.63050E+02  -1.29068E+05

1000.00   3.02043E+01   2.06810E+04   1.66214E+02  -1.45533E+05

1100.00   3.05319E+01   2.37171E+04   1.69108E+02  -1.62302E+05

1200.00   3.09281E+01   2.67897E+04   1.71781E+02  -1.79348E+05

1300.00   3.13615E+01   2.99040E+04   1.74274E+02  -1.96652E+05

1400.00   3.18115E+01   3.30625E+04   1.76614E+02  -2.14197E+05

1500.00   3.22641E+01   3.62664E+04   1.78824E+02  -2.31970E+05

1600.00   3.27094E+01   3.95151E+04   1.80921E+02  -2.49958E+05

1700.00   3.31406E+01   4.28078E+04   1.82917E+02  -2.68151E+05

1800.00   3.35526E+01   4.61426E+04   1.84823E+02  -2.86539E+05

1900.00   3.39415E+01   4.95175E+04   1.86648E+02  -3.05113E+05

2000.00   3.43045E+01   5.29300E+04   1.88398E+02  -3.23866E+05
```

REACTOR (REACTOR_SIMULATOR) Commands

In this section:

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CREATE_DIVIDERS



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Define the segment boundaries and the ways on how to distribute phases between various segments and to split the feeds of heat and mass.

Syntax	CREATE_DIVIDERS
Prompts	`Number of dividers /4/: <The number of dividers>` Specify the number of dividers (boundaries between various segments) in the reactor. It is normally the segment number plus one: for example, if the stage box number is defined as 4, the divider number should be defined as 5.
	`Number of outputs for divider # /3/: <The number of outputs>` Specify the number of outputs for a specific divider #.
	`Percent of input to output 1 /100/: <Percent of input>` Define the percentage of input to the output 1 in the current divider #.
	`Percent of input to output ## /100/: <Percent(s) of input(s)>` Define the percentages of inputs to the outputs ## in the current divider #. It is repeated till the last output is specified.

CREATE_PIPES



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Define the pipes between various segments and the ways on how the mass and heat transport between the surroundings (with the record number as 0) and the reactor, among various segments in the reactor, and along various dividers (segment boundaries in the reactor).

Syntax	CREATE_PIPES
Prompts	`From record: <A record number>` Specify a record number. If there are four segments in the reactor, these records are available: • `0` surroundings • `1-4` stage boxes (segments) • `5-9` dividers (segment boundaries)
	`Pipe to record: <Another record number>` Specify another record number to which the mass or heat flows from the current record (specified above). Before this prompt, a message shown on the screen indicates what kind of mass or heat flow (according to the definitions of stage boxes and dividers, which have already been created prior to this command) should be specified in the pipe. This is repeated for all inputs and/or outputs for mass and/or heat in current record.

CREATE_STAGE_BOXES

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Create several reaction stages as boxes (segments), where the you define the feed in either mass input and initial temperature or heat input from surroundings, as well as the mass out and initial temperature in each of the segments.

Syntax	CREATE_STAGE_BOXES
Prompts	`Number of stage boxes /4/: <The number of stage boxes>` Specify the number of stage boxes in the reactor. Then define the feed of mass and/or energy (from surroundings to) the rector.
	`Give feed to system: <Feed>` One feed (of mass or heat) to the reactor must be specified here. Two types of feeds can be used: • As input amount of heat (enthalpy): `H=Value`. • As input amount of specific species or element and its initial temperature: `N(SPECIES)=Value, Input temperature` (in one line, or the input temperature in the next prompt).
	`Input temperature /298.15/: <Input temperature>`

	`Give feed to system: <Feed>`
	Specify other feeds (mass or energy) to the reactor. Press <Enter> to finish the feed inputs, and then:
	`Give for stage box #`
	Now start to define the type of stage box (segment is specifically numbered as #), and to specify a guess of initial temperature and an output for each phase in the segment.

	`Type of box/Equilibrium/: <Type of box>` Only the `EQUILIBRIUM` type is allowed. Press <Enter> to accept it.
	`Is the stage heat controlled? /Y/: <Yes or No>` Y means the current segment is heat controlled.
	`Initial guess of temperature? /1000/: <Initial temperature>` Give a guess of initial temperature (in K) for the current segment; press <Enter> to accept the default.
	`Give initial amount: <Initial amount of mass or heat>` The initial amount of mass and/or heat in the current segment can be specified here. Two types of initial amount can be used: • As initial amount of heat (enthalpy): `H=Value`. • As initial amount of specific species or element and its initial temperature: `N(SPECIES)=Value, Input temperature` (in one line, or the input temperature in the next

Syntax	CREATE_STAGE_BOXES
	prompt).
	`Input temperature /298.15/: <Input temperature>`

	`Give initial amount: <Initial amount of mass or heat>`
	Specify initial amount (mass or energy) in the current segment. Press <Enter> to finish the initial amount inputs, and then this message displays:
	`Each phase may have a separate output, give these`
	Now start to define the output for each phase.

	`Phase name /Rest/: <Name of phase>` Specify a phase that has a separate output, e.g. `GAS`; by pressing <Enter> to accept that all `REST` phases do not have separate outputs. Then the program asks for further definitions of all the other segments (one by one), repeating some of the above questions, till the last segment in the reactor is defined.

EXECUTE_POLY3_COMMAND



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Syntax	EXECUTE_POLY3_COMMAND
	To directly use all kinds of POLY commands inside the REACTOR module. Any legal POLY commands can be entered. POLY Module Commands

LIST_RECORDS

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Syntax	LIST_RECORDS
	Lists all the already-created records for the reactor (including stage boxes, dividers, pipes, etc.).

READ_WORKSPACE



This command is for the REACTOR_SIMULATOR (REACTOR) module.

The REACTOR workspace (along with the related POLY and GIBBS workspaces) and the simulated results from the SIMULATE command can be read by this command from a binary file where they must be saved with SAVE_WORKSPACE. The *.RCT file is not printable.

Syntax	READ_WORKSPACE
Options	`File name`: The name of a saved *.RCT file where the REACTOR and POLY/GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default .RCT, otherwise type the whole *.RCT file name. An **Open** window displays if a file name is not given after the command or its path is incorrect, so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. RCT) cannot be changed.

SAVE_WORKSPACES

This command is for the REACTOR_SIMULATOR (REACTOR) module.

The POLY module and Gibbs (GES) module also have a command with the same name.

The workspaces are saved to a file with this command. In the REACTOR workspace, all definitions of multi-stage steady-state rector and its distribution coefficients are saved, together with the GIBBS and POLY workspaces.

After using this command, you can always return to the state when you issued the command by giving a READ command.

After saving the workspaces to a file, you can exit the software and at a later time READ the file and continue from the saved state.

START_SIMULATION automatically saves on the work file with the most lately specified name. To avoid destroying the simulated results, do not SAVE after a START_SIMULATE command is enforced, similar to that you should not use SAVE after a STEP or MAP command. You may append several results by START_SIMULATE without destroying the previous results but SAVE erases them all.

Syntax	SAVE_WORKSPACES
	`File name` A file name must be specified. The default extension of the RCT file is .RCT, while or any other extension as required.
	A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** (i.e. RCT) cannot be changed. If there is already a file with the same file name under the directory a warming message displays. Click **OK** to overwrite the current REACTOR (and POLY3/GIBBS) workspaces onto the existing *.RCT file. Click **Cancel** to return to the REACTOR module. You can use the SAVE command with an unspecified name (i.e. through `SAVE ,,,` command-sequence) to save the REACTOR (and POLY3/GIBBS) workspaces.

START_SIMULATION

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Start the reactor simulation, and list the results for all iterations. The output for each iteration consists of the conditions set in each segment, and you can also select some state variables to list. After each loop, the temperatures in all segments are listed.

Syntax	START_SIMULATION
Prompts	`Max number of loops /10/: <The max number of loops>` Give the max number of loops. The reactor simulation repeats until this loop number is reached.
	`Output to screen or file /Screen/: <File name or return>` Decide on either listing simulation results on the screen (by pressing <Enter>) or saving them on an experimental file (with the default extension .EXP). The conditions in each segment are not saved in the file, only on the screen.
	`Output variables /T BP($)/: <Variable name(s)>` Specify the variable name(s) that is also listed on the screen together with the conditions in each segment, or in the output experimental file.

Example

For a four-stage reactor, the output at a certain iteration may look like this:

```
H=-991745.1, P=100000, N(C)=2.8468936, N(N)=6.78399966E-4, N(O)=3.8171615,
N(SI)=1.77031
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588099,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-924751,87, P=100000, N(C)=2.0594558, N(N)=5.17999978E-4, N(O)=4.0142358,
N(SI)=2.7551438
```

```
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-813239., P=100000, N(C)=1.6592668, N(N)=3.59999988E-4, N(O)=3.7549293,
N(SI)=2.896635
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=7374.6403, P=100000, N(C)=8.84911857E-1, N(N)=1.99999996E-4, N(O)=1.9379203,N
(SI)=1.853872
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175982, BP(C_S)=8.1588097,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
10  1788.03  2065.69  2086.91  2208.31     0.00     0.00     0.00
```

POST Module Commands

The POST module (post-processor) is available from the these modules: POLY, TAB, BIN, TERN, POT, SCHEIL and POURBAIX.

- Using the POST Module

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ADD_LABEL_TEXT

Add a text to an area in a phase diagram or a property diagram. The label is written starting from the specified coordinates. Optionally, you can also let the program automatically add the text by first calculating an equilibrium state at the specified coordinates and then making a label out of the stable phase names.

The label texts and coordinates, either added by this command or modified with MODIFY_LABEL_TEXT (or manually edited in the **Console Results** window), are stored in the workspace, and these may later be saved onto an *.EXP file (with MAKE_EXPERIMENTAL_DATAFILE).



In some cases such an optional calculation for automatic phase region labeling may not work. It is not possible to automatically add labels for certain sets of axes, like entropy, enthalpy, pH, Eh, etc.

Plot Labels

Syntax	ADD_LABEL_TEXT
Prompts	`Give X coordinate in axis units: <Value of the X coordinate>` Specify the value of the X coordinate where the label is to start.
	`Give Y coordinate in axis units: <Value of the X coordinate>`  The labels disappear if any axis is changed after wards. Specify the value of the Y coordinate where the label is to start.
	`Automatic phase labels? /Y/:` By default the program automatically calculates the equilibrium at the given coordinates and generates a label with the names of the stable phases. However, the automatic calculation works only for phase diagrams that are mapped with two axes in the POLY module, and sometimes it may not work correctly especially for complex heterogeneous interaction systems; in such cases, a message displays.

	`Text: <Text for the label>`
	If you answer N enter text at the prompt. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.
	LaTeX: You can use LaTeX commands to enter text and symbols. First enter the command followed by the expression or string, for example to display Al2O3 as subscripts:
	`\latex Mole-fraction Al_2O_3`

Syntax	ADD_LABEL_TEXT

	For a list of supported LaTeX commands, see http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html.
	
	By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.
	
	To add a mixture of plain text and equation text, you can exit math mode using the string `\textrm` followed by the text to display enclosed in curly brackets. For example `\latex \textrm{Mole-fraction }Al_2O_3` displays this label Mole-fraction Al_2O_3.
	
	Rotate the text: If you want to rotate the label, start a text string with the rotation command (which is case sensitive and must be in lower case letters) then enter the number of degrees to rotate the label. For example, to rotate the label 45 degrees enter:
	
	`\rotation 45`
	
	To rotate the text and use LaTeX, the rotation command must be used first. For example:
	
	`\rotation 45 \latex Mole-fraction Al_2O_3`
	
	Rotates the text 45° and includes subscripts in the title Mole-fraction Al2O3.

	`Text size: /.35/: <Size for the label>` A smaller size of the text may be necessary to fit the label text into the diagram. A default size is given using the latest size in adding label texts, or .35 if the command is called for the first time. A recommended size is e.g. 0.25. These changes to plot labels can also be manually edited in the **Console Results** window.

APPEND_EXPERIMENTAL_DATA

Add experimental data and text onto a calculated diagram. This is done by placing the experimental data and text on a formatted textual file (always having an extension of EXP) that is prepared outside of Thermo-Calc software (Console Mode and Graphical Mode), according to the syntax of the DATAPLOT Graphical Language.

The picture generated from the data is superimposed on the ordinary graphical output from the postprocessor. Such an experimental data file (*.EXP) may be created by an ordinary textual editor.

Another important usage of this command is to superimpose plots from several independent calculations. For this purpose, there is a command MAKE_EXPERIMENTAL_DATAFILE, which dumps a calculated diagram on an EXP file according to the DATAPLOT syntax. With the aid of a normal text editor, many such files may be merged together. Remember that you can only have one prologue section on each such EXP file.

- *DATAPLOT User Guide* included with this documentation set.

Syntax	APPEND_EXPERIMENTAL_DATA
Prompts	`Use experimental data (Y or N) /N/:` By default, no experimental data are plotted. Enter Y to use the data from an experimental data file in the next plot. An **Open** window displays to specify the name of the file with the experimental data.
	`Prologue number: /0/: <Prologue number>` Select which prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on.  By answering -1, a list of all prologues on the file is given; and by 0, no experimental data are appended.
	`Dataset number(s) /-1/: <Dataset number(s)>` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and by 0, no experimental data are appended.

CHANGE_LEGEND

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

LIST_EQUILIBRIUM also displays `ORD` (ordered) or `DISORD` (disordered) (when available).

In some cases the legend only shows the phase name for a line when SET_LABEL_CURVE_OPTION is set to `F`.

Syntax	CHANGE_LEGEND
Prompt	`Set suffix for phase names in legend? (All, None, Constitution, Ordering)/None/:` • `None`: the legend includes the standard information about the phases. • `All`: the Constitution description and the Ordering description (when there is ordering) are also included. • `Constitution`: it is added to the standard description. • `Ordering` (when applicable): it is added to the standard description.
	For examples and more details about what these options show, see About Legend Styles and Legend and Label Styles where it is described for Graphical Mode.

DUMP_DIAGRAM

This is an alternative command used to create output. First use the PLOT_DIAGRAM command to send output to the Results window. Then you can save it to a file either using this command or right-click the diagram in the Results window and select Save as.



Similar to PRINT_DIAGRAM, it does not matter what graphic device/printer is set up. The command can convert the diagram shown in the Results window to the selected format.

Syntax	DUMP_DIAGRAM
Prompt	`Output format/: (jpg,ps,pdf,svg,emf,gif,png) /png/`
	Enter a format or press <Enter> to accept the default (png).  If you choose to enter the parameters and file name in one line (i.e. when you are entering the command), the **Save** window does not open as described below. For example, if you enter `dump_diagram png test` at the prompt, an image file called **test.png** is output to the same folder where the macro file is stored. If a file with the specified name already exists, you are prompted to overwrite the old file. You can alternatively add `Y` or `N` to the command string to specify whether to overwrite the file or not e.g. `dump_diagram png test y`. A **Save** window opens if you have not specified a file name. Select a directory path and enter a **File name**. If a file with the specified name already exists, then you are prompted whether to overwrite the old file or not. The third argument of the command (Y) allows you to specify whether to overwrite the old file or not (N).



After the output is done, the temporarily set graphic device for conversion and printing is switched back to the one set by the command SET_PLOT_FORMAT, so that you can save the graph in file(s) using PLOT_DIAGRAM.

ENTER_SYMBOL

This command is for the POST module.

There are also a GES and POLY module commands with the same name.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command STEP_WITH_OPTIONS) or mapping calculation (enforced by MAP). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using EVALUATE_FUNCTIONS before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.



See example 44 for an example of using variables and functions.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Syntax	ENTER_SYMBOL
Prompt	`Constant, Variable, Function or Table? /Function/: <Keyword>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION` or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER_CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable

Syntax	ENTER_SYMBOL
	with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST.  There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`Name: <Name of the symbol>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.  For different types of symbol (constant, function, variable or table), the questions have different prompts.

	`Function: <Definition for a function or variable>`
	Functions and *variables* are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).
	Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS` and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).
	Examples of function expressions:
	• `GM(LIQUID)`: The Gibbs energy of liquid per mole component
	• `H.T/4.184`: The heat capacity of the system in calories
	• `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
	• `T-273.15`: The temperature in Celsius
	`&: <Continuation of the definition for the symbol>`
	The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.

	`Value: <Value for a constant>` A *constant* can only be assigned a numeric value once.
	`Value or expression: <Value of expression for a variable>`

Syntax	ENTER_SYMBOL
	A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

	`Variable(s): <Variable(s) in a table>`
	
	A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.
	
	Example:
	
	`ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)`
	
	Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.
	
	To show the temperature in Celsius in a table, give the command ENTER_FUNCTION `TC=T-273`; and then use the symbol `TC` in the table.
	
	`& <Continuation of the definition for the table>`
	
	The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press `<Enter>` again.

FIND_LINE

Identifies various property curves on a plotted property diagram (after a stepping calculation); it also works well in find stable phase regions on a phase diagram (after a mapping calculation).

Syntax	FIND_LINE
Prompts	`X coordinate /.484623611/: <Value of the X coordinate>` Specify the `value of the X coordinate` where you want to find the details of property curve (or phase region).
	`Y coordinate /.5153737962/: <Value of the Y coordinate>` Specify the `value of the Y coordinate` where you want to find the details of property curve (or phase region). The POST module displays the identified property (for a property curve on a property diagram), or the identified stable phase-assemblage (for a phase region on a phase diagram).

LIST_DATA_TABLE

This is a POST module command.

This command is used for listing various properties (i.e. the Y-axis variable on a property diagram) that change with an independent variable (i.e. the X-axis variable on a property diagram), which have already been defined in the POST module (and often are plotted on the **Console Results** window), but only after a STEP calculation.

The listing output can be either on screen or in a spreadsheet file in the MS Excel format (under specified file name with the default file extension of XLS), which can be further edited or used for graphical handling by opening the file (using the MS-Excel program) outside of the Thermo-Calc software system.

Syntax	LIST_DATA_TABLE
Prompt	`Output to screen or file /Screen/: <File name or return >` Specify a file name if you want to save on a spreadsheet file (in the MS Excel format, with the default extension of `XLS`) on which the already-defined properties on a property diagram (after a STEP calculation) is saved, or press <Enter> if want to see a simple textual table on screen (for the already-defined properties that change alone with an independent variable). This command only works for a property diagram after a stepping calculation but not for any phase diagram after a mapping calculation.

LIST_PLOT_SETTINGS



This is a POST module command.

Syntax	LIST_PLOT_SETTINGS
	Lists the present values of most parameters specifying the type of diagram to be plotted.

LIST_SYMBOLS



This command is for the POST module.



There is also a POLY module command with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

MAKE_EXPERIMENTAL_DATAFILE

Write the graphical information onto screen or a formatted text file (always having an extension of .EXP) using the DATAPLOT graphical format. In order to merge two or more diagrams from separate calculations, you can write them out on files with this command, and then add/edit them together with a normal text editor.



There is another type of experimental data file that is generated in Thermo-Calc when working with the PARROT module. For more information seeExperimental Data Files (*.POP, *.DOP).

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	`Output to screen or file /Screen/: <Name of a file or return>` Specify the name of the desired file. Press <Enter> for a list. Otherwise enter a file name where the graphical information is written. The default file extension is `EXP` (for Windows) or `exp` (for Linux).

MODIFY_LABEL_TEXT

Move a label created with the command ADD_LABEL_TEXT to another position, or replace its text with another one.

The label texts and the coordinates, either added by ADD_LABEL_TEXT command or modified by this command or manually edited on the Console Results window, are stored in the workspace, and can be saved onto an *.EXP file (through MAKE_EXPERIMENTAL_DATAFILE).

Syntax	MODIFY_LABEL_TEXT
Prompts	`Which label to modify? /#/: <Number of the label>` Before this prompt, all the labels created by the ADD_LABEL_TEXT command is listed with an identifying number. Specify the `Number of the label` you want to modify. The default one (#) is the last added label.
	`New X coordinate: /xxx/: <New X position>` Specify the `New X position`. The previous X coordinate is displayed. Press <Enter> to accept.
	`New Y coordinate: /yyy/: <New Y position>` Specify the `New Y position`. The previous Y coordinate is displayed. Press <Enter> to accept.
	`New text /ABCDEFGH.../: <New labeling text>` Specify the `New labeling text`. The previous text is displayed. Press <Enter> to accept.  The new label text must not be longer than the previous text.

PLOT_DIAGRAM

After you use the SET_PLOT_FORMAT command to define the default graphic device (the printer) you can use a PLOT_DIAGRAM command to either save the calculation output to a file or display the output in the Results window.



The diagram axes must be set first.

The functionality of this command is shared in two ways:

- in PLOT_DIAGRAM for normal screen display and file saving and
- *Windows OS*: If the device is not defined, you can alternatively use PRINT_DIAGRAM for a hard copy.

Syntax	PLOT_DIAGRAM
Prompt	`Output to screen or file /Screen/: <Name of a file or return for screen>` `Specify the name of the file`
	 For Linux users, the prompt is `PLOTFILE /SCREEN/`). A file with a proper extension for the selected graphic format (set by SET_PLOT_FORMAT) is saved under the current working directory. If no extension is given in the file name, the default extension e.g. ps for Postscript portrait/landscape modes, P7 or p7 for HPGL landscape, P8 or p8 for HPGL portrait, etc.) is automatically given to the file name. If the default device is set (SET_PLOT_FORMAT), press <Enter> to plot the diagram on the screen in the Console Results window or give a file name to save it.

PRINT_DIAGRAM

Saving and Printing the Output in Console Mode

First use PLOT_DIAGRAM to create a diagram that displays in the **Console Results** window. Then after entering the PRINT_DIAGRAM command, the **Print** window opens where you can choose additional settings for a hard copy of the diagram.



PRINT_DIAGRAM functions in the same way as in the **Console Results** window where you can right-click a diagram and choose **Print**.

QUICK_EXPERIMENTAL_PLOT

This is similar to APPEND_EXPERIMENTAL_DATA but can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axes, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

- Plotting Experimental Data Files in the *DATPLOT User Guide* included with this documentation set.

Syntax	QUICK_EXPERIMENTAL_PLOT
Prompts	`Prologue number: /0/: <Prologue number>` An **Open** window displays. Select the prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and with 0, no experimental data are appended.
	`Dataset number(s) /-1/: <Dataset number(s)>` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering `-1`, a list of all datasets on the file is given; and with `0`, no experimental data are appended.

REINITIATE_PLOT_SETTINGS

The REINITIATE_PLOT_SETTINGS command gives default values to all parameters describing the diagram. All plot settings made in the POST module are deleted, and it returns to the initial settings when the POST module is entered.

RESTORE_PHASE_IN_PLOT

Restores a phase previously suspended from the plot with SUSPEND_PHASE_IN_PLOT. It works only after at least one phase is suspended.

Syntax	RESTORE_PHASE_IN_PLOT
Prompt	`Phase name: <Name of a phase>` Give the name of the phase to be restored.

SELECT_PLOT

Select a plot (diagram) within the current **Results** tab in the **Console Results** window.

Syntax	SELECT_PLOT
Prompt	`Plot <N/New>` Where `N` is a positive integer. Enter the number of the plot that is selected in the **Console Results** window (in the currently selected **Results** tab). If a plot with that number does not exist, it is created. The default parameter value is `NEW`. If this is entered, then a new plot is created. Create a new plot can also be done by pressing <Ctrl+Shift+T>.

SET_AXIS_LENGTH

Change the real length of an axis in inches. The default number of tic-marks on an axis is 10 when the relative length is 1. The number and units per tic-mark must be a multiple of 1, 2 or 5 to obtain a reasonable scaling of an axis.

Syntax	SET_AXIS_LENGTH
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis to set the length.
	`Axis length /11.5/: <New relative axis length>` Specify the new real axis length in inches. The relative length 1 corresponds to 10 tic-marks on the axis.

SET_AXIS_PLOT_STATUS

Specify whether the axis title texts and axis label texts are to be plotted or not on a diagram. It does not work for the axis lines and tic-marks. If you want to plot a diagram without tic-marks, use SET_TIC_TYPE first.

This can be used to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default status is that all the set axes are to be plotted.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	`Axis plot (Y or N) /Y/: (Y or N)`

SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to a text.

- ADD_LABEL_TEXT

Syntax	SET_AXIS_TEXT_STATUS
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis text status to change.
	`Automatic axis text (Y or N) /N/:` Specify if automatic axis text is to be used.
	`Axis text: <Enter axis text>` You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.

SET_AXIS_TYPE

Change the axis type among linear, logarithmic and inverse axis.

Syntax	SET_AXIS_TYPE
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis to change the axis type.
	`Axis type /Linear/: <New axis type>` Specify which new axis type to set. Select `LIN`ear (default), `LOG`arithmic or `INV`erse. Only the three first characters are relevant.

SET_COLOR

Some devices support colours or line thickness. With this command, select different colors or line types on some types of information on a diagram.



This command can fail if a chosen device does not support colors or line thickness.

This command gives four sequential prompts (i.e. text and axis, invariant equilibria, tie-lines, and all other lines), with the keyword and default option (both listed below). Depending on if the switched-on graphic device (by SET_PLOT_FORMAT) supports colors or line types, the POST automatically switches on the appropriate Keyword.

Syntax	SET_COLOR

Prompt	`Text and axis keyword /Default option/`
	`<Return or new option>`
	`Invariant equilibria keyword /Default option/: <Return or new option>`
	`Tie-lines color keyword /Default option/: <Return or new option>`
	`Keyword of all other lines /Default option/: <Return or new option>`
	This is usually for the solubility lines.

	 The `Keyword` is either `Color` or `LineType`, depending on if color or line type is supported by the switched-on graphic device (by SET_PLOT_FORMAT); the POST module *automatically* switches on the appropriate `Keyword` .

Color Options

The options for `Color` are:

BACKGROUND	BLUE	PURPLE	GRAY
FOREGROUND (default)	YELLOW	GOLD4	ORANGERED3
RED (default for invariant equilibria)	MAGENTA	TURQUOISE4	MAROON
GREEN (default for tie lines)	CYAN	PINK	PLUM
	SIENNA	OLIVEDRAB	SEAGREEN
	ORANGE1	CORAL1	USERDEF

LineType Options

The options for `LineType` are:

INVISIBLE	VERY_THICK (default for invariant equilibria)
NORMAL (default)	THIN (default for tie lines)
THICK	VERY_THIN
DASHED	DOTTED

SET_CORNER_TEXT

Adds text to the corners on a plotted diagram. Normally, you can write such texts as a subtitle.

The primary database (not the appended ones) used in calculations and the calculated conditions are automatically plotted at the upper-left corner as a part of the header on all plotted diagram. Unless the plotting option WRITE CONDITIONS is switched off by the command SET_PLOT_OPTIONS, the calculated conditions are always written on plotted diagrams; and only when the plotting option PLOT HEADER is switched off by the command SET_PLOT_OPTIONS, the used database also always appear. Under such circumstance, avoid writing texts at the UPPER_LEFT corners.

Syntax	SET_CORNER_TEXT
Prompt	`Corner/Lower_Left/: <Return or new option>` Choose an option: • LOWER_LEFT • UPPER_LEFT • UPPER_RIGHT • LOWER_RIGHT • TOP_OF_TRIANGLE
	`Text: <Texts as a subtitle or a note>` Write the texts that are to be written on the specified diagram corner.

SET_DIAGRAM_AXIS

Specify an axis variable for a plot or a listing. To be able to plot a diagram, at least two axis variables (X and Y) must be specified. In Console Mode, three axes (X, Y, and Z) can be specified for a diagram.



The axis variables in the plot can be different from the number of axis used for the mapping.

If you want to plot a phase diagram with tie-lines in the plane after a MAP calculation, then the composition axis must be `mole-fraction` or `weight-fraction`, or `mole-percent` or `weight-percent` of one specific component. You must not use the stable variable `x(comp)` or `w(comp)` even if that is what you used when calculating the diagram, because that only gives one side of the two-phase region. It may be sufficient to indicate that mole-fraction is the same as the stable variable `x(*,comp)`, and weight-fraction is the same as the stable variable `w(*,comp)`.

If you plot a phase diagram where the tie-lines are not in the plane after a MAP calculation, then `mole-fraction` and `x(comp)` are identical.

When you plot a property diagram after a STEP calculation and want a composition axis variable, you should normally use x(comp) and not mole-fraction.

The axis must have exactly the same number of columns, or one axis must have one column. In the first case the columns are plotted matching them one by one; in the latter all columns on one axis is plotted against the single column. For example, you can have the temperature on one axis and the amount of each phase on the other. The amount of each phase is the state variable `NP(*)` in mole fraction or `BPW(*)` for mass fractions of phases.

Automatic diagram axis: The POST module can set automatic diagram axis identical to those used in the MAP command.

If the state variable `x(comp)` is used in a MAP calculation, then mole-fraction of the component is used as diagram axis; if a potential or some other state variables are used, then that is used as a diagram axis.

After a STEP calculation, automatic diagram axis is not set as there is only one axis used in the calculation.

Syntax	SET_DIAGRAM_AXIS
	`Axis (X, Y or Z): <Axis name>` Specify which axis (X or Y or Z) to set with a variable.
Prompts	`Variable type: <Variable name>`

Syntax	SET_DIAGRAM_AXIS
	Specify a variable for the chosen axis here. The valid variables are: • TEMPERATURE-CELSIUS as temperature in °C • TEMPERATURE as temperature in K • PRESSURE as pressure in Pa • ACTIVITY for a component • LNACTIVITY for a component [ln(ACR(component)] • MOLE-FRACTION for a component • MOLE-PERCENT for a component • WEIGHT-FRACTION for a component • WEIGHT-PERCENT for a component • ENTHALPY as enthalpy in J/mol • ENTROPY as entropy in J/mol/K • NONE to clear the axis • Any valid state variable including those with wildcards, e.g. NP(*) or x(*,component). Due to the use of wildcard * in such a state variable, the program asks for a column number. • Any entered function or variable. • Any entered table.
	If you specify an entered table as the variable, then you are given these prompts: `For component: <Component name>` When an activity, mole or weight fraction or percent of a component shall be plotted, the component name must be supplied here.
	`Column number: <Column number(s)>` Specify the column number(s) in the chosen table that are to be plotted onto the earlier specified axis. For example: • `1` for column 1 • `2,3` for columns 2 and 3 • `2,3 >5` for column 2,3 and all columns above column 5 • `*` for all columns

SET_DIAGRAM_TYPE

Choose the diagram type as perpendicular plot or triangular plot (Gibbs triangle, especially for ternary systems). The default is with a perpendicular axes.

For phase diagrams of ternary or pseudo-ternary systems, it is usually need to plot isothermal sections as triangular grams. If desired, all lines outside the region limited by a line joining the end points of the X- and Y-axis is removed.

Syntax	SET_DIAGRAM_TYPE

Prompts	`Triangular diagram (Y or N) /N/:`
	The default is to set a perpendicular axis. Perpendicular diagrams have (almost) the same scaling on both axes.
	`Create tetrahedron WRML file (Y or N) /N/:`
	  The 3D plotting in Console Mode does not work. Enter Y to specify a triangular plot instead.

	`Plot 3rd axis (Y or N) /N/:` If a triangular plot is selected, enter Y to specify a 3rd axis and to connect (and plot) the end points of the X- and Y-axes.
	`Clip along 3rd axis (Y or N) /N/:` If a triangular plot is selected, enter Y so that all lines outside the region limited by a line joining the end points of the X- and Y-axis are removed.

SET_FONT

Select the font to use for labels and numbers when plotting the diagram under the currently selected graphic device (SET_PLOT_FORMAT). For some devices there may be other fonts available and these are selected by SET_PLOT_FORMAT.

Syntax	SET_FONT
Prompts	`Select font number /1/: <#>` Specify an available font number # as the default font for the current graphic device, or accept the font number 1 by pressing <Enter>. By typing a question mark `?` here, the program lists the available fonts under the currently selected graphic device.
	`Font size /.34/: <##>` The size of the chosen font is specified. A value around 0.34 is recommended.

SET_INTERACTIVE_MODE



In the POLY module this is called SET_INTERACTIVE.

Use the SET_INTERACTIVE_MODE command to use it in demonstration or macro files to stop the execution of the command file and pass over input focus to the keyboard.

SET_LABEL_CURVE_OPTION

Identify the curves drawn in the post-processor by marking each curve with a digit and then list the meaning of these digits beside the plot.



The number of digits can be quite large in some cases. If so, use SET_FONT and reduce the font size; usually, 0.2 is sufficient.

Syntax	SET_LABEL_CURVE_OPTION
Prompt	`Curve label option (A, B, C, D, E, F OR N) /A/: <Option>`

	The options:
	• `A`: List stable phases along line
	• `B`: As A but curves with same fixed phase have same number
	• `C`: List axis quantities
	• `D`: As `C` but curves with same quantities have same number
	• `E`: As `B` with changing colors
	• `F`: As `D` with changing colors
	• `N`: No labels
	This question is rather cryptic but usually the option B or E is good for phase diagrams (after a MAP command) and option D or F for property diagrams (after a STEP command). Those interested can try out the option A and C by themselves.
	  Option B or E lists the fixed phases along each curve, whereas option D or F gives the axis variables used along each curve. E provides varied colors for different stable-phase curves on phase diagrams (after a MAP command); F provides varied colors for different property curves on property diagrams (after a STEP command). The option `N` (NONE) disables all curve labels and lists.
	If, for example, you use `T` (temperature in K) as the variable axis in a STEP command and then plot the amount of stable phases (with SET_DIAGRAM_AXIS `Y NP(*)`) on the Y-axis versus `T-C` on the X-axis, then the list may have lines like:
	`1: T-273.15, NP(LIQUID)`
	`2: T-273.15, NP(FCC_A1)`
	This means that for curve `1` the X-axis is `T-273.15` (the same for all curves, of course) and `NP(LIQUID)` on the Y-axis. Curve `2` has the same X-axis but `NP(FCC_A1)` on the Y-axis.

SET_PLOT_FORMAT

Adjust the format of the graphical output to another graphical device. This default can be changed with the SET_PLOT_ENVIRONMENT command in the SYSTEM MONITOR.

Syntax	SET_PLOT_FORMAT
Prompt	`Graphic device number /#/: <Number of the device>` Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark `?`. For some formats there can be additional sub-prompts (Y or N) about the available fonts being used for the chosen format. Also enter Y for further specifications, e.g. font type and size.

SET_PLOT_OPTIONS

You are prompted for and can toggle on (`Y`) or off (`N`) the plotting of some options on all subsequently generated diagrams.

For the `Always initiate POST on re-entering` prompt, the default is Y which implies that the POST module automatically reinitiates whenever the POLY3 workspace is changed upon re-entering. If answered N the same diagram axis variables are kept even if the workspaces in the POLY module are read from or written to a *.POLY3 file. The N answer is useful when there are several sets of *.POLY3 files with the same calculation but for different sets of model parameters.

For the `Always solid line` prompt, the default answer is `N` which means that the POST module plots solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When the alternative answer Y is chosen, all the lines are always plotted in solid lines.

Syntax	SET_PLOT_OPTIONS
Prompts	`Plot header /Y/:` Toggle the plotting of the header text above a diagram.
	`Plot logo /Y/:` Toggle the plotting of the Thermo-Calc logo at the lower-left corner of a diagram.
	`Plot footer /Y/:` Toggle the plotting of the footer identifier text at the right margin of a diagram.
	`White-Contoured-PS-CHARS /Y/:` By default, the PostScript characters are written as a white contoured status.
	`Plot remote exponent(s) /Y/:` By default the remote exponent on the axis is plotted.
	`Plot symbols at node points /0/: <#>` This makes it possible to plot symbols at the node points on plotted lines on a diagram.
	`Symbol size /.1/: <.#>` Set the size of symbols which are plotted at the node points.
	`Write condition? /Y/:` By default, the initial equilibrium conditions for the current calculations are automatically plotted at the upper-left corner as a part of the header. If you enter N, the calculated conditions are not included on a plotted diagram.
	`Write database name? /Y/:`

Syntax	SET_PLOT_OPTIONS
	By default, the primary database (not appended ones) used in the current calculations are plotted at the upper-left corner as a part of the header. If you enter N, the database name is not included on a plotted diagram.
	`Always initiate POST on re-entering: /Y/:` By default the POST module automatically reinitiates whenever the POLY3 workspaces are changed upon re-entering. If you enter N, the same diagram axis variables are kept even if the workspaces in the POLY module is read from or written to a *.POLY3 file. This can be useful when there are several sets of *.POLY3 files with the same calculation but for different set of model parameters.
	`Always solid line: /N/:` By default the POST module plots solid lines for stable phases and dashed lines for metastable phases. This is normally for plotting property diagrams after a STEPPING calculation. However, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. Enter Y to always plot solid lines in this case, for example.

SET_PLOT_SIZE

Change the size of the diagram by specifying a global plot size (as a relative scaling factor). The default value of the relative scaling factor is 1, while the real size of the plotted diagram depends on what output device is chosen with SET_PLOT_FORMAT. The default plot size (corresponding to the default global plot size 1) is adjusted to the chosen device.

Syntax	SET_PLOT_SIZE
Prompt	`Global plot size /1/: <Relative scaling factor>` Enter the relative scaling factor as a numerical number (e.g. `0.5`, `0.8`, `1.0`, `1.5`, etc.). By pressing <Enter>, the default relative scaling factor (`1`) is accepted.

SET_PREFIX_SCALING

Specify on which axis is to have a prefix scaling then set the scaling of remote exponents with certain powers.

Syntax	SET_PREFIX_SCALING
Prompt	`Axis (X, Y or Z): <Name of an axis>` Specify which axis is to have a prefix scaling.
	`Use prefix scaling /Y/: (Y or N or #)` • `NO` switches off its action. • `YES` arranges the prefix scaling so that the axis scaling is done with the remote exponents being powers of three, i.e. `. . . , -6, -3, 0, 3, 6, . . .` . The default is 3. • # is an integer number that sets the remote exponents as being powers of # (as the powers for the remote exponents).

SET_RASTER_STATUS

Plot a raster (i.e. with gridlines on both axis directions) in the diagram.

Syntax	SET_RASTER_STATUS
Prompt	`Raster plot (Y or N) /N/:` By default no raster is plotted. Enter Y to plot using a raster plot.

SET_REFERENCE_STATE

This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials, and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature, and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials, and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC (O2,GAS), LNACR(O2,GAS).

For the POST module, and after calculating with the STEP_WITH_OPTIONS or MAP commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. MUR(comp), MUR (comp,ph), ACR(comp), ACR(comp,ph) or the common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`Component: <Name of the component>` The name of the component must be given.
	`Reference phase: <Name of a phase used as the new reference state>`

Syntax	SET_REFERENCE_STATE
	Enter the `Name of a phase` for the system. For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed. If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy. The following are example using temperature. Pressure is used in the same way: • In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C. • If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1. • Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state.
	`Temperature /*/: <Temperature for the reference state>` Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation. The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.
	`Pressure /1E5/: <Pressure for the reference state>` Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.

	Examples
	
	`S-R-S Fe SER`
	`S-R-S Cr FCC * 100000`
	`S-R-S H2O AQUEOUS * 100000`
	`S-R-S ZE REF_ELECTRODE * 100000`

SET_SCALING_STATUS

When an axis variable is selected by SET_DIAGRAM_AXIS, the scaling status for the axis is always set to automatic scaling. By this command, choose between manual or automatic scaling on a specified axis. If manual scaling is chosen, specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram.

Syntax	SET_SCALING_STATUS
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis that you want to set the scaling status.
	`Automatic scaling (Y or N) /N/:` The default is manual scaling. Enter Y for automatic scaling (N). For manual scaling specify the Min and Max values.
	`Min value: <Minimum value>` The minimum value at the start point of the specified axis.
	`Max value: <Maximum value>` The maximum value at the end point of the specified axis.

SET_TIC_TYPE

Change the drawing of the axis tics. You may alter the placement of tic marks on the axis, e.g. inside or outside or no tic marks. The size of tic marks cannot be altered by this command, but these are adjusted based on the selected graphic device and the defined relative scaling factor (global plot size).

Syntax	SET_TIC_TYPE
Prompt	`TIC Type /1/: <1 or -1 or 0>` The tic type 1 is default, i.e. the tics are drawn outside the diagram. -1 means that the tics are inside the diagram and 0 means no tics.

SET_TIELINE_STATUS

If the tie-lines are in the plane of the calculation, you can select to plot the tie-lines in two-phase fields with this command.

Syntax	SET_TIELINE_STATUS
Prompt	`Plotting every tie-line no. /0/: <Number of tie-lines>` The tie-lines plotted are not equally spaced by the graphics software. Instead, you can select to plot a subset of the calculated tie-lines, i.e. every one (1), every second (2), every three (3), etc. By accepting the default value 0, no tie-line is plotted.

SET_TITLE

Specify a title that displays on all listed tables and plotted diagrams from the POST module.

- ADD_LABEL_TEXT

Syntax	SET_TITLE
Prompt	`Title` Enter the title you want to appear on all tabulation or graphic outputs.  There is a maximum length of about 60 characters for the title. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.

SET_TRUE_MANUAL_SCALING

The tic-marks on the axes are normally placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. If such an automatic adjustment behaviour is unwanted, it can be avoided by using this command (followed by a message showing the TRUE MANUAL SCALING set for a specific axis).

The command works like a toggle. To reset the automatic scaling behaviour, repeat the command a second time for that specific axis (followed by a message saying the SEMI_ MANUAL SCALING set for the specific axis.

Syntax	SET_TRUE_MANUAL_SCALING
Prompt	`Axis (X, Y or Z): <Name of an axis>` Specify which axis (X or Y or Z) you want to toggle between automatic adjustments or avoid the adjustment of the given maximum and minimum values.

SUSPEND_PHASE_IN_PLOT

Specify that lines originating from the presence of a certain phase shall not be plotted on a diagram. If you want to bring the suspended phase back to the diagram, use RESTORE_PHASE_IN_PLOT.

Syntax	SUSPEND_PHASE_IN_PLOT
Prompt	`Phase name: <Name of a phase>` Specify the name of the phase to be suspended from the diagram.

TABULATE

This command is available for a table entered in either the POLY or POST module.

For any entered table, this command gives a table of values from equilibria calculated with a STEP command.

Unlike the TAB module's command (also called TABULATE) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	`Name: <Name of a table entered in either POLY or POST>` Specify a table name that is entered in either the POLY or POST module.
	`Output on screen or file /Screen/:` Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

Technical Notes

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Technical Note: Pipe or Redirect Output Data from Console Mode

Audience:	Advanced Programmers and Users
OS:	Windows, Linux, or macOS
Application:	For users who want to pipe or redirect data from Thermo-Calc running a macro in Console Mode. For example, you can start the application with the `Thermo-Calc.bat` file and the entire application closes when you enter the EXIT command in the Console prompt.

Command examples:	**WINDOWS**
	`Thermo-Calc.bat macro.tcm > results.log`
	LINUX
	`Thermo-Calc.sh -E < macro.tcm > results.log`
	MACOS
	`Thermo-Calc.command -E < macro.tcm > results.log`

Command line definitions	
`E`	For Linux and Mac users, the Emacs style editing feature must be disabled (turned off) using the switch `-E` in order for redirection and piping to work correctly with Thermo-Calc. For Windows this flag is not necessary.
`<>`	Redirection commands. The direction of each arrow indicates the flow of data. For example in `./Console.sh -E < my_commands.tcm > results.log`, the contents of `my_commands.tcm` is used as input to the `Console.sh` script file and the resulting output is then written to `results.log`.

Console Mode Examples

In this section:

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Thermo-Calc Console Mode Examples

There are many examples to examine and to help you learn Thermo-Calc in Console Mode. Some of the examples in the table below are included with specific sections, whereas some of the general examples are included (repeated) in more than one section.

Each topic has a brief description of the example and includes some or all of the commands used in the macros.

- About the Examples
- Opening Console Mode Macro Files



All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > All Thermo-Calc Documentation** and open *Thermo-Calc Console Mode Example Macros*.

Topic	TCEX Examples included
Binary Phase Diagram Examples	1, 4, 13, 16, 17, 26, 31, 34, 50
Property Diagram Examples	2, 8, 9, 11, 12, 22, 23, 25, 28, 29, 32, 41, 49, 50
Ternary Phase Diagram Examples	3, 5, 14, 17, 19A, 19B, 21, 33, 37, 42, 43
Multicomponent Phase Diagram Examples	6, 10, 23, 27
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Topic	TCEX Examples included
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Binary Phase Diagram Examples

tcex01 - Calculating the Binary Fe-C Phase Diagram

This example calculates the binary Fe-C phase diagram using the Binary module. The TCBIN database is used and included with your installation.

Some of the main commands used:

- LIST_EQUILIBRIUM
- LIST_STATUS
- LIST_CONDITIONS
- CHANGE_STATUS
- COMPUTE_EQUILIBRIUM
- SET_DIAGRAM_AXIS
- SET_TIELINE_STATUS
- PLOT_DIAGRAM
- SET_SCALING_STATUS
- SET_LABEL_CURVE_OPTION
- ADD_LABEL_TEXT
- MODIFY_LABEL_TEXT

tcex04 - Calculating the Fe-Cr Miscibility Gap

This example calculates the miscibility gap in the Fe-Cr system. The FEDEMO database is used and included with your installation.

These commands are used:

- SWITCH_DATABASE
- GET_DATA
- LIST_EQUILIBRIUM
- SET_AXIS_VARIABLE
- DEFINE_SYSTEM
- AMEND_PHASE_DESCRIPTION

- SET_CONDITION
- SAVE_WORKSPACES
- REJECT
- LIST_STATUS
- COMPUTE_EQUILIBRIUM
- SET_TIELINE_STATUS

tcex13 - The Binary Al-Ti Phase Diagram and its G Curve

This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

tcex16 - Second Order Transition of the Al-Fe System

This example calculates the second order transition line in the Bcc field of the Al-Fe system.



This uses the SSOL database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- ADVANCED_OPTIONS
- SET_SCALING_STATUS
- DEFINE_SYSTEM
- MAKE_EXPERIMENTAL_DATAFILE
- LIST_EQUILIBRIUM
- APPEND_EXPERIMENTAL_DATA
- STEP_WITH_OPTIONS

tcex17 - The Pseudo-binary System - CaO-SiO2

This example calculates the pseudo-binary system CaO-SiO_2 using the OXDEMO database, which is included with your installation.

The oxide demo (Oxdemo) database can be used both for pseudo-binary systems like the one in this case, $CaO\text{-}SiO_2$, or for full ternary systems like Ca-Fe-O.

These commands are of note and used in this example:

- LIST_SYSTEM
- REJECT and RESTORE
- AMEND_PHASE_DESCRIPTION
- LIST_STATUS
- DEFINE_COMPONENTS
- SET_CONDITION
- COMPUTE_EQUILIBRIUM and LIST_EQUILIBRIUM

tcex26 - The As-Ga Phase Diagram: Plotting the Partial Pressures of a Gas Species

This example uses the PG35 Binary Semi-Conductors database and is an example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga.

These commands are of note and used in this example:

- REJECT
- RESTORE
- SET_DIAGRAM_AXIS
- SET_SCALING_STATUS
- SET_AXIS_TEXT_STATUS
- SET_LABEL_CURVE_OPTION

tcex31 - Using GES to Calculate CVM

Using the Gibbs Energy System (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

These GES commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SPECIES
- ENTER_SYMBOL
- ENTER_PHASE
- ENTER_PARAMETER
- LIST_PHASE_DATA

tcex34 - The Al-Zn Phase Diagram and its G Curve

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

Property Diagram Examples

tcex02 - Plotting Thermodynamic Functions

This example shows how to plot thermodynamic functions in unary, binary and ternary systems. It also involves working with partial derivatives and partial quantities.



This uses the SSOL database. A license is required to run the example.

These commands are used and may be of interest:

GOTO_MODULE	GET_DATA	SET_CONDITION
SWITCH_DATABASE	AMEND_PHASE_DESCRIPTION	LIST_EQUILIBRIUM
DEFINE_SYSTEM	COMPUTE_EQUILIBRIUM	SET_AXIS_VARIABLE
SAVE_WORKSPACES	STEP_WITH_OPTIONS	SET_DIAGRAM_AXIS
ENTER_SYMBOL	PLOT_DIAGRAM	SET_LABEL_CURVE_OPTION
REJECT	RESTORE	LIST_SYSTEM
LIST_STATUS	CHANGE_STATUS	SHOW_VALUE
SET_INTERACTIVE		

tcex08 - Property Diagrams for a High Speed Steel

This example shows how to calculate property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, and so forth.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_DIAGRAM
- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- REINITIATE_PLOT_SETTINGS

tcex09 - Calculating a Dew Point with POLY3

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

The STEP_WITH_OPTIONS and MAP commands are of note and used in this example.

tcex11 - Oxidation of Cu2S with an H2O/O2 Gas Mixture

This example demonstrates the oxidation of Cu_2S with an H_2O/O_2 gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu_2S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu_2S and H_2O using a command SET_INPUT_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

These commands are of also of note and used in this example:

- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex12 - Tabulation of Thermodynamic Data for Reactions

This example shows a number of independent cases using the TABULATE_REACTION (TAB) module to tabulate thermodynamic data for reactions.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- TABULATE_REACTION
- DEFINE_SPECIES
- ENTER_FUNCTION
- QUICK_EXPERIMENTAL_PLOT
- SET_SCALING_STATUS
- LIST_SUBSTANCES
- TABULATE_SUBSTANCE

tcex22 - Calculating an Adiabatic Flame Temperature

This example examines a heat balance when C_3H_8 is burned in oxygen by calculating the adiabatic flame temperature.



This uses the SSUB database. A license is required to run the example.

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

tcex25 - Simulating the Refinement of Steel

This example is based on a typical steel refining process. Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment).

This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping

the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.



This uses the SLAG database. A license is required to run the example.

tcex28 - Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- EVALUATE_FUNCTIONS
- SET_START_CONSTITUTION

tcex29 - Calculating the Speciation of a Gas

This example shows how to calculate the speciation of a gas.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION

tcex32 - Calculating Oxide Layers on Steel

This example calculates oxide layers on a steel and shows how to append databases.



This uses the TCFE and SSUB databases. These licenses are required to run the example.

These commands are of note and used in this example:

- SET_START_CONSTITUTION
- SET_REFERENCE_STATE
- APPEND_DATABASE

tcex41 - Calculating a Solubility Product

Calculation of a solubility product.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_ELEMENTS
- REINITIATE_PLOT_SETTINGS
- SET_DIAGRAM_AXIS

tcex49 - Quasichemical Model Using GES

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.

These commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SYMBOL
- AMEND_ELEMENT_DATA
- ENTER_PARAMETER
- ENTER_SPECIES
- SET_REFERENCE_STATE
- SHOW_VALUE

Ternary Phase Diagram Examples

tcex03 - Calculating an Isothermal Section

This example calculates an isothermal section using the Ternary module. The FEDEMO database is used and included with your installation.

These commands are used:

- AMEND_PHASE_DESCRIPTION
- ADD_LABEL_TEXT
- PLOT_DIAGRAM
- SET_DIAGRAM_AXIS; SET_DIAGRAM_TYPE; and SET_AXIS_TYPE
- SET_REFERENCE_STATE
- CHANGE_STATUS
- SET_SCALING_STATUS

tcex05 - Calculating a Vertical Section in the Al-Cu-Si System

This example calculates a vertical section in the Al-Cu-Si system and of a vertical section from Al to 10% Cu_2Si. The ALDEMO database is used and included with your installation.

tcex14 - Variations in Solidification of an Al-Mg-Si Alloy

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

These commands are of note and used in this example:

- LIST_SYSTEM
- LIST_CONDITIONS
- SET_AXIS_TEXT_STATUS

tcex17 - The Pseudo-binary System - CaO-SiO2

This example calculates the pseudo-binary system CaO-SiO_2 using the OXDEMO database, which is included with your installation.

The oxide demo (Oxdemo) database can be used both for pseudo-binary systems like the one in this case, CaO-SiO_2, or for full ternary systems like Ca-Fe-O.

These commands are of note and used in this example:

- LIST_SYSTEM
- REJECT and RESTORE
- AMEND_PHASE_DESCRIPTION
- LIST_STATUS
- DEFINE_COMPONENTS
- SET_CONDITION
- COMPUTE_EQUILIBRIUM and LIST_EQUILIBRIUM

tcex19a and tcex19b - Mapping of Univariant Equilibria with the Liquid in Al-Cu-Si

- Part A. Step-by-step calculation using the POLY3 module.
- Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.

These commands are of note and used in these examples:

- DEFINE_SYSTEM
- GET_DATA
- AMEND_PHASE_DESCRIPTION
- SET_CONDITION and LIST_CONDITIONS
- ADVANCED_OPTIONS
- SAVE_WORKSPACES and READ_WORKSPACES
- APPEND_EXPERIMENTAL_DATA
- MAKE_EXPERIMENTAL_DATAFILE

tcex21 - Calculating a Ternary Isotherm in Fe-Cr-Ni

This example calculates a ternary isotherm in Fe-Cr-Ni with a user-defined database included with the example in the file named *tcex21.TDB*.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- GET_DATA
- SET_CONDITION
- SET_DIAGRAM_TYPE

tcex33 - An Fe-Cr-C Isopleth

This example is a benchmark calculation of an isopleth in the Fe-Cr-C system. The FEDEMO database is used and included with your installation.

tcex37 - Calculating an Isothermal Section

This example shows how to use command lines to enter and calculate an isothermal section using the POLY3 module. The FEDEMO database is used and included with your installation.

tcex42 - Paraequilibrium Calculation - Formation of Para-pearlite - Isopleth



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

tcex43 - Paraequilibrium Calculation - Formation of Para-pearlite - Isothermal



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 700 C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP_ WITH_OPTIONS command using the Paraequilibrium option.

Multicomponent Phase Diagram Examples

tcex06 - An Isopleth in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

This example calculates a multicomponent phase diagram using the DEFINE_MATERIAL command in POLY and the TCFE steel database. The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C (by weight). These conditions and the temperature are set by the DEFINE_MATERIAL command.

After the first equilibrium results, a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.



This uses the TCFE database. A license is required to run the example.

tcex10 - Preventing Cr2O3 Clogging in a Continuous Casting Process

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr_2O_3 clogging in a continuous casting process.



This uses the SLAG database. A license is required to run the example.

The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr_2O_3 was formed.

Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential. In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- CHANGE_STATUS
- COMPUTE_EQUILIBRIUM
- DEFINE_SYSTEM
- DEFINE_SYSTEM
- LIST_CONDITIONS

- LIST_EQUILIBRIUM
- LIST_STATUS
- SET_CONDITION
- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

tcex27 - Calculating Chemical Vapor Depositions (CVD)

This example calculates the chemical vapor deposition (CVD).



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_COMPONENTS
- SET_CONDITION
- ADD_INITIAL_EQUILIBRIUM
- LIST_AXIS_VARIABLE
- LIST_INITIAL_EQUILIBRIA

Examples Calculating Thermodynamic and Related Quantities

tcex02 - Plotting Thermodynamic Functions

This example shows how to plot thermodynamic functions in unary, binary and ternary systems. It also involves working with partial derivatives and partial quantities.



This uses the SSOL database. A license is required to run the example.

These commands are used and may be of interest:

GOTO_MODULE	GET_DATA	SET_CONDITION
SWITCH_DATABASE	AMEND_PHASE_DESCRIPTION	LIST_EQUILIBRIUM
DEFINE_SYSTEM	COMPUTE_EQUILIBRIUM	SET_AXIS_VARIABLE
SAVE_WORKSPACES	STEP_WITH_OPTIONS	SET_DIAGRAM_AXIS
ENTER_SYMBOL	PLOT_DIAGRAM	SET_LABEL_CURVE_OPTION
REJECT	RESTORE	LIST_SYSTEM
LIST_STATUS	CHANGE_STATUS	SHOW_VALUE
SET_INTERACTIVE		

tcex13 - The Binary Al-Ti Phase Diagram and its G Curve

This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

tcex14 - Variations in Solidification of an Al-Mg-Si Alloy

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

These commands are of note and used in this example:

- LIST_SYSTEM
- LIST_CONDITIONS
- SET_AXIS_TEXT_STATUS

tcex18 - A3 Temperature of a Steel

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.

 This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- COMPUTE_TRANSITION
- DEFINE_MATERIAL
- ENTER_SYMBOL
- SHOW_VALUE

tcex22 - Calculating an Adiabatic Flame Temperature

This example examines a heat balance when C_3H_8 is burned in oxygen by calculating the adiabatic flame temperature.

 This uses the SSUB database. A license is required to run the example.

tcex26 - The As-Ga Phase Diagram: Plotting the Partial Pressures of a Gas Species

This example uses the PG35 Binary Semi-Conductors database and is an example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga.

These commands are of note and used in this example:

- REJECT
- RESTORE
- SET_DIAGRAM_AXIS
- SET_SCALING_STATUS
- SET_AXIS_TEXT_STATUS
- SET_LABEL_CURVE_OPTION

tcex34 - The Al-Zn Phase Diagram and its G Curve

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

tcex39 - Calculating Reversible Carnot Cycles of a Heat Engine

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3 and POST modules are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

These commands are of note and used in this example:

- REINITIATE
- ENTER_PARAMETER
- ENTER_SPECIES
- SET_PLOT_FORMAT
- ENTER_PHASE

tcex51 - Calculation of Molar Volume, Thermal Expansivity and Density

This example uses the POLY3 module to calculate the molar volume, thermal expansivity and density of the FCC_A1, BCC_A2 LIQUID and liquid phases of C-Fe.



This uses the TCFE database. A license is required to run the example.

Single Equilibrium Calculation Examples

tcex07 - Single Equilibria in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

This example shows how to calculate a single equilibria in a low alloyed Fe-Mn-Si-Cr-Ni-C steel. There are two common ways to perform a single equilibrium calculation:

- Get data from a database, then in POLY use SET_CONDITION and COMPUTE_ EQUILIBRIUM.
- Go directly to POLY and use DEFINE_MATERIAL.

The COMPUTE_TRANSITION command is also used to determine the temperature or composition where one phase forms or disappears. It is the same as the CHANGE_STATUS → SET_CONDITION→ COMPUTE_EQUILIBRIUM sequence of commands.

A STEP_WITH_OPTIONS command using the option *normal* is also used in addition to the other commands that should be becoming more familiar as you work through the examples.



This uses the TCFE database. A license is required to run the example.

tcex18 - A3 Temperature of a Steel

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- COMPUTE_TRANSITION

- DEFINE_MATERIAL
- ENTER_SYMBOL
- SHOW_VALUE

tcex20 - Adiabatic Decompression in a Geological System

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- DEFINE_COMPONENTS
- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION
- SHOW_VALUE

Potential Diagram Example

tcex35 - Calculating a Potential Diagram

This example uses the POTENTIAL module to calculate a potential diagram. Note that there are no commands for this module, you just follow the prompts. The SUBDEMO database is used and included with your installation.

Examples of Scheil-Gulliver Calculations

- About the Scheil-Gulliver Solidification Simulations

tcex15 - Simulating the Solidification of a Cr-Ni Alloy

This is an example of a solidification simulation of a Cr-Ni alloy. This is a classic Scheil-Gulliver simulation.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- START_WIZARD
- COMPUTE_TRANSITION
- ADD_INITIAL_EQUILIBRIUM
- ENTER_SYMBOL
- ADVANCED_OPTIONS
- STEP_WITH_OPTIONS
- MAKE_EXPERIMENTAL_DATAFILE
- CHANGE_STATUS

tcex30a and 30b - Scheil Calculation for an Al-4Mg-2Si-2Cu Alloy

The Equilibrium Calculation Module (POLY3) and About the Scheil-Gulliver Solidification Simulations

These examples show two ways to do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy. In part A, you use the POLY3 module and the STEP_WITH_OPTIONS command with an EVALUATE option. Then in part B you use the SCHEIL module commands to do the same thing. Data from the COST2 database is used and included with the example in the file named *tcex30_cost2.TDB*.

tcex48 - Scheil Solidification with C Back Diffusion

This is an example of Scheil solidification with C back diffusion in solid phases. The results are compared between a simple Scheil and equilibrium calculation. The FEDEMO database is used.

tcex54 - Scheil Solidification of an Al-2.1Cu-1Si Alloy including Back Diffusion

This is an example of a solidification simulation of a Al-2.1Cu-1Si alloy. The back diffusion option in the Scheil module is used, i.e. there is back diffusion in the primary phase. The example uses both the thermodynamic ALDEMO and mobility MALDEMO demo databases included with your installation.

tcex57 - Scheil Solidification with Solute Trapping

This is an example of a solidification simulation of a Al-7.5Si-0.2Cu system. The solute trapping option in the Scheil module is used. The example uses the thermodynamic ALDEMO demo database included with your installation.



See the Graphical Mode example T_13: Scheil Solidification with Solute Trapping for an additional comparison to Classic Scheil.

Example Calculating Chemical Ordering

tcex16 - Second Order Transition of the Al-Fe System

This example calculates the second order transition line in the Bcc field of the Al-Fe system.



This uses the SSOL database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- ADVANCED_OPTIONS
- SET_SCALING_STATUS
- DEFINE_SYSTEM
- MAKE_EXPERIMENTAL_DATAFILE
- LIST_EQUILIBRIUM
- APPEND_EXPERIMENTAL_DATA
- STEP_WITH_OPTIONS

Examples of Gibbs Energy System (GES)

tcex31 - Using GES to Calculate CVM

Using the Gibbs Energy System (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

These GES commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SPECIES
- ENTER_SYMBOL
- ENTER_PHASE
- ENTER_PARAMETER
- LIST_PHASE_DATA

tcex38 - Calculating the Morral "Rose"

This example uses the Gibbs energy system (GES) module to calculate the Morral rose, which are miscibility gaps.

These commands are of note and used in this example:

- REINITIATE
- ENTER_ELEMENT
- AMEND_ELEMENT_DATA
- ENTER_PARAMETER
- ENTER_PHASE

tcex39 - Calculating Reversible Carnot Cycles of a Heat Engine

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3 and POST modules are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

These commands are of note and used in this example:

- REINITIATE
- ENTER_PARAMETER
- ENTER_SPECIES
- SET_PLOT_FORMAT
- ENTER_PHASE

tcex49 - Quasichemical Model Using GES

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.

These commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SYMBOL
- AMEND_ELEMENT_DATA
- ENTER_PARAMETER
- ENTER_SPECIES
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex52 - Changing the Excess Models for Interaction Parameters in a Solution Phase

- Solution Models in the GIBBS (GES) Module

This example shows how to change the excess models for binary and ternary interactions in a solution phase, either

- through direct interactive amendments of phase descriptions within the GIBBS_ ENERGY_SYSTEM (GES) module, or
- enforced by specific type-definitions given in a database file retrieved by the DATABASE_RETRIEVAL module (also called the TDB module).

For binary excess models, the example changes it from the default *R-K model* to a *Mixed-Excess-Model*. The phase has to be a substitutional phase in this case.

For ternary extrapolation models, the example changes it from the default *R-K-M model* to a *Toop_Kohler model*.

Notes Related to the Example

The following is included in the macro file as part of the instructions but may be of use to new users:

Amending the binary excess model

The default binary excess model is the Redlich-Kister Model for all the three associated binary interaction pairs (A-B, A-C and B-C) in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

Before changing this default binary excess model for the ternary LIQUID solution phase, one must have already entered the G parameters (for standard Gibbs energies of all pure end-members) and L parameters (for binary R-K excess interaction energies), as shown in the example.

In this particular example, we want to change from the default R-K binary excess model to the Mixed-Excess-Model (with three different binary excess models, namely Legendre, Polynom and Redlich-Kister models, applied to the A-B, A-C and B-C binaries, respectively), as demonstrated below:

For the A-B interaction, the Legendre binary excess model should be used (rather than the default Redlich-Kister Model), with the first species (i.e. A) as the independent constituent and the second species (i.e. B) as the dependent constituent, while the L parameters for the A-B interaction shall remain the same as those handled by the R-K model.

For the A-C interaction, the Polynom binary excess model should be used (rather than the default Redlich-Kister Model), with the second species (i.e. C) as the independent constituent and the first species (i.e. A) as the dependent constituent, while the L parameters for the A-C interaction shall remain the same as those handled by the R-K model.

Amending the ternary extrapolation model

The default ternary excess model is the Redlich-Kister_Muggianu Model (i.e., the MUGGIANU_RESTOR method for ternary extrapolation based on binary parameters) for the associated ternary interaction terms; when no ternary L parameter is entered for that, such a default Redlich-Kister_Muggianu Model is thus to be used for extrapolation from binary excess energies to ternary interactions in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

However, in this particular example as illustrated in the following, we shall change from this default R-K-M ternary excess model to the TOOP-KOHLER method for the ternary extrapolation method, with the species C as the Toop constituent, while the species A and B as the Kohler constituents (entering A and B, or B and A, as the basis constituent and first interacting constituent). This will implicitly enforce that, during the ternary extrapolation, only the A-B binary interaction parameters are utilized in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction

parameters used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions). This makes the extrapolated ternary excess interaction terms different from those handled either by the default MUGGIANU_RESTOR method or by the alternative KOHLER-ALL method.

Note that only when all the relevant binary excess energies in a ternary system are treated by the default Redlich-Kister Model (i.e., the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the Redlich-Kister_Kohler Model.

Example Calculating the T0 Temperature

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

Examples Calculating Paraequilibrium

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

tcex42 - Paraequilibrium Calculation - Formation of Para-pearlite - Isopleth



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

tcex43 - Paraequilibrium Calculation - Formation of Para-pearlite - Isothermal



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 700 C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP_ WITH_OPTIONS command using the Paraequilibrium option.

Example Using Functions and Variables

tcex44 - Exploring Variables and Functions

This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550° C). The example was created using an expression from Eliasson and Sandström (2000).

REFERENCE

J. Eliasson and R. Sandström, “Proof strength values for austenitic stainless steels at elevated temperatures,” Steel Res., vol. 71, no. 6–7, pp. 249–254, 2000.



This uses the TCFE database. A license is required to run the example.

Example Using PARROT and EDIT_EXPERIMENT

tcex36a - Using PARROT and EDIT EXPERIMENTS



The example is divided into parts corresponding to the files in the **tcex36a** folder. It is recommended you open *tcex.36.readme* before continuing with this advanced exercise.

Also see the *Data Optimization User Guide*.

Each problem has "selected" experimental data. The example uses a fictitious binary A-B system where element A is BCC until it melts. Element B is BCC up to 1100 K and FCC above. There is a compound A2B stable in a limited temperature range.

- The creation of the "setup" file is described (*tcex36a.TCM*) where you enter the elements and phases into the Gibbs Energy System (GES) module
- The creation of the experimental data file is described (*tcex 36b.TCM*). When you run the TCEX36a macro, the contents of this macro file is automatically launched and the experimental data file created.
- The actual run in the PARROT module in order to obtain the result (*tcex 36cpd.TCM*)

There are many commands used in this advanced example (listed in alphabetical order):

ADVANCED_OPTIONS	AMEND_ELEMENT_DATA	AMEND_PHASE_DESCRIPTION
APPEND_EXPERIMENTAL_DATA	COMPILE_EXPERIMENTS	
CONTINUE_OPTIMIZATION	CREATE_NEW_EQUILIBRIUM	CREATE_NEW_STORE_FILE
DEFINE_COMPONENTS	EDIT_EXPERIMENTS	ENTER_PARAMETER
ENTER_PHASE	LABEL_DATA	LIST_ALL_VARIABLES
LIST_PHASE_DATA	LIST_RESULT	MACRO_FILE_OPEN
OPTIMIZE_VARIABLES	QUICK_EXPERIMENTAL_PLOT	READ_WORKSPACES
RESCALE_VARIABLES	SAVE_PARROT_WORKSPACES	SAVE_WORKSPACES

SELECT_EQUILIBRIUM	SET_ALL_START_VALUES	SET_ALTERNATE_CONDITION
SET_ALTERNATE_MODE	SET_FIX_VARIABLE	SET_OPTIMIZING_VARIABLE
SET_STORE_FILE	SET_WEIGHT	

Pourbaix Diagram Examples

tcex40

This is the first in a series of examples to demonstrate the advanced POURBAIX module calculations and plotting. This example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25° C and 1 bar. Other diagrams, along various phase boundaries for the same interactions resulted from the same Pourbaix module calculation, are also plotted.



It is recommended you read the text file *TCEX40-README.txt*, which is located in the **Extended** subfolder.

Also see the *Pourbaix Diagrams Educational Material Guide.*

A so-called Pourbaix diagram is actually a phase diagram with independently-varied acidity (pH) and electropotential (Eh), for a heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water dissolving a specified amount of metals and other solutes), under a defined temperature and pressure condition.

The PAQ2 Database

The example uses the PAQ2 (TCS Public Aqueous Solution Database using the SIT aqueous solution model) included with your installation. The database contains an AQUEOUS solution phase and REF_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 is specially designed for these example calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of phase diagrams or property diagrams in some aqueous-bearing multicomponent heterogeneous interaction systems within the limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H2O-NaCl, via the Single-Database Option in the advanced POURBAIX module or through the normal TDB-GES-POLY-POST routine.

Additional Examples in this Series

Additional examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D and TCEX40E) are provided to demonstrate options and features in the Pourbaix module and to show more advanced

applications of the TCAQ and AQS aqueous solution databases [in the Multiple-Database Option, i.e., with appended data from the SSOL and SSUB databases]. See Pourbaix Examples TCEX40A to 40E.

tcex53 - Pourbaix Diagram Calculations for a Heterogeneous Interaction System

Also see the *Pourbaix Diagrams Educational Material Guide.*

This example uses the PAQ2 database to calculate some Pourbaix diagrams. The DATABASE_RETRIEVAL (TDB), GIBBS_ENERGY_SYSTEM (GES), POLY3, and POST modules are used for the Fe-X-H2O-NaCl heterogeneous interaction system, where X = Cr-Ni-Co.

The initial bulk composition of Fe-based alloy in this calculation is just preliminarily assigned, in which the BCC_A2 and/or FCC_A1 solution phase(s) are considered as of primarily interest. For practical calculations, one shall have more precise inputs for the initial bulk compositions of alloys.

Step 1: Single-Point Calculations for H2O-NaCl system

To demonstrate how to define the molality of NaCl in an aqueous-bearing heterogeneous interaction system.

Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system

To demonstrate how to define the initial amount of alloy in an aqueous-bearing heterogeneous interaction system. In this example, we are interested in only the BCC_A2 and FCC_A1 phases in the Fe-based alloy.

Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl system

Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl system - define the variables

From the same mapping calculations you arrive at by the end of the example, you can plot more diagrams using a variety of X-Y axis variables.

For a list of pre-defined symbols, go to the end of the tcex53.TCM macro file (open it in a text editor).

Pourbaix Examples TCEX40A to 40E

These are the extended examples that are described in Pourbaix Diagram Examples.

TCEX 40A

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses a single database. The Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25C and 1 bar is automatically calculated and plotted.

A more advanced version of 40A can be found in TCEX40E, which also uses Option 1 but with multiple databases. However, licenses are required for three types of commercial Thermo-Calc databases.

See POURBAIX_DIAGRAM Commands for Options 1 to 4.

A so-called Pourbaix diagram is actually a phase diagram with independently-varied electropotential (Eh) and acidity (pH), for an heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water solving a specified amount of metals and other solutes), under defined temperature and pressure conditions. Some property diagrams, along various phase boundaries for the same interactions resulting from the same Pourbaix module calculation, are also plotted, without leaving Option 1.

At the end of this example, a new POLY3 file called *POURBAIX.POLY3* is automatically saved. The following examples (TCEX40B, TCEX40C and TCEX40D) use this same POLY3 file for the calculations. Therefore it is important to make four copies of this file and rename these to TCEX40A.POLY3, TCEX40B.POLY3, TCEX40C.POLY3 and TCEX40D.POLY3. This must be done outside of the Thermo-Calc software and after the TCEX40A calculation and plotting is complete. This is so that the required POLY3 file structure is not lost.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE TCEX40A.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

TCEX 40B

This example shows you how to use Option 2 where you **Open an old (existing) file and plot other property diagrams**.

Example 40A calculated and plotted the Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25° C and 1 bar. Example 40B reads the original POURBAIX.POLY3 file , and uses the calculated results to plot property diagrams for the same heterogeneous interaction system.

For example 40B, the POLY3 file is not modified. However, it is still recommended that a copy of the original POLY3 file is used so you do not lose the file structure and calculated results.

If you have a POLY3 file generated after choosing Option 4, that file can also be used for Option 2, and vice versa.

TCEX 40C

This example shows you how to use Option 3 where you **Open an old file and make another Pourbaix calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make another Pourbaix calculation and plot.

The same chemical system is used (Fe-H2O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and without the GASeous mixture phase. The new conditions are 0.01 m Fe in a 1 m NaCl solution at 200° C and 1 kbar.

In this example, the GASeous mixture phase for the Pourbaix diagram is not considered.

The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file and rename it (e.g.TCEX40C.POLY3) so you do not lose the file structure and new calculated results.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

After the default Pourbaix diagram is generated and refined, you can also use Option 3 to plot property diagrams along different phase boundaries for the same system. These settings are possible from within Option 3 and you do not need to go back to Option 2.

TCEX 40D

This example shows you how to use Option 4 where you **Open an old file and make another stepping calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make a stepping calculation and plot.

The same chemical system is used (Fe-H2O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and using a POLY3 stepping calculation. The new conditions are 0.01 m Fe in a 0.1 m NaCl solution at 1 kbar and under varied temperature (from 0 to 400° C). The equilibrium conditions are modified and two stepping calculations are done. The same stepping calculation is used to plot property diagrams for the heterogeneous interaction system.

The example also explores settings such as editing the definitions for some system components and their initial bulk composition conditions. This is done through the direct and internal POURBAIX-POLY3 intersection, for a Stepping (or Mapping) calculation inside the Pourbaix module.

The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file (from example TCEX40A) and rename it (e.g. to TCEX40D.POLY3) so you do not lose the file structure and new calculated results.

If you have a POLY3 file generated after choosing Option 2, that file can also be used for Option 4 and vice versa.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

TCEX 40E

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses multiple databases (TCAQ, SSUBand SSOL). The Pourbaix diagram for 0.001 m $Fe_{90}Co_5Ni_5$ alloy (9E-3 m Fe + 5E-4 m Co + 5E-4 m Ni) in an aqueous solution with 2E-2 m H_2S and 3 m NaCl at 25° C and 1 bar is automatically calculated and plotted.

You need licenses for three Thermo-Calc databases, i.e.

- A: AQS (TGG Aqueous Solution Database; HKF model) or TCAQ (TCS Aqueous Solution Database; SIT model);
- B: SSUB (SGTE Pure Substances Database)
- C: SSOL (SGTE Alloy Solutions Database) or TCFE (TCS Steels/Fe-Alloys Database) or similar.

The TCAQ database contains only an AQUEOUS solution phase (using the SIT model) and REF_ELECTRODE phase (as a reference state for electron in aqueous electrolyte systems). The SSUB database is appended for the GASeous mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and the SSOL database is appended for various solid solution phases.

The Pourbaix module inside the software also accepts the AQS2 aqueous solution database (using the complete Revised HKF model) in the Multiple Database Option, in addition to the TCAQ2 aqueous solution database (using the SIT model).

POURBAIX_DIAGRAM Commands for Options 1 to 4

Option 1: Start a Completely New Pourbaix Diagram Calculation

Option 1 is used to make a completely new Pourbaix diagram calculation and automatically plot a pH-Eh diagram. i.e., define a new chemical system; specify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh and various property diagrams.



Many of the commands in Option 1 are also repeated for Options 2 to 4. The details for each command are included with this section unless it is specific to one of the other option choices. The order that the commands display on screen is also different and based on what is entered at the prompts. These prompts are also available in other commands and when applicable a link to that command is included.

`Consider the GAS phase in calculating a Pourbaix diagram? /Y/`

You can choose to ignore the GAS mixture phase on a calculated/plotted Pourbaix diagram. However, such a plot is actually not a complete Pourbaix diagram because the thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will not be calculated.

- If you enter `Y` (the default), GAS mixture phase is always considered.
- If you enter `N` the GAS mixture phase is completely ignored.

`Use single database? /Y/`

If you keep the default you are prompted for a database.

`Combined database: /PAQ2/`

The default is PAQ2, a database included with all installations.

The following information is provided on screen if you chose Y at the first prompt, `Need any instruction on the POURBAIX module? /N/`.

Define a Chemical System and its Initial Bulk Composition

Normally a Pourbaix diagram and its related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition, which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS)

- Default defined elements (solvent H2O): H and O and specially assigned ZE (electron) and VA(vacancy).
- Prompt specified elements (solutes ELEM): Fe Ni Co Cr C N S Na Cl

INITIAL BULK COMPOSITION

- Default defined composition (solvent): 1.0 kg of H2O
- Prompt specified composition (solutes): x mole of ELEM
- Mass of Water (weight) = 1 kg



When entering solutes in chemical formulas, the first element's letter must be in UPPER case, and second in lower case, for example `NaCl`, `CO2`, `CoCl3`, `Fe0.93S`, `NaSO4-1`, and `H2SO4`.

```
First solute
```

Enter a solute, e.g. `Fe`.

```
Molality of <first solute> [mol/kg] /.001/
```

Enter a molality for the first solute, e.g. Fe.

```
Second solute
```

Enter a second solute and its molality on the same line, e.g. `NaCl .1`.

```
Next solute
```

You can continue to enter solutes. Press <Enter> to skip to the next prompt.

The following information is provided on screen if you chose Y at the first prompt, `Need any instruction on the POURBAIX module? /N/`.

Defined Chemical System and Initial Bulk Composition

Solutes have been split up into chemical elements and their mole numbers. If confirmed, the Pourbaix module will, in further steps, count the initial bulk composition in terms of chemical elements.

```
Confirm defined system and initial bulk composition? /Y/
```

If you keep the default (Y) thermodynamic data is retrieved from the database. Then it lists the database's phases for the defined system.

You can then reject or restore phases as required with the next prompts.

```
Reject phase(s) /NONE/
```

```
Restore phase(s): /NONE/
```

Then the program lists the phases retained in the system and you prompted whether this is OK or not.

```
OK? /Y/
```

If you answer Y, then a list of references for the assessed data is displayed on the screen. The next prompt is related to miscibility gap checks, global minimization, saving the information to a POLY3 file, and setting numerical limits.

```
Should any phase have a miscibility gap check? /N/
```

The database usually creates two or more "composition sets" for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase specify this here. It costs some computation time and may make subsequent MAP or STEP processes more difficult to converge. To keep the default (not to have any such phase) press <Enter>. Otherwise answer Y and follow the additional prompts.

```
Enforce Global Minimization Technique in calculations? /N/
```

If you choose Y, the Global Minimization is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

```
Save all functions, variables and tables in POLY3 file? /Y/
```

Choose Y if you want to save all the defined symbols (functions, variables and tables) into the POURBAIX.POLY3 file, for further normal POLY3 calculations or normal POST post-processing. Choosing yes may result in a large POLY3 file.

```
Set numerical limits? /N/
```

- SET_NUMERICAL_LIMITS

The Pourbaix module has a default setting for numerical limits.

- Maximum number of iterations: 20000
- Required accuracy: 1E-6
- Smallest fraction: 1E-15
- Approximate driving force for metastable phases: Y

If you kept the defaults for the above prompts, the program lists the default and pre-defined calculation conditions and you are prompted to confirm.

```
Confirm defined conditions? /Y/
```

Now Thermo-Calc calculates the start points. This can take a few moments. Near the end of the calculation there is a list of the default axis variables. The maximum pH limit is calculated precisely and determined automatically by the Pourbaix module as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system. You are prompted to accept these settings.

```
Accept the default settings for two mapping variables? /Y/
```

The program now lists the initial equilibria for mapping and continues to calculate the mapping. Then it sets the automatic diagram axes and starts to plot the diagram. But first there are several prompts to guide you.

```
Any missing phase boundary you could possibly think of? /N/
```

Sometimes the Pourbaix module may miss some phase boundaries during the mapping process. If you answer `Y` you can add additional starting point(s) into the calculation. You are now prompted to specify a pH-Eh coordinate pair, for instance (4.0, -0.15), which is close to the expected phase boundary. However, such additional pH-Eh point should not outside the AQUEOUS/GAS(O2) or AQUEOUS/GAS(H2) boundaries; otherwise, the module will fail in finding any new starting point.

The next set of prompts relate to plotting.

```
Change the pH/Eh steps for smoother curves? /N/
```

You can modify the mapping steps of X/Y axes for smoother curves; sometimes it may help finding missing phase boundaries by decreasing the pH and Eh increments.

```
Zoom in? /N/
```

Change the scaling status for both X and Y axes. The program then asks for minimum and maximum values for the axes. In some cases values are suggested.

```
Change Curve-Label Option for the diagram? /N/
```

Change the Curve-Label option to one of the following:

- A: List stable phases along phase boundaries
- B: As A, but curves with same fix phase have same number
- C: List axis quantities
- D: As C, but curves with same quantities have same number
- E: As B, but curves with changing colours
- F: As D, but curves with changing colours
- N: No labels

Usually, Option E or B is good for phase diagrams such as pH-Eh plots, and F or D is good for property diagrams like pH-RC(Fe+2).

SET_LABEL_CURVE_OPTION

```
Add Label-Texts onto the Pourbaix diagram? /N/
```

Add label text to an area in the diagram. The label is written starting from the specified coordinates. Optionally, let the program automatically add the text by calculating an equilibrium at some specific coordinates and also make a label as the stable phase names in the area. However, such an automatic calculation may fail, especially for a Pourbaix diagram where either pH or Eh is not an intensive variables.

In most cases, the program is able to write the label if the coordinates and texts are specified.

```
Change the Subtitle of the diagram? /N/
```

This is the same as the POST module commandSET_CORNER_TEXT → UPPER_RIGHT <SUBTITLE>. The default subtitle is automatically assigned by the POURBAIX module and is based on the defined conditions in the system (temperature, pressure and initial bulk compositions).

If you choose `Y` then the existing subtitle is displayed and you are prompted to enter a new subtitle or to have None.

```
New Subtitle /NONE/
```

You can change the subtitle for all the diagrams in the same POURBAIX run (i.e., within the same Option). The new subtitle that can be altered later at the same option, when further modifying the present graph or when refining any sequentially defined plot. By entering text (empty space at any position is allowed), the new subtitle is defined. By typing OLD, the existing subtitle is kept.

By pressing <Enter> (i.e., accepting None), the subtitle is deleted from all sequential plots, which can be set back later at the same option, too.

```
Change Axis-Texts? /N/
```

Change the axis text for both X and Y axes.

```
Further Refine the diagram in POST Module? /N/
```

With this option, you can further change the appearance the plot and use any command in the normal POST Module.

POST Module Commands

```
Hard copy of the diagram? /N/
```

Recommended Responses

- Hard copy of the diagram? /N/: Y
- CURRENT DEVICE: MS-Windows
- GRAPHIC DEVICE NUMBER /1/: 5
- NEW DEVICE: Postscript portrait mode
- USE POSTSCRIPT FONTS /YES/: Y
- SELECT FONTNUMBER /9/: 27
- NEW FONT: Times-Bold
- FONT SIZE /.35833/: .32
- PLOTFILE : /defaultname/: yourfilename

```
Save X-Y coordinates of curve on text file? /N/
```

Write all the current graphic information (generated and modified in the above procedure) on a text file using the DATAPLOT format (see the *DATAPLOT User Guide* or search the online help). This also makes it possible to merge two or more diagrams from separate but similar calculations, or put some experimental data points onto a calculated diagram. You do this by first writing them onto text files with this option and then edit them together (using a general text editor). The program asks for a file name. Accept the default (usually POURBAIX) or use another name. If an extension is not given, the written file is given an extension of *.EXP.

```
Modify the diagram? /N/
```

Further modify the appearance of the created plot. This brings you back to the above prompts for changing various features.

```
Any more diagram? /N/
```

Make many other plots using the same POURBAIX module calculation file.

Option 2: Open an Existing File and Plot Other Property Diagrams

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <*FILE NAME*>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Open an existing POLY3 file created by the Pourbaix module (from a previous Pourbaix calculation Option 1 or 3 or a previous Stepping calculation Option 4), and selectively plotting other property diagrams. i.e., open the old GES and POLY3 workspaces; plot pH-Eh or various property diagrams.

```
File name /ABCDEF/
```

The name of a previously saved POLY3 file where the POLY3 and GES5 workspaces is to be read must be specified. You do not need to enter the file extension if it is the default .POLY3 name. The default file name (e.g. ABCDEF) is the most recent specified POLY3-file name or RESULT if there is no workspace already saved in the run. You can press <Enter> or type a specific file name to read the POLY3 and GES5 workspaces from the file.

For Windows, and at the prompt, an **Open file** window displays if a file name is not given or the file path is incorrect. The file type (i.e. POLY3) cannot be changed. Click **Open** or **Cancel** to continue with the selected file.

When the file opens, it confirms on screen what kind of calculation is contained in the POLY3 file. For example: *The loaded POLY3 file is of POURBAIX-MAPPING Calculation*.

On screen it also lists the system components and the default and predefined calculation conditions to enable you to review these.

Next you are given a set of properties that are available to be selected as axis variables for making other diagrams from the same calculation.

Abbreviation	Definition
pH	Acidity
Eh	Electronic potential (V)
Ah	Electronic affinity (kJ)
pe	Electronic activity [log10ACRe)
IS	Ionic strength
TM	Total concentration
Aw	Activity of water
Oc	Osmotic coefficient
MF (AQsp)	Mole fractions of aqueous species
ML (AQsp)	Molalities of aqueous species
AI (AQsp)	Activities of aqueous species
RC (AQsp)	Activity coefficients of Aq species
Where AQsp is the name of a specific aqueous species, and "*" can be used as a wild sign for all AQSp. It is not necessary to give a complete aqueous species name. However, the entered AQsp name must be unique. If neither AQsp nor * is given, all species are searched.	



The rest of the prompts are the same as with Option 1 and relate to plotting. Enter ? at any prompt for details.

Option 3: Open an Existing File and Make Another Pourbaix Calculation

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <*FILE NAME*>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Open an existing POLY3 file created by the Pourbaix module and make another Pourbaix diagram calculation i.e. open the old GES and POLY3 workspaces, adopt the defined chemical system, modify the T-P-X conditions, calculate the initial equilibria, perform the pH-Eh mapping calculation and plot pH-Eh or other property diagrams.

The rest of the prompts are the same as with Option 1 or Option 2. Enter ? at any prompt for details.

```
Modify Label-Texts on the Pourbaix diagram? /N/
```

Once some labels are written by the Add-Label-Text command onto the diagram, you can also modify the labels (changing their positions and text contents). The text-size cannot be changed. The program asks which label and you enter its new X/Y coordinates with the new text. The new text must not be longer than the old one.

```
Modify Label-Curve-Option on the Pourbaix diagram? /N/
```

Because some phase-region labels have been written onto the diagram, the Label-Curve-Option might need to be modified, normally to the Option N.

Important Information About Option 3

The default definitions of the Eh and pH quantities in the advanced Pourbaix module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

```
Eh = MUR(ZE)/RNF
pH = -log10[AI(H+1,AQUEOUS)]
= -log10[ACR(H+1,AQUEOUS)*AH2O]
```

where RNF is the Faraday constant (96485.309 C/mol), and AH2O is the molecular weight of H2O (55.508435 g). MUR(ZE) is the electrochemical potential (ECP; in the unit of J/mol; w.r.t. the standard hydrogen electrode). ACR(H+1,AQUEOUS) is the site-fraction-based activity of the H+1 aqueous species in AQUEOUS solution phase, but AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is the molality-based activity of the H+1 aqueous species that should be used for defining the pH quantity.

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H2O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H2S). The reference state for the H2O component must always be defined as the solvent species H2O in the AQUEOUS solution phase under the current temperature (*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

```
ML = Y(AQUEOUS,I)*AH2O/YH2O
RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)
AI = RC*ML
= ACR(I,AQUEOUS)*AH2O
```

where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

```
Axis No 1: LNACR(H+1)Min: -34.532525Max: 2.3025851 Inc: 0.8
Axis No 2: MUR(ZE)   Min: -150000   Max: 200000    Inc: 7718.85
```

The default settings (listed above) for two mapping variables [in terms of lnACR (H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

```
pH:  0.00 -> 14.00, at a step of 0.35
Eh: -1.55 ->  2.07, at a step of 0.08 (V)
```

The maximum pH limit has been calculated precisely and determined automatically by the Pourbaix module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

Option 4: Open an Existing File and Make another Stepping Calculation

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation. i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; specify one of the T-P-X conditions as the stepping variable; calculate the initial equilibria; perform the stepping calculation; plot various property diagrams.

Many prompts are the same as with Option 1 or Option 2. Enter ? at any prompt for details.

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE *<FILE NAME>*.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

The stepping calculation modifies the POLY3 file but this can be used for other Stepping calculations inside the Pourbaix module (e.g. repeating Option 4) or in normal POLY3 module.

Stepping Parameters

The following parameters are suitable for a STEPPING calculation for the defined aqueous-bearing system. Choose one of them as the stepping variable:

```
T Temperature (C)
P Pressure (bar)
pH Acidity
Eh Electronic Potential (V)
N(Comp) Mole of One Component
```

where "Comp" is the name of a specific component as listed below. One should not use any key component (H2O or H+1 or ZE) as such a stepping variable, because of that their compositional definitions and variations are determined by the AQUEOUS solution phase in the POURBAIX Module.

An interacting component defined as an element (such as Fe or Na or Cl) can be selected as a stepping variable.

However, if you want to make a stepping calculation with a non-element chemical formula (such as NaCl or CaS2) as the stepping variable, one must have made some necessary modifications in the POLY3 Module, before reaching this point, by conducting some POLY3 commands as given below (as an example for the system Fe-Na-Cl-H-O):

```
POLY_3: def-component H2O H+1 ZE Fe NaCl Cl
POLY_3: set-ref-state H2O AQUEOUS * 1E5
POLY_3: set-ref-state ZE REF_ELEC * 1E5
POLY_3: change-status phase REF-ELEC=SUSPEND
POLY_3: set-cond b(H2O)=1000 n(H+1)=0 n(ZE)=0
POLY_3: set-cond P=1E5 T=298.15**
POLY_3: set-cond n(Fe)=1E-3 n(Cl)=0 n(NaCl)=3 **
```

** Here the P-T-n(Fe) conditions can be set as what you wanted, while the initial n(NaCl) value must be set as between its minimum and maximum values that you are interested in. Later on, it will be prompted for specifying the n(NaCl) Min-Max-Step values of the stepping calculation.

```
Stepping variable: /T/
```

The chosen stepping variable must be one of the suitable parameters listed above.

```
Minimum temperature (C) /15/
Maximum temperature (C) /35/
Increment in temperature (C) /1/
```

The AQUEOUS solution phase under the defined bulk composition and pressure condition is stable only between 0 and 99° C. However, you can make a stepping calculation outside this temperature range, where the AQUEOUS solution phase become metastable. In this case, the resulting POLY3 file is possibly able to be opened by any other option within the Pourbaix module.

Example Using Tabulate Reaction (TAB)

tcex12 - Tabulation of Thermodynamic Data for Reactions

This example shows a number of independent cases using the TABULATE_REACTION (TAB) module to tabulate thermodynamic data for reactions.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- TABULATE_REACTION
- DEFINE_SPECIES
- ENTER_FUNCTION
- QUICK_EXPERIMENTAL_PLOT
- SET_SCALING_STATUS
- LIST_SUBSTANCES
- TABULATE_SUBSTANCE

Example Using REACTOR

tcex24 - Simulation of the Silicon Arc Furnace

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_SPECIES
- CREATE_STAGE_BOXES
- CREATE_DIVIDERS
- CREATE_PIPES
- START_SIMULATION

Examples with Database Properties

tcex55 - Plotting Viscosity of Cr-Ni at 1873 K

This is an example of including viscosity in the calculations. This property, and others, are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

Using the FEDEMO database, which is the free demonstration version of the TCS Steel and Fe-alloys Database (TCFE), the viscosity of metallic liquids is plotted at 1873 K for Cu-Ni and compared to experimental data from Sato (2005).



Not all databases have this property although it is being added to databases as these are updated over time. Currently it is available with the latest versions of TCFE, TCHEA, TCNI and TCAL.

Reference

[2005, Sato] Y. Sato, K. Sugisawa, D. Aoki, T. Yamamura, "Viscosities of Fe–Ni, Fe–Co and Ni–Co binary melts," Meas. Sci. Technol. 16, 363–371 (2005).



You can learn more about the viscosity model by searching the help (press F1 when in Thermo-Calc).

The example includes an experimental data (`*.exp`) file called `Cr-Ni_1873K.exp`.



The same example is also provided in Graphical Mode as **T_12_Viscosity_in_Cr-Ni.tcu**.

tcex56 - Plotting Surface Tension of Cu-Zr at 1373 K

This is an example of including surface tension in the calculations. This property, and others, are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

Using the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL), the surface tension of liquid metallic is plotted at 1373 K for Cu-Zr and compared to experimental data from Krasovskyy (2005).



Not all databases have this property although it is being added to databases as these are updated over time. Currently it is available with the latest versions of TCNI and TCAL.

Reference

[2005, Krasovskyy] V. P. Krasovskyy, Y. V. Naidich, N. A. Krasovskaya, "Surface tension and density of copper–Zirconium alloys in contact with fluoride refractories," J. Mater. Sci. 40, 2367–2369 (2005).



You can learn more about the surface tension model by searching the help (press F1 when in Thermo-Calc).

The example includes an experimental data (`*.exp`) file called `Cr-Zr_ALDEMO.exp`.



The same example is also provided in Graphical Mode as **T_11_Surface_ tension_in_Cu-Zr.tcu**.

Application Examples

tcex09 - Calculating a Dew Point with POLY3

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

The STEP_WITH_OPTIONS and MAP commands are of note and used in this example.

tcex10 - Preventing Cr2O3 Clogging in a Continuous Casting Process

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr_2O_3 clogging in a continuous casting process.



This uses the SLAG database. A license is required to run the example.

The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr_2O_3 was formed.

Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential. In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- CHANGE_STATUS
- COMPUTE_EQUILIBRIUM
- DEFINE_SYSTEM
- DEFINE_SYSTEM
- LIST_CONDITIONS
- LIST_EQUILIBRIUM
- LIST_STATUS
- SET_CONDITION

- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex11 - Oxidation of Cu2S with an H2O/O2 Gas Mixture

This example demonstrates the oxidation of Cu_2S with an H_2O/O_2 gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu_2S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu_2S and H_2O using a command SET_INPUT_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

These commands are of also of note and used in this example:

- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex20 - Adiabatic Decompression in a Geological System

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- DEFINE_COMPONENTS
- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION
- SHOW_VALUE

tcex24 - Simulation of the Silicon Arc Furnace

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.

 This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_SPECIES
- CREATE_STAGE_BOXES
- CREATE_DIVIDERS
- CREATE_PIPES
- START_SIMULATION

tcex25 - Simulating the Refinement of Steel

This example is based on a typical steel refining process. Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment).

This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.

 This uses the SLAG database. A license is required to run the example.

tcex27 - Calculating Chemical Vapor Depositions (CVD)

This example calculates the chemical vapor deposition (CVD).

 This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_COMPONENTS
- SET_CONDITION
- ADD_INITIAL_EQUILIBRIUM
- LIST_AXIS_VARIABLE
- LIST_INITIAL_EQUILIBRIA

tcex28 - Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- EVALUATE_FUNCTIONS
- SET_START_CONSTITUTION

tcex29 - Calculating the Speciation of a Gas

This example shows how to calculate the speciation of a gas.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION

Data Optimization User Guide

Thermo-Calc Version 2021b



Introduction

In this section:

Introduction to Data Optimization 3
Data Optimization 4
The Least-Squares Method 5
The CALPHAD Approach 6

Introduction to Data Optimization

This guide describes the basic idea behind data optimization, contains brief descriptions of the modules and file types that you work with while doing your optimization, as well as rough outline of overarching workflow that you typically follow when working with optimization.

This guide assumes that you are familiar with using Thermo-Calc Console Mode. It also assumes that you understand the principles of thermodynamics and are familiar with the theoretical foundations of computational thermodynamics.



Press F1 to search the help for information about all the commands available in the Thermo-Calc Console Mode, including PARROT and ED_EXP. Note that the commands listed under PARROT and ED_EXP are only commands that are specific to PARROT and/or ED_EXP. These modules also contain some commands that are also available in POLY.



Thermo-Calc Console Mode example tcex36 is a detailed example of assessment and optimization in Thermo-Calc.



More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website.

Data Optimization

In a thermodynamic database, each phase in a system is characterized using a mathematical model of its Gibbs energy. The Gibbs energy of a phase depends on various state variables. It can be defined individually even in a heterogeneous system with many stable phases since the properties of one phase are completely independent of the properties of the other phases in the system. In most alloy systems, the thermodynamic properties of a phase can be modeled by expressing how the Gibbs energy depends on temperature and composition. State variables such as pressure, volume or entropy can also serve as parameters in the Gibbs energy expression. The Gibbs energy of the whole system is the sum of the products of the Gibbs energy of each phase multiplied by the amount of that phase.

How the Gibbs energy of the phase varies with various state variables is determined by a mathematical model and how various adjustable parameters of the model is set. By optimizing these parameters, you can calculate the thermodynamic properties of a system under various conditions (by calculating phase diagrams for example). The thermodynamic properties themselves are functions of temperature, pressure or composition. They include, among other properties, standard enthalpy of formation, entropy, heat capacity, molar volume, thermal expansivity, compressibility and Curie temperature for magnetic transformations.

Data optimization is about adjusting the model parameters so that calculated equilibria fit well with experimental data. An important part of a data optimization is therefore collecting and assessing available experimental and theoretical information about phase equilibria and thermochemical properties of a system.

When you optimize the parameters of the model of a phase, you put what is called optimizing variables into the Gibbs energy expressions of those parameters. During the optimization, the values of these variables are varied in order to find a fit between the calculated equilibria and the experimental data that you base the optimization on. Once you have settled on a Gibbs energy expression for a certain parameter of a phase of the element, then you must stick to this expression in all future optimizations involving the element. If you do not do this, then you must re-optimize all previous systems that involve this element when the expression is changed.

The Thermo-Calc software allows you to optimize parameters that characterize not only binary systems, but also ternary system and systems of even higher orders. You can even optimize parameters that characterize systems of different orders at the same time.



More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website.

The Least-Squares Method

Data optimization in Thermo-Calc is based on the least-squares method for fitting values calculated on the basis of a model with observed quantities. The software is accordingly trying to find the optimizing variable values that lead the minimized sum of the squares of the differences between the calculated values and the observed quantities (that is, of the errors or residuals).

The least-squares method works best under the following conditions:

- The observed quantities have a Gaussian probability distribution.
- The observed quantities are only subject to random errors.
- The different observations (experiments) are uncorrelated
- The standard deviation of each observation can be estimated.
- The number of observations is large.
- The models used give precise predictions.

Of course, these conditions are usually not all met in a normal thermodynamic assessment. But even in non-ideal conditions, there is no known method that works better than the least-squares method.

The CALPHAD Approach

CALPHAD is originally an abbreviation for *CALculation of PHAse Diagrams*, but was later expanded to refer to *computer coupling of phase diagrams and thermochemistry*. More about the CALPHAD methodology, including some of its history, is available on the Thermo-Calc Software website.

The data optimization functionality in Thermo-Calc works according to the CALPHAD approach to computational thermodynamics. This approach builds on the development of models that accurately represent thermodynamic properties for various phases. These models enable you to predict the thermodynamic properties of multicomponent systems-based data concerning binary and ternary subsystems. The predictions can take many factors into accounts, such as, for example, crystallography, type of bonding, order-disorder transitions and magnetic properties.

References

For in-depth information about CALPHAD as well as data optimization, see *Computational Thermodynamics – The Calphad Method* by Hans Leo Lukas, Suzana G. Fries and Bo Sundman (Cambridge University Press, 2007). CALPHAD was given its first general description in *Computer Calculations of Phase Diagrams* by Larry Kaufman and Harold Bernstein (Academic Press, 1970). The book contains some case studies of optimizations using Thermo-Calc.

Information about the concept of 'lattice stability' (which is important for the development of multicomponent thermodynamic databases) can also be found in the paper *Hume-Rothery and Calphad Thermodynamics* by Larry Kaufman, published in *Calphad and Alloy Thermodynamics*, edited by Patrice E.A. Turchi, Antonios Gonis, Robert Shull (The Minerals, Metals & Materials Society, 2002), pp. 3-19.

Working with Data Optimization in Thermo-Calc

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Data Optimization in Thermo-Calc

More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website.

The actual performance of the optimization of a system is primarily done in the PARROT module, and in its sub-module ED_EXP. The POLY and POST modules are used to calculate and plot property or phase diagrams based on the optimized variables. This allows you to visually assess how good a fit you have achieved between your calculated results and your experimental data.

The end result of a successful optimization is typically an updated Thermo-Calc database file (with filename extension *.TDB) or a new database file.

Data Optimization Workflow

When you carry out an optimization using Thermo-Calc, you typically follow a workflow as outlined below.

1. Collect experimental data about your system from various sources such as journal articles and reports.
2. Create a POP file in which you enter the experimental data you have collected.
3. Create a setup macro file in which you define your system and the variables you want to optimize. A useful general procedure is to first find a minimum set of variables that allows you to calculate most of the experiments.
4. Run the setup macro file.
5. Compile your POP file. This file often contains errors, which need to be corrected, and the file recompiled several times before the compilation is completed without errors.
6. In the ED_EXP module, check that the experiments in your POP file reach equilibrium with reasonable results. If any experiments do not reach equilibrium with reasonable results, then try changing the starting values on equilibrium conditions (such as composition) to see whether the equilibrium can be computed after all. If this does not work, then you can temporarily exclude the experiment from the optimization. At a later stage in the optimization, when the optimizing variables have different values, you can check whether the experiments can be computed with reasonable results.
7. Back in the PARROT module, run the first optimization cycle and evaluate the feedback in the console. You can also plot diagrams in the POLY module that allow you to visually inspect the fit between calculated optimization results and the experimental data. If you are not satisfied with the fit, then enter the ED_EXP module again and adjust the weights of the experiments in a way that is likely to improve the fit and run another optimization cycle. Reiterate until you are satisfied with the fit.
8. Once you get the optimization stable and smooth with the minimum set of variables chosen in step 3 above, try using different sets of variables to see whether improvements are possible.
9. When you are satisfied with the fit between calculated results and experimental data with your final set of optimizing variables, update your setup file and POP file. In the setup file, enter the calculated optimizing variable values as the variables' start values. In the POP file, enter the final weights of the experiments. With these files updated, you can easily regenerate the parameter values of your optimized system. Having the files updated also makes it easier to optimize the system again in light of

new data or new theoretical models.

10. Finally, update the database with your calculated results or create a new database with information about the system that you have optimized.

The PARROT Module

More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website.

The PARROT module consists of a comprehensive subroutine package for data evaluation of thermodynamic model parameters from experimental data. The module has 99 variables that you can use for optimization and the module can handle a thousand experimental measurements in an optimization. However, there are limits on the simultaneous numbers of variables and experiments. These limits are listed at each optimization.

The PARROT module is part of the Thermo-Calc software. The module is not included in the software development kits (SDKs).

The experimental data is entered and edited in a sub-module of PARROT: The EDIT_EXPERIMENTS Module.

The EDIT_EXPERIMENTS Module

The EDIT_EXPERIMENTS module, or ED_EXP for short, is used for entering, evaluating, and editing experimental data. To enter the module, go to The PARROT Module and then issue the command EDIT_EXPERIMENTS.

Since ED_EXP uses the POLY module for doing equilibrium calculations of experimental data points, many POLY commands are also available in the ED_EXP module. However, the commands may work somewhat differently in the two modules. There are also unique ED_EXP commands which are not found in POLY.

When you execute ED_EXP commands, the PARROT workspace is modified. However, note that you must always first use READ_WORKSPACES in ED_EXP before doing anything in the module. The command loads the experimental data that you are going to work with during the optimization. Furthermore, before leaving ED_EXP you must use SAVE_WORKSPACES or the results of your work in the ED_EXP module is lost.

Data Optimization in Other Modules

All kinds of thermodynamic data, calculated equilibrium states or dynamic parameters are transferred back and forth between the PARROT and the GIBBS module as well between these and the POLY module. Whenever an optimization run is performed, PARROT calls the GIBBS module for stored system definition data and model parameters.

In Thermo-Calc, the GIBBS module (the Gibbs Energy System) handles the models of the various phases that can form in a multicomponent system. It stores thermodynamic data and performs various Gibbs energy equilibrium calculations. It contains subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any set of variables. Many thermodynamic models for various types of substances are implemented in the module. Some commands that are available in the PARROT module are also available in the GIBBS module.

In the GIBBS module, parameters of the Gibbs energy models are referred to as *TP-functions*.

PARROT calls the POLY module for equilibrium calculations. The POLY module is used for calculating and storing complex heterogeneous equilibria.

Optimization File Types

These are the important files you work with when optimizing.

File type	Description
POP file	The POP file (Parrot OPtimization file) is the file that contains all the experimental data that you use for optimizing Gibbs energy values for your system. The POP file is a plain text file that contains ED_EXP commands. By default, the file has the filename extension *.POP in Thermo-Calc.
Setup file	The setup file is a Thermo-Calc macro file (*.TCM). This file typically contains commands that define your system, opens the PARROT workspace (and associated GIBBS and POLY workspaces) and sets optimizing variables.
Other macro files	It is often useful to have other macro files than the setup file at hand while you are doing your optimization. For example, it is convenient to have a macro file that automatically plots phase diagrams or other diagrams based on the latest values of your optimizing variables. An optimization process typically involves many optimization cycles, so this operation needs to be done many times during a typical optimization.
Workspace files	The PARROT module has its own workspace with dynamic memories, similar to the workspaces of POLY and GIBBS. It is stored and updated in a PARROT workspace file with the filename extension *.PAR. The workspace file is a binary file whose format is hardware dependent. This means that the format is unique for each type of CPU. Hence, a workspace file saved on a computer with one type of CPU cannot be used on a computer with another type of CPU.
EXP-file	The EXP-file is a plain text file with information in the form of DATAPLOT Graphical Language commands. These commands can specify some or all of the data points in your POP file. This allows you to plot these data points on top of your plotted optimization results (with the POST commands APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT). You can then visually assess the fit between these results and the experimental data. The PARROT workspace is not influenced in any way by the creation or use of EXP-files. ▶ *DATPLOT User Guide* included with this documentation set.

Optimization Workspaces

When writing the setup file, you enter a CREATE_NEW_STORE_FILE command which creates a PARROT workspace file. Alternatively, select an existing PARROT workspace file with SET_STORE_FILE. The workspace file is automatically updated and saved with the latest optimization results (after each use of the OPTIMIZE_VARIABLES command). You can also explicitly instruct Thermo-Calc to save the workspace using SAVE_PARROT_WORKSPACES. If you want to get rid of your latest changes and return to the state of your workspace when it was last saved, use READ_PARROT_WORKSPACES.

When the PARROT workspace is saved, parts of the POLY and GIBBS workspaces are also saved to the PARROT workspace file, along with the PARROT workspace itself. Using the POLY command SAVE_WORKSPACES creates a new POLY3 file, nothing is saved to the PARROT workspace file.

If you do any POLY calculations based on data in the current workspace file, then a *.POLY3 file is created, which contains a copy of the current set of parameters. If you continue on your optimization and read the old *.POLY3 file, then the new set of parameters is overwritten with the old set. It is therefore recommended that you never read a *.POLY3 or *.GES5 file while you are doing an optimization.

Method for Optimization and Simulation

The PARROT module typically uses ordinary POLY minimization for equilibrium calculations. The global minimization technique that is used in POLY cannot be used because it automatically creates new composition sets which corrupt the PARROT workspace. Furthermore, the equilibrium definitions that you use as input for your optimization must each be attributed to a specific phase. Some of these definitions may specify some local or partial equilibrium state rather than a global minimum. However, it is possible to use the global minimization technique for some equilibrium calculations by using the ED_EXP command ADVANCED_OPTIONS with the `Toggle_Alternate` option.

Optimization in PARROT is performed on the basis of a 'maximum likelihood' principle. According to this principle, the best fit between various calculated results and all the input of experimental data is found where the sum of the square of the weighted residuals is at its minimum.

Typically, the results of an optimization is considered to be better the fewer optimizing variables that are needed to get the same level of fit between computed results and experimental data. If you can get almost the same fit using eight instead of twelve parameters, then this should be considered to be a significant improvement. When more parameters are used, the values of the individual parameters tend to become unrealistic. This is particularly true when it comes to temperature-dependent parameters. However, relatively small differences in the number of parameters are often insignificant. For example, it does not typically matter whether you used 24 or 25 parameters to reach a certain degree of fit.

It is often difficult to compare the quality of different optimizations based on the number of optimizing variables that have been optimized. Since you may rely more or less heavily on different pieces of available experimental data (and do so with good reason), it is possible that two different users could end up with very different numbers of parameters for the same system. For example, suppose you optimize the Fe-Al system to incorporate it into an Al database, while someone else optimizes the same system to incorporate it into an Fe database. In this situation, the two of you would probably make different judgements about which experimental information your calculated results must have a good fit with.

Creating the POP File

Before starting an optimization in Thermo-Calc, you must collect relevant experimental data about your system that is available in the research literature. This data is then entered in the POP file. The experimental data points and measurements are entered in this plain text file in the form of ED_EXP commands.

The syntax of the POP file is in principle independent of the models used for describing the phases in the system.

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Experimental Information

An optimization of thermodynamic model parameters should be based on a range of reliable experimental results that is as wide as possible, as well as on empirical or semi-empirical correlations and theoretical considerations. During an optimization in Thermo-Calc, many kinds of thermochemical and thermophysical data can be mixed and used together.

The information needed for an optimization represent measurements of thermodynamic parameters in the system at equilibrium. These can be measurements of any of the thermodynamic quantities that can be set as conditions in Thermo-Calc. The information may represent measurements of activities or enthalpies in single-phase regions for example, or solubilities or transformation temperatures in a multi-phase region.

For each equilibrium that is used in the optimization, at least one quantity must have been measured and you also need to know the conditions that must be set to compute the system's equilibrium state. For example, consider a binary system in a single-phase region. Suppose that you have measured the temperature, pressure, composition and the chemical potential. Three of these quantities are necessary to specify the equilibrium state and the forth can be used as experimental information to model the phase.

If you have a two-phase region and know the temperature and pressure conditions, as well as which the stable phases are, then you could use the compositions of one or both phases as experimental data. The former information about the conditions is sufficient to determine the equilibrium. The experimental information can then be used to optimize the parameters that are used to characterise and model the system.



For examples how to enter various kinds of experimental data in the POP file, see Experiments and Experimental Data.

Conflicting or Missing Information

You are likely to sometimes have inconsistent or conflicting experimental information. In principle, all available experimental data should still be entered into the POP file, unless you have good reasons to exclude some information. For example, if you have reason to believe that the samples used in some experiments were not pure, then these experiments could be excluded from the POP file.

For some systems, you have very little experimental data to go on. When this is the case, do not try to fit the available data uncritically with high accuracy without considering possible errors. You can look for data in systems with similar elements to get an idea about what the reasonable estimates of data that is lacking could be. Or you can use calculations from first principles or semi-empirical methods to get reasonable estimates that can be used as experimental data.

Invariant Equilibria Information

The most valuable experimental information for an optimization is information about stable invariant equilibria. An invariant equilibrium is such that neither pressure, temperature nor composition can be changed without there being a change in the set of phases present in the system. It is recommended that all information about invariant equilibria for a system is included in the POP file. These equilibria need not all be based on explicit experimental measurements of thermodynamic properties.

Reasonable estimates from available experimental data are often useful to include in the POP file. Such estimates, which should be based on the available experimental data, helps Thermo-Calc find a good set of start values on the optimization variables. However, at the end of the assessment, these estimated equilibria should be excluded and you should complete the optimization based only on the experimental information that is based on measurements.

With some experience from phase diagram evaluation, it is possible to make reasonable estimates of metastable invariant equilibria. Such estimates helps reduce the number of phases that are assessed simultaneously during the optimization. For example, you may assume that a certain intermediate phase does not form in a system. Then extrapolate the liquidus curves below the stable three-phase equilibria and finally, estimate temperatures and compositions of metastable three-phase equilibria between two other phases and the liquid.

Another useful technique is to extrapolate a liquidus line from a peritectic equilibrium to estimate the congruent melting temperature of a compound. This estimate may be more useful than the information about the peritectic equilibrium itself as the equilibrium involves only two phases.

Equilibria in Higher-Order Systems Information

When you optimize a binary system, the available experimental information can often be described equally well by very different sets of parameters. Information about ternary and higher order systems that include the components of the binary system are then often useful for optimizing the binary system (the same is true of information about quaternary system with respect to optimizing ternary systems). Often, it is only when you extrapolate the optimized parameters to a higher-order system that you can judge which of the sets of model parameters that is best. Sometimes information from several ternary systems is required to make a reliable judgement about which set of parameters best describes a particular binary system.

Heat Capacities Information

If you want to optimize your system based on data about heat capacities, then the corresponding parameters should first be optimized separately before you perform the general optimization of your system. The parameters should be kept fixed during the general optimization. This is because it is normally not possible to optimize heat capacity data together with other data in a meaningful way. If you do this, then it is very likely that the parameters related to the heat capacity are badly determined.

POP File Syntax

It is recommended that you specify an experimental equilibrium as close as possible to actual experimental conditions. Ideally, there is information about the set of stable phases, temperature, pressure and some or all compositions for the equilibrium.

In addition, it is recommended that you keep the POP file well-organised and extensively commented. This is especially important if someone else reassesses the system when new experimental information is available.

If you have too many equilibria defined in your file, or if you define equilibria with different sets of components in the same file, then you must divide the POP file in *blocks* (using the FLUSH_BUFFER command). You know whether you have defined too many equilibria for one block when you compile the file. A too large number of equilibria leads to an error message when the file is compiled.

If you use the DEFINE_COMPONENTS command, then it must be the first command in the POP file (or if you have several blocks, DEFINE_COMPONENTS can also be put as the first command after FLUSH_BUFFER). This is because the command automatically reinitiates the current workspace, so the effect of any commands placed before it are not saved.



The last command in the POP file should always be SAVE_WORKSPACES .

Legal Commands in a POP File

The following commands can be used in a POP file.

- ADVANCED_OPTIONS
- CHANGE_STATUS
- COMMENT
- CREATE_NEW_EQUILIBRIUM
- DEFINE_COMPONENTS
- ENTER_SYMBOL
- EVALUATE_FUNCTIONS
- EXPERIMENT
- EXPORT
- FLUSH_BUFFER
- IMPORT

- LABEL_DATA
- SAVE_WORKSPACES
- SET_ALL_START_VALUES
- SET_ALTERNATE_CONDITION
- SET_CONDITION
- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SET_START_VALUE
- SET_WEIGHT
- TABLE_HEAD, TABLE_VALUES and TABLE_END

Entering Experimental Information

A POP file in Thermo-Calc (*.POP) mainly consists of descriptions of equilibria, each equilibrium describing a data point that is based on an experiment from the existing literature on your system. An equilibrium is specified using ED_EXP commands.

The following is an example of a specification of an equilibrium with a single stable phase in the Au-Cu system. Equilibria with a single stable phase are often from experiments where enthalpies of mixing or chemical potentials have been measured.

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQUID=FIX 1
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
EXPERIMENT HMR=-1520:200
COMMENT Measurement by Topor and Kleppa, Met trans 1984
```

Creating a New Equilibrium

The first command in an equilibrium specification is always CREATE_NEW_EQUILIBRIUM. This command takes two integers as arguments. The first integer should specify a unique identifier that can be used later to refer to the equilibrium in question. The second integer is an initialisation code 0, 1 or 2:

- Code 1: This means that all components are entered but all phases are suspended. This code is appropriate in most cases.
- Code 0: This means that all components and phases in the equilibrium are suspended initially. This code is needed if you are using experimental data about systems of different orders simultaneously, such as data about both binary and ternary systems for example.
- Code 2: This means that all components and phases are initially entered.

For example, the first command in the example above creates an equilibrium data point with the unique identifier 1. All components of the system are entered but all phases are suspended:

```
CREATE_NEW_EQUILIBRIUM 1 1
```

Setting Equilibrium Conditions and Uncertainty

All the equilibrium-related commands that are placed in between two CREATE_NEW_EQUILIBRIUM commands are interpreted as specifying the conditions of the equilibrium created by the first command. The values of these conditions should be based on the conditions specified in the experiment that you base the equilibrium definition on.

In the example, the CHANGE_STATUS command specifies that the equilibrium is a single-phase equilibrium with the liquid phase.

```
CHANGE_STATUS PHASE LIQUID=FIX 1
```

Furthermore, the temperature is 1379 K, the pressure is 1 bar (1E5 Pa) and the mole fraction of Au is 0.0563.

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
```

Sometimes you have reason to think that some information about an equilibrium condition may not be accurate. If this is the case, then you specify the degree of uncertainty for a condition with a colon after the condition quantity, directly followed by either an absolute value or a percentage. For example, if you have reason to doubt the reliability of the Au mole fraction measurement, then you could write:

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563:10%
```

This indicates that you think the Au mole fraction is between 0.0507 and 0.0619. PARROT calculates the equilibrium twice, once for 0.0507 and once for 0.0619, and then computes the change of each experimental value between these two equilibria. This change is used to modify the uncertainty specified for the experimental value.

- Entering the Experimental Value and its Uncertainty

The possibility of specifying uncertainties on conditions may be useful when you have experimental data about a ternary system. In a binary system, a tie-line is determined by the two phases, the temperature and the pressure. Measurements of the compositions of both phases can then be used as experimental data. To specify the tie-line in a ternary two-phase equilibrium one of the four compositions must also be set as a condition. If the measurement of this composition has the same uncertainty as the other compositions, then you can assign this same degree of uncertainty both to the composition selected as a condition and the compositions selected as experimental data. Alternatively, the sample (overall) composition could be used as a condition and all four phase compositions could be used as experiment values. These phases must have the status *entered* (not fixed) since the relative amount of each is unknown.

Setting Reference States

If you want to specify a non-default reference state for one or several of your system components, then you do this with the SET_REFERENCE_STATE command. In the following example, the reference states for Au and Cu are set to the liquid phase at current temperature (*) and a pressure of 1E5 Pa.

```
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
```



In order for these reference states to be taken into account, the `R` suffix must be used when the measurement of the enthalpy per mole of the system is entered for an experiment.

The Reference State Suffix R

Suffixes

You can use the reference state suffix R for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the SET_REFERENCE_STATE command in POLY (or in response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the R suffix depends on the reference states of all the components in the defined system.



It is possible to use an R suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then MUR(comp)= MU (comp), ACR(comp)= AC(comp) and LNACR(comp)= LNAC(comp).

In the case of some thermodynamic variables, you can also use the R suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

Entering the Experimental Value and its Uncertainty

The EXPERIMENT command is used to specify the quantity that the calculated results should be fitted to. When specifying this quantity, you both specify the measured quantity itself and your estimation of the uncertainty of this value.

In the example, the EXPERIMENT command specifies the enthalpy per mole of the system, where this value is specified with respect to non-default reference states that you have set in the equilibrium specification:

```
EXPERIMENT HMR=-1520:200
```

The value before the colon is the quantity of the variable. The value after the colon is an assessment of the uncertainty of this quantity. A higher value means a greater uncertainty. In the example, the uncertainty has been specified with an absolute value but it could also be specified in percent of the quantity:

```
EXPERIMENT HMR=-1520:13%
```

Several experiments can be specified after the experiment command. Besides assigning values to conditions, it is also possible to specify that a certain quantity is greater than or less than a certain value. For instance, the following command would specify that the activity of the C-component is less than 0.01 and the mass fraction of the BCC phase of Ag is greater than 0.05:

```
EXPERIMENT ACR(C)<0.01:0.001 W(BCC,AG)>0.05:10%
```

Note that an experimental quantity can typically also be treated as an equilibrium condition, and vice versa. Which measured quantities that you treat as conditions and which quantities you treat as experimental data should be based on the accuracy of the different measurements. In most cases, the quantity that is based on the experimental technique with the lowest accuracy should be used as the experimental value.

Entering Many Equilibria as a Table

When one thermodynamic variable (e.g. heat capacity) has been measured as a function of another (e.g. temperature), then experimental data is often presented as a table. By using the TABLE_HEAD, TABLE_VALUES and TABLE_END commands, you can enter such experimental information into the POP file in the form of a table. These three commands should always be used together and must be entered in the right order. See TABLE_HEAD, TABLE_VALUES and TABLE_END.

The TABLE_HEAD command is followed by a number. This number identifies the table as a whole, but also uniquely identifies the first equilibrium that is included in the table. This numeric identifier is incremented by one for each additional equilibrium in the table. Each row in the table represents one equilibrium. Thus, the equilibrium defined by the first row in the table above (on the line immediately below TABLE_VALUE) is uniquely identified with the number 1, the equilibrium defined by the second row by number 2, and so on until the last equilibrium on the sixth row, which is identified by the number 6.

Since the unique identifiers of the equilibria in the table are automatically generated from the unique numerical identifier that you give to the table, the unique numerical identifier that is normally given to the CREATE_NEW_EQUILIBRIUM command is replaced by two at signs (@@).

At least one of the equilibria conditions specified with the SET_CONDITION command must be a condition whose value is set by the numbers in one of the table columns. To assign the numbers in a column to a condition, use the syntax SET_CONDITION <condition>=@<column number>. For instance, in the example above, the mole fraction of X(ALO3/2) is for each equilibrium given by the number in the first column of the table.

At least one of the measured variables that are entered with the experiment command must be a variable whose value is set by the numbers in a table column. To assign the numbers in a column to a measured variable, use the syntax EXPERIMENT <variable>=@<column number>. In the example above, the measured temperature for each equilibrium is given by the number in the second table column.

The actual table should be entered between TABLE_VALUES and TABLE_END. Separate the columns with tabs or any number of spaces. The columns do not have to contain numbers, but can also contain other types of values, such as phase names for example. If a column contains text with spaces or special characters, then the text must be surrounded by double quotes ("ABC DEF&ghi", for example). The table may have columns that are not used, but each row must have exactly the same number of columns.

The following block of commands exemplifies how a table can be entered into a POP file:

```
TABLE_HEAD 1
CREATE_NEW_EQUILIBRIUM @@ 1
CHANGE_STATUS PHASE TETR=FIX 0
CHANGE_STATUS PHASE ION=ENT 1
SET_CONDITION P=101325 N=1 ACR(O2,GAS)=.21 X(ALO3/2)=@1
EXPERIMENT T=@2:5
TABLE_VALUE
0.46082476
0.57142380
0.66822276
0.7496 2176
0.50382426
0.63132249
TABLE_END
```

Setting Site Fraction Start Values

In some systems, you have to set non-default composition start values on some experiments in order to get them to converge properly during optimization. This may be important if your system has a miscibility gap for example, in which case several equilibria with different

compositions exist at certain temperatures. In such cases, you have to make sure it is specified in the POP file which side of the miscibility gap the equilibrium is on. The calculated equilibrium could otherwise end up on the wrong side, resulting in a large error.

In the POP file, you can set the site fraction of a constituent on an equilibrium with SET_START_VALUE.

For example, the following command sets the composition start value of VA constituent of the FCC_A1 phase to 0.99:

```
SET_START_VALUE Y(FCC_A1,VA#2)=0.99
```

Setting the mole fraction for a component in a phase is not as reliable as setting the site fraction.

Additional equilibria entered after the last SET_START_VALUE command are automatically given a similar start value if the following command appears previously in the POP file:

```
SET_ALL_START_VALUES Y
```

If start values are not set automatically for phase constituents, then you may have to set the composition start value for each equilibrium (or table of equilibria) separately.

Commenting About an Equilibrium

The COMMENT command inserts a comment about the equilibrium that is saved to the PARROT workspace file when the POP file is compiled. The comment must be entered on one line.

Comments can also be entered immediately after a dollar sign ($), but these are not saved to the PARROT workspace. Instead, these comments are ignored by Thermo-Calc when the POP file is compiled.

Simultaneous Use of Binary and Ternary Experiments

You can use experimental information about binary and ternary systems (as well as systems of even higher order) in the same POP file and optimization. To do this, you must inform the PARROT module that not all components of the ternary system (or system of even higher order) should be considered. This allows you, for example, to use experimental information about a binary equilibrium that exists within a ternary system.

Use CHANGE_STATUS with the keyword component and which components that should be entered. You should also give the initialization code 0 (rather than 1) to the CREATE_NEW_EQUILIBRIUM command. This code indicates that all components must be entered.

For example, the following set of ED_EXP commands characterises a binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C). It can be used in a POP file that otherwise only contain experimental information about the ternary system (A-B-C):

```
CREATE_NEW_EQUILIBRIUM 1 0
CHANGE_STATUS COMPONENT A B = ENTERED
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=1177:10
COMMENT from A-B
```

Using Stability Conditions

Early in the optimization when parameter values are not so good it is often useful to set the driving force for precipitation of a phase (per mole of components) to make sure that it appears where it should. The DGM condition is very useful for making sure that phases appear where they should. It can be removed when the optimization becomes stable.

The DGM condition is also useful for suppressing phases that appear where they should not appear. Do this by setting the value and the uncertainty to something reasonable. For example, the driving force for precipitation of the BCC phase could be set as follows:

```
DGM(BCC)<-0.1:0.1
```

This produces an error even before BCC becomes stable and the weight of the experiment in question can be adjusted as needed. If you specify that the driving force for the BCC phase should be below 0 (DGM(BCC)<0:1E-4 for example), then the optimization converges extremely slowly (if at all). With such a sharp error condition, calculating the equilibrium is like finding the minimum point on a lawn that gently slopes towards a rock wall. The optimization keeps bouncing into the wall.

Another useful stability condition is the phase stability function, abbreviated QF. This can be used to specify that a phase is outside the miscibility gap for a solution phase. If QF(phase) is negative, then the phase is inside the miscibility gap; if QF(phase) is positive, then it is outside the miscibility gap.

Grouping Equilibria with Labels

If you have several equilibria describing experiments that you want to be able to treat collectively, you can give all of the equilibria one and the same label.

Use LABEL to give an equilibrium a label. The label must start with the letter A and can only be up to four characters long. For example, you can insert the following command in several equilibria specifications:

```
LABEL ALH
```

During the optimization, you could use this label to, for example, set all the equilibria that have it to the same weight in the ED_EXP module.

Dividing the POP File into Several Blocks

For two different reasons, you may have to divide your POP file into different blocks:

- PARROT uses a buffer for storing compiled experimental data. If there is not enough memory in this buffer for storing all the experiments from the POP file, then the POP file can be divided into several blocks. When PARROT encounters the end of a POP file block, it saves the experimental data that has been compiled to PARROT workspace, clears out the memory buffer and then proceeds to read the next block in the POP file. This goes on until the experimental data from all the blocks have been saved to the PARROT workspace.
- If you want to put equilibria with different sets of components in one and the same POP file, then you must divide the file up into blocks. Each block should only contain equilibria that all have the same set of components.

To divide the equilibria in the POP file into different blocks, enter the FLUSH_BUFFER command between two equilibria. This command marks the beginning of new block. When the command is encountered during the compilation of the POP file, the compilation of the current block is terminated, the equilibria saved to the PARROT workspace file and a new block is initiated. That the buffer is reinitiated means that all functions and constants that were entered in the previous block must be entered again in new block in order to be used.

When editing your experimental data in the ED_EXP module, you can select which block to load and edit using READ_WORKSPACES `<block number>`. The block before the first instance of FLUSH_BUFFER is block number 1, the block after the first instance and before the second instance is block number 2, and so on.

The Setup File

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Creating the Setup File

The second step is to create the setup file. This is an ordinary Thermo-Calc macro file (*.TCM). Typically, your setup file should contain the following:

- A system definition.
- A section where you enter model parameters and optimizing variables.
- A GO PARROT command.
- A section where initial values are assigned to the optimizing variables for the first optimization cycle.
- A CREATE_NEW_STORE_FILE `<filename.par>` which creates the PARROT workspace file onto which the results of your optimization are continuously saved and updated. By default this workspace file has the same filename as the setup file, but with the *.PAR filename extension.
- A COMPILE_EXPERIMENTS `<filename.pop>` command. Since you often encounter syntax errors when you first try to compile a POP file, it may be useful to execute this command from the console rather than as part of the setup macro file.
- Normally, you also have a SET_INTERACTIVE at the end of the setup file. This command returns control over Thermo-Calc to the console.

It is possible to interactively execute all these commands one at a time in the console. It may be instructive to enter the commands that would normally go into the setup file interactively while using the on-line help while you are learning to use the PARROT module.

Defining the System

If you have an existing database with information about your system, then you can write the system definition part of your setup file in two different ways.

- If you have an unencrypted user database, then you can define your system by entering DATA module commands directly in the setup file. Use the DATA commands that you normally use to define a system when doing equilibrium calculations in Thermo-Calc Console Mode.
- Define your system by entering DATA module commands directly in the console, then generate a macro file with the GIBBS command LIST_DATA `<name of setup file>.tcm p` . This command saves all the data that has been loaded in the GIBBS workspace as a macro file. This file can then be modified as required into an optimization setup file.

Creating Additional Composition Sets of a Phase

If you need several composition sets of a phase, then these should be created with the GIBBS command AMEND_PHASE_DESCRIPTION `<phase name> composition_sets <composition set number>` in the setup file.



If you add composition sets of a phase after the POP file has been compiled, the data structure in the workspace is corrupted and you have to recompile the POP file.

Entering the Optimizing Variables

When you have retrieved the data about your system for the setup file, you must manually enter the model parameters that you want to optimize. This is done using the GIBBS command ENTER_PARAMETER, but when you specify the Gibbs energy expression for the parameter, you enter variables that can be given various values into the expression. It is the values of these variables (and thus, the Gibbs energy of the parameter) that you are optimizing.

How you in detail specify the optimizing variables in your set up file depends on which phase you are trying to optimize and what thermodynamic model that is used in the optimization.

- Thermodynamic Models

Entering Optimizing Variables in Parameter Specifications

There are ninety-nine predefined variables in the PARROT module which you can use in your optimization. These variables are referred to as `V1`, `V2`, `V3`, … `V98` and `V 99`. When the GIBBS workspace is initialized, all optimizing variables are set to a fixed numerical value of zero. When you do an optimization, there is always some variable for which you want to evaluate the best value, but you can assign fixed values to optimizing variables too. It is often useful to enter all the variables that you can conceivably want to optimize, and then you can interactively select and change which variable to focus at various stages of the optimization.

The setup file excerpts that follow show how optimizing variables are entered. However, before the optimizing variables are introduced in this example, the following command enters an ionic liquid solution phase (a phase for which you have some experimental information):

```
ENTER_PHASE IONIC_LIQ  Y,
AL+3,ZR+4 ; ALO2-1,O-2 ; N N
```

This ENTER_PHASE command enters a phase called IONIC_LIQ into the GIBBS workspace. This phase is of the type ionic liquid solution, which is specified by type code `Y`. Such a phase is modeled by the *Ionic Two Sublattice Liquid Model*. The next two arguments specify the two sublattices, in this case the cations AL+3,ZR+4 and the anions ALO2-1,O-2. Components that interact in a sublattice are separated by a comma. The first `N` at the end means that no additional constituents are added to the phase. The second `N` means that a list of possible parameters for the phase should not be shown in the console.

There are model parameters that describe the phase which you do not want to optimize, in which case the Gibbs energy expression of the parameter does not contain any optimizing variables.

Example 1

For example, the following parameters of the IONIC_LIQ phase do not contain any optimizing variables:

```
ENTER_PARAMETER G(IONIC_LIQ,AL+3:ALO2-1;0) 298.15 +2*GAL2O3_L; 6000 N
ENTER_PARAMETER G(IONIC_LIQ,AL+3:O-2;0) 298.15 +GAL2O3_L+400000; 6000
N
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:O-2;0) 298.15 +2*GZRO2L; 6000 N
```

These parameters define the Gibbs energy expressions for three constituents in the constituent array, namely AL+3:ALO2-1, AL+3:O-2 and ZR+4:O-2. The names that occur in these expressions—that is, GAL2O3_L and GZRO2L—are the names of complex functions of temperature that are entered in the GIBBS workspace with the ENTER_SYMBOL command.

The numbers that frame the Gibbs energy expressions specify the temperature range within which the expression should be applied. In the above, the expressions are applied in a temperature range from 298.15 K to 6000 K.

Example 2

In this example, suppose that you want to optimize the model parameter for the ZR+4:ALO2-1 combination, then you could enter the variables V1 and V2 in the Gibbs energy expression for that parameter in the following way:

```
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:ALO2-1;0) 298.15 +GZRO2L +2*GAL2O3_L
+V1+V2*T; 6000 N
```

You normally have different optimizing variables in different parameters, but in some cases you may want several parameters to vary together, in which case you can use the same variable in the Gibbs energy expressions of several parameters.

Entering Interaction Parameters

For some systems, you have to consider interaction parameters in order to take excess Gibbs energy into account and correctly model the phase. By default, the software uses a Redlich-Kister expression for the excess Gibbs energy. The coefficient is entered after the constituent array when you use the ENTER_PARAMETER command. In the last section, all the parameters were entered with a coefficient of zero (0).

To take account of the excess Gibbs energy, you might enter the following:

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;0) 298.15  +V11+V12*T;
6000 N
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;1) 298.15  +V13+V14*T;
6000 N
```

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;2) 298.15  +V15+V16*T;
6000 N
```

Parameters with interaction coefficients are referred to as *interaction parameters*. The regular parameter has a coefficient of 0. The subregular parameter has a coefficient of 1. It is possible to interaction coefficients up to a value of 9, but you are advised not to use more than three coefficients (that is, with coefficient values of 0, 1 and 2).

Initializing Optimizing Variables in PARROT

Variables that have been entered into Gibbs energy expressions for model parameters in the setup file have to be initialized and given start values before they are optimized.

You have to estimate what start values to give to the optimizing variables based on your knowledge of the system or of relevantly similar systems. There are no general rules for what start values your optimizing variables should have. If you are not able to make any informed estimation about what start values to use, then you may not be able to find a good fit between your experimental data and your calculated results. In this case, it is often best to start the optimization in the so-called alternate mode. In alternate mode, the PARROT module helps you find some reasonable start values for your optimizing variables.

- About Alternate Mode

Even if you are starting your optimization in alternate mode, you still have to initialize the optimizing variables though (you can all give them a start value of 0).

To initialize an optimizing variable and to give it a start value, use either SET_OPTIMIZING_VARIABLE or SET_SCALED_VARIABLE. Using SET-OPTIMZING_VARIABLE results in a scaling factor equal to the current value of the parameter unless the current value is zero, in which case the scaling factor is 1000. This is typically appropriate for enthalpic parameters, but not necessarily for other parameters. The scaling factor is the factor by which the optimizing variable value is varied during the optimization.

For example, if you want to optimize the variables V1, V2, V11, V13 and V17, then you could enter the following in the setup file:

```
SET_OPTIMIZING_VARIABLE 1 +43000
SET_OPTIMIZING_VARIABLE 2 -35.2
SET_OPTIMIZING_VARIABLE 11 +72000
SET_OPTIMIZING_VARIABLE 13 +27000
SET_OPTIMIZING_VARIABLE 17 -100000
```

The value given to each optimizing variable (+43000 for variable V1 for example) is also that variable's initial scaling factor. If you want to set the initial scaling factor of a variable to a value that is lower or higher than its start value, then use SET-SCALED_VARIABLE `<start value><scaling factor><min value><max value>`.

Creating the Workspace File

In the setup file, after the system definition and the entered optimizing variables, use the PARROT command CREATE_NEW_STORE_FILE to create and save a PARROT workspace file for the system defined in the setup file. For example, the following command saves all current data on system definitions (elements, species, components, phases), symbol definitions (constants, variables, functions, tables) and parameters that are stored in the workspace used by GIBBS, POLY and PARROT into a file called AL2O3-ZRO2.PAR:

```
CREATE_NEW_STORE_FILE AL2O3-ZRO2
```



The experimental information in the POP file is not saved to this PARROT workspace file.

Compiling the POP File

At the end of the setup file, use the command COMPILE_EXPERIMENTS followed by the name of your POP file to compile the data in that file and save it to the current PARROT workspace file. Note that you must first have opened or created a new PARROT workspace file before you compile your POP file. The other argument to the command can typically be given default values with comma signs (,):

```
COMPILE_EXPERIMENTS AL2O3-ZRO2.POP,,,
```

If Thermo-Calc encounters errors in the syntax of the POP file, then error messages are displayed in the console. Normally, the compilation also stops when syntax errors are encountered. If this happens, then you must correct the errors and recompile the file. It is useful to have two console windows open when you do this. That way, you can use one console for editing the experimental data and another console for compiling and reading any further error messages.

Returning Control to the Console

Put the command SET_INTERACTIVE at the end of the setup file if you want to return control to the console when the commands in the setup file have all been executed.

Optimizing in PARROT

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Optimizing the System in PARROT

When you have created a POP file, a setup macro file, and (optionally) EXP files, you should start doing optimization runs interactively in the console. This process can be divided into a number of steps (such as running optimization, evaluating optimization results, modifying weights and models and adding new information), but usually, you have to go through many optimization cycles before achieving a satisfactory fit between calculation results and experimental data.

Typically, it is not obvious when an optimization is finished. You must exercise your judgment about when the fit you have achieved is good enough.



It is possible to interactively change almost everything in the initial setup macro file and in the POP file. For example, you can add more parameters to be optimized and modify or add more experimental information.

Changes that Require POP File Recompilation

Some changes that you do interactively in the PARROT module or the ED_EXP sub-module destroys the data structure in the workspace. For example, if you add more composition sets to a phase, then the number of phases actually change and the links break between the experimental data and the thermodynamic models. Note that if the global minimization technique is used in POLY, then new composition sets that corrupts the PARROT workspace may be created automatically. If this happens, then you have to compile the POP file again.

If you recompile the POP file, then the experimental equilibria are calculated with the default start values.

Optimization Workflow

Normally, the workflow during an optimization is the following:

1. In the PARROT module, run the setup macro file using MACRO_FILE_OPEN.
2. Go to ED_EXP with EDIT_EXPERIMENTS, use READ_WORKSPACES to load your experimental data and then execute .
3. If an equilibrium cannot be computed, then this either means that the start values (site fractions, for example) were inappropriate or that the equilibrium cannot be calculated with the current set of parameters. If the latter, then the equilibrium may have to be excluded from the optimization. However, you should make an effort to exclude the possibility that the reason is just that you do not have the appropriate start values for the equilibrium.
4. When each equilibrium is either successfully computed or excluded from the calculation, go back to the PARROT module and run the OPTIMIZE_VARIABLES command. Give the number of optimization iterations you want the Thermo-Calc program to carry out as an argument to the command. This number specifies how many different sets of values for the optimizing variables that PARROT tries to fit with the experimental data. It is recommended that you run 0 iterations first to see the discrepancy between the experimental data and the initial calculated results. The current workspace file is automatically updated with the last set of optimized variables and calculated results.
5. List and evaluate the result of the optimization using LIST_RESULT. Typically, what is of interest in the results are the relative standard deviation of the optimizing variables and the error values in the list of calculated experimental data results. If the relative standard deviation for an optimizing variable is very large, this means that the variable doesn't have any effect on the computed results and that the variable should not be used (you can make PARROT ignore the variable by setting its value to 0 with SET_FIX_VARIABLE). If the relative standard deviation is close to zero for a variable, then this might indicate that you need to use more variables. When it comes to errors in the calculated equilibrium results, these can be decreased by lowering the weight that PARROT gives the experiment in the calculation (the more weight, the more the experiment affects the calculated results).
6. Use OPTIMIZE_VARIABLES or CONTINUE_OPTIMIZATION to carry out a new optimization cycle. Go back to step 5 above and continue to do optimization cycles until you judge that there is a good enough fit between your calculated results and your experimental data. It is recommended that you do not only rely on feedback from LIST_RESULT but also frequently plot various diagrams and compare them visually to some of your experimental data.

Ensuring Computation of all Equilibria

When you have run the setup macro file, you should start by trying to compute all the equilibria that were created when your POP file was compiled. To do this, you must first go to the ED_EXP submodule, and load the experimental data from the current PARROT workspace file with the READ_WORKSPACES `<block #>` command (normally, the block number is `1`).

When you have loaded all equilibria, you should try to compute them all using the ED_EXP command . A list of calculated equilibrium results are shown in the console, but the software is not able to reach an equilibrium for an experiment, then the program cancels the calculations and displays an error message.

The following list shows an example output where the first two experiments in the POP file have been successfully computed, but an equilibrium is not reached for the third experiment. No other equilibria are computed, since the calculations are aborted when the error occurs.

```
Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
  1 A1    22   1.    2575.3      IONIC_ FLUORI TETR
  2 A1    18   1.    2156.9      IONIC_ CORUND TETR
*** ERROR  1614 IN QTHISS
*** CONDITIONS CAN NOT BE FULLFILLED
```

When this happens, try to find out why the equilibrium calculation fail. Are the condition start values that you have given the equilibrium inappropriate for example? If you have a similar equilibrium that has already been successfully computed, then you can select the equilibrium that does not work, use the ED_EXP command SET_ALL_START_VALUES and accept all the suggestions for the site fractions. Alternatively, use TRANSFER_START_VALUE `<equilibrium number>` to make the currently selected equilibrium inherit the start values of the indicated equilibrium. Run COMPUTE_EQUILIBRIUM again to see if the equilibrium can be computed with the inherited start value.

If you cannot find an explanation of why the equilibrium cannot be computed, then it may be that the experiment is faulty. If so, then this experiment should be excluded from the optimization by being given a weight of 0. You should then run COMPUTE_EQUILIBRIUM again to make sure that all equilibria can be computed. However, experiments that fail to reach equilibria could succeed in doing so if the optimizing variables have other values. It is therefore sometimes worth trying to include experiments later in the optimization process (when the optimizing variables are relatively close to their final values), even if they had to be excluded at its start. In some cases, it might also be appropriate to change the error tolerance for in an experiment (using the ED_EXP command EXPERIMENT).



You must save the PARROT workspace with SAVE_WORKSPACES before you exit the ED_EXP module.

Setting Weights

To change the weight of an experiment, first enter the ED_EXP module from PARROT using EDIT_EXPERIMENTS. Then use the SET_WEIGHT command to set the weight for a specific equilibrium (equilibrium number `3` for example), for a range of equilibria (the equilibria `10-19`) or all the equilibria that have a certain label (such as all the equilibria with the label `A1`). To save the new weight(s), use SAVE_WORKSPACES .

By default, all the experimental information in your POP file is treated equally: each experiment has a weight of `1`. However, experiments that you excluded because they did not reach equilibrium now have a weight of `0`. The higher the weight of an experiment is, the more Thermo-Calc tries to ensure that the computed result fits the condition measured in that experiment.

The contribution of an experiment's error to the sum of errors is multiplied by the square of the weight set for that experiment. In other words, if you want to cut the error of an experiment with weight 1.0 by half, then you should use a weight of 0.7. This makes the experiment's error 0.49. Setting the weight to 1.4 instead makes the error twice as large (1.96).

Note that if you use READ_WORKSPACES after you have changed weights on the experiments, your changes are lost unless you have saved those changes. In the ED_EXP module, you can get a list of all the experiments in the console if you first read the experimental data from the workspace file (with READ_WORKSPACES) and then use LIST_ALL_EQUILIBRIA.

Optimizing and Evaluating Results

When you have ensured that all the experimental data points can reach equilibrium, go back to the PARROT module and use OPTIMIZE_VARIABLES `<number of iterations>` with `0` iterations. Present the result of this initial optimization by using LIST_RESULT.

When evaluating the optimization results, the most important information is found in the list of experiments at the end of the listed results. The rightmost column shows the difference between the value of the experimental data and the value computed by Thermo-Calc in the last optimization cycle.

The following shows part of list of experiments in the output of a LIST_RESULT command:

```
106 ACR(B)=0.34                0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964          3.6380E-12  5.00E+02   1964.      3.928
111 HMR(LIQUID)=-3500           0.000      5.00E+02   3500.      7.000    *
112 HMR(LIQUID)=-4588           0.000      5.00E+02   4588.      9.176    *
113 HMR(LIQUID)=-5239          7.2760E-12  5.00E+02   5239.      10.48    *
114 HMR(LIQUID)=-5454         -3.6380E-12  5.00E+02   5454.      10.91    *
115 HMR(LIQUID)=-5233          1.8190E-12  5.00E+02   5233.      10.47    *
116 HMR(LIQUID)=-4575         -1.8190E-12  5.00E+02   4575.      9.150    *
117 HMR(LIQUID)=-3481         -1.8190E-12  5.00E+02   3481.      6.962    *
118 HMR(LIQUID)=-1950           0.000      5.00E+02   1950.      3.900

PARROT:
```

The experiments for which the optimization has not found a good fit are marked with an asterisk (*) or a hash sign (#) in the rightmost column. An asterisk in this column indicates that the experiment has an error that is larger than the error tolerance and a hash sign indicates that the error is much larger. The error tolerance depends on the degree of accuracy set for that particular piece of experimental information. The error values are presented in the next to rightmost column.

Note that if you are optimizing in *alternate mode*, then you usually do not need to change the weights for the experiments. Instead, you can simply run OPTIMIZE_VARIABLES again, specifying, say, thirty iterations, evaluate the results again, and continue in that way until you are satisfied with the results.

- About Alternate Mode

The Critical Set of Experiments

The set of weighted experiments that you end up with as a result of your optimization is referred to as the *critical set* of experiments. When you work to determine this set and the weights of the experiments, the following factors should be reflected in both the selection of experiments and the weights of those experiments:

- The reliability of the experimental technique.
- The extent of agreement/disagreement between independent measurements of the same quantity.
- The extent of agreement/disagreement between data obtained with different experimental methods.

Continuing the Optimization and Resetting Variables

To continue the optimization after you have used OPTIMIZE_VARIABLES, you can either use this command and enter `<Number of iterations>` again or CONTINUE_OPTIMIZATION `<Number of iterations>`.

If you use CONTINUE_OPTIMIZATION, then PARROT continues the optimization using the same Hessian matrix. If the optimization is going well but you run out of iterations, then continuing with the same Hessian matrix may be useful.

As before, use LIST_RESULT to inspect the fit between the calculated and the experimental values for your experiments. If necessary, adjust the weights of the experiments again in the ED_EXP module. You may even discover that you have to exclude additional experiments from the optimization.

Besides looking at the rightmost column in the list of experiments (that is produced when you use LIST_RESULT), it is also useful to look at the *sum of squares* of the errors of all the variables. This is shown in the output of OPTIMIZE_VARIABLES and CONTINUE_ OPTIMIZATION. This sum should be as low as possible.

The following shows part of the output that you get when using LIST_RESULT:

```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      6.94641846E+05    4.30000000E+04    4.30000000E+04    1.42299558E+00
V2     -3.32619842E+02   -3.52000000E+01   -3.52000000E+01    7.91369573E-01
V11     8.37422071E+04    7.20000000E+04    7.20000000E+04    2.02212692E-01
V13     2.65253341E+04    2.70000000E+04    2.70000000E+04    1.45201828E-01
V17    -3.66637428E+05   -1.00000000E+05   -1.00000000E+05    8.04279315E-01

NUMBER OF OPTIMIZING VARIABLES :   5
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   3.50196879E+05 TO   3.49096720E+05
DEGREES OF FREEDOM   14.  REDUCED SUM OF SQUARES   2.49354800E+04
```

In the example you can see that the sum of squares have decreased slightly. (The final sum of squares that you get after an optimization run is also presented directly in the output from OPTIMIZE_VARIABLES and CONTINUE_OPTIMIZATION.) As long as the sum of squares figure is decreasing, the optimization is working as it should.

When your calculated results have been improving for a while, that is, when the sum of squares has been decreasing, and you are confident that you are making definitive progress, then you should use the PARROT command RESCALE_VARIABLES to reset the starting values of the optimizing variables to their current values. When you do this, the start values and

scaling factors of the optimizing variables (shown in the table's third column in the preceding screen shot), are all set to the current values (shown in the table's second column).

If your optimization is not going well, then you may want to reset the values of your optimization variables to their current start values. To do this, use RECOVER_VARIABLES.

After rescaling the variables, continue the optimization using OPTIMIZE_VARIABLES again. Cycle through calls of the commands OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION, CONTINUE_OPTIMIZATION, RESCALE_VARIABLES and OPTIMIZE_VARIABLES again until your set of optimizing variables does not seem to improve anymore. Even when it seems to you that you have reached this point, it is recommended that you use OPTIMIZE_ VARIABLES/CONTINUE_OPTIMIZATION a few extra times to make sure that the variable values cannot be further improved, that is, that the sum of squares of the errors of all the variables cannot be reduced further. If the final solution is repeatedly calculated after the same number of iterations and reaching the same result, then it is generally reasonable to accept the current variable values.

Updating the Set of Optimizing Variables

Besides evaluating the fit between the calculated results and the experimental data, you should also ensure that you have the right number of optimizing variables. If you have too many or too few optimizing variables, then you may not be able to use your model to accurately extrapolate thermodynamic properties in a wide range of temperature, pressure and composition conditions.

With more optimization parameters, the sum of errors usually decrease, but the parameters also tend to become less precisely determined. A measure of this precision is the Relative Standard Deviation (RSD) of each optimizing variable. However, the RSD is only significant if you have used RESCALE_VARIABLES followed by an optimization which converges and the values of the variables do not change much. The RSD tells you how much the parameter can be changed in either a positive or in a negative direction without changing the reduced sum of errors with more than one unit.

A large RSD value thus means that the parameter has not been determined well.

```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      2.01820948E+04    2.01874462E+04    2.01874462E+04    2.60519742E-02
V2     -2.90936164E+01   -2.90969472E+01   -2.90969472E+01    1.41576516E-02
V11    -2.18127453E+04
V12     1.55559524E+01
V15     2.36701148E+04    2.37258719E+04    2.37258719E+04    1.00528931E-01
V16    -7.56541897E+00   -7.64417807E+00   -7.64417807E+00    3.17218507E-01
V17     3.00342429E+03    3.02274918E+03    3.02274918E+03    2.60675550E-01
V19     2.20133190E+04    2.14534347E+04    2.14534347E+04    6.92923849E-01
V20    -6.72498276E+00   -6.31334932E+00   -6.31334932E+00    1.79242248E+00

NUMBER OF OPTIMIZING VARIABLES :   7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   1.51360340E-01 TO   1.44420287E-01
DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.02334928E-03
```

If such a significant RSD has a value larger than 1, then this typically means that you are using too many optimizing variables. However, the RSD values also depend on the weighting of the experiments, so it is sometimes possible to reduce the RSD by changing weights.

The RSD should not be too low either. If one or more of them is very close to 0, then this suggests that you are trying to optimize the system with too few optimizing variables. You can add optimizing variables interactively using ENTER_PARAMETER in GIBBS. However, it is

recommended that you add a sufficient number of variables in the setup file from the start so that do not need to do this. You can fix variables to a value of 0 until you discover that they are needed.

Besides the RSD, you should also keep an eye on the variable values themselves (shown in the VALUE column, next to the leftmost column in the table shown in the preceding screenshot). If the value of a variable is in the order of 1E5 or higher and this variable has been put in the temperature-independent part of an interaction parameter's Gibbs energy expression, then you may not have the right weights on your experiments or you are using too many optimizing variables. This is also typically the case if a variable with a value in the order of 10 or more (per mole atoms) is in the temperature-dependent part of the Gibbs energy expression of an interaction parameter. Such a high parameter value may lead to inverted miscibility gaps or re-stabilisation of a phase at high temperature. It is important to keep an eye on this since the temperature-independent and the temperature-dependent interaction parameter often varies together. If the temperature-dependent interaction parameter cannot be reliably determined, you may have to fix its value.

Note that even if you have found a good enough fit between calculated and experimental values after an optimization run, a parameter value may suddenly start to change by several orders of magnitude when you use OPTIMIZE_VARIABLES is used again. If this happens, then careful reconsideration of the weighting of the experiments of the set of optimizing variables is required. However, when the optimization has converged and the parameter values remain stable after repeated use of OPTIMZE_VARIALBES, this should usually not happen.

Reducing the Number of Optimizing Variables

If you have one or more optimizing variables with RSD larger than 1, then you should remove one or more of the variables by setting them to a value of 0, or alternately, set them to a reliably estimated value (estimated based on, for example, semi-empirical methods).

To fix an optimizing variable to certain value, use the PARROT command SET_FIX_VARIABLE `<variable number> <value>`.

Plotting Intermediate Results

It is typically not sufficient to look at the plain text output of LIST_RESULT to reliably judge how the optimization is progressing. Plotting a phase or property diagram of the system you are optimizing using the POLY and POST modules is often very useful.

It is recommended that you create a macro file for plotting the diagram since you probably want to repeatedly plot the diagram as you progress with the optimization. This macro file can then be called directly from the PARROT module with the MACRO_FILE_OPEN command.

Superimposing Experimental Data from EXP Files

If you create one or several EXP files based on the experiments in your POP file, you can visually compare the fit your plot and the experimental data you are optimizing the system against. An EXP-file contains data points specified in the DATAPLOT format. You could make an EXP-file for each type of data that you are using in the optimization.

Use the POST command APPEND_EXPERIMENTAL_DATA to superimpose the data points in an EXP-file on a phase or property diagram that you have plotted. For example, to put the experimental data points from a file entitled DP.EXP onto a plotted diagram, you could enter the following:

```
APPEND_EXPERIMENTAL_DATA Y DP.EXP 0 1
```

Such a command call tells Thermo-Calc to superimpose the data points in dataset 1 of DP.EXP onto the plot in the Console Results window, but not to impose any information about axis scaling, labels and other information which is normally found in the prologue of the DP.EXP file.

The POST command QUICK_EXPERIMENTAL_PLOT can also be used to superimpose data points on a plotted phase or property diagram.

- *DATPLOT User Guide* included with this documentation set.

Finalizing the Optimization

In this section:

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Rounding off Optimizing Variable Values 62
Updating the Database File 63
Creating a Database File 64
Updating the Setup File and the POP file 65

Finishing the Optimization

When to stop optimizing is a matter of judgment. It is rarely the case that you finish optimizing a system with the feeling that it cannot be improved.

The final step is to update your files with the final results. Besides updating your database file (or alternatively, creating a new database file), it is advised that you also update your setup and POP files with the final weights and optimizing variable values.

Rounding off Optimizing Variable Values

When you save the optimizing variable values, it is important that you round off the values correctly. When you have a metallic system, it is usually best to keep whatever number of decimal digits that you need to make less than one J/mol difference at 1000 K. When you have an aqueous system or a system that you are optimizing based on data from very different temperature ranges, then this is not always the only appropriate guideline. However, rounding off the values in such a way that it gives a difference that is larger than one J/mol may lead to differences in the phase diagram.

Another approach you can take when rounding off variable values is by progressively fixing the value of more and more of the variables. This allows you to round-off all but one of the variables values so that each only has a few significant digits. Variables whose values have been rounded off in this way are easier to handle compared with those that that are rounded off so that they continue to have many significant (non-zero) digits.

To round off the variable values according to this second approach, first use SET_FIX_VARIABLE to set the variable(s) with the highest RSD to a rounded off value (such as, say, 0.4). When you then re-optimize using OPTIMIZE_VARIABLES, the sum or errors changes. However, you should get almost exactly the same sum of errors as before after you rescale the variable values using RESCALE_VARIABLES. (If the sum of errors is different, then this means that the variable with the highest RSD was not rounded off in a good way.) If you successfully round off the first variable value, then continue to round of the optimizing variable which now has the highest RSD. Continue doing this until you have fixed all but one of the optimizing variables to their rounded-off values. The final sum of errors that you get after having fixed the variable values should not deviate significantly from the initial sum of errors you had before starting to round-off the variable values.

Updating the Database File

About the Database Files

To update the database file (with filename extension TDB) open it in a text editor and enter or update each of the parameters that you have optimized.

For example, suppose you have the following command in your setup file:

```
ENTER_PARAMETER L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15  +V17; 6000 N
```

If you then end up with a value for optimizing variable V17 of -100000, then you should enter the following under the IONIC_LIQ phase in the database file:

```
PARAM L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 -100000; 6000 N REF !
```



If you often need to round-off the optimizing variable value in some way, see Rounding off Optimizing Variable Values.

When you have updated or entered the parameters that you optimized, save the database file.

Creating a Database File

In some circumstances you may want to save all the information about your system into a new database file. To do this, go to the GIBBS module and use LIST_DATA `<Filename> N`. This creates a new user database file that contains all the information about the system that is in the workspace.

The N-argument tells the LIST_DATA command to save the output into database file rather than some other type of file, such as a macro file for example. Note that the output database file that you get from LIST_DATA have to undergo some manual editing before it can be used as proper database file.

Updating the Setup File and the POP file

It may be useful for you to be able to recreate your optimization from scratch. It is therefore recommended that you do the following when you are done with the optimization:

- Update your POP file so that it contains the weights of your critical set of experiments. Use SET_WEIGHT to set the weights directly in the POP file. You may also have to use SET_START_VALUE for some conditions in the POP file. Otherwise, you may not be able to compute the equilibria with .
- Copy the final values of your optimizing variables and set them as start values of the variables in the setup macro file (with SET_FIX_VARIABLE).



It is important that you round off the values of the optimizing variables correctly. See Rounding off Optimizing Variable Values. When you have done this, you can run the setup macro file to recreate the final result of the optimization.

Alternate Mode

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About Alternate Mode

To turn Alternate Mode ON or OFF, use the PARROT command SET_ALTERNATE_MODE.

When you have one or more multi-phase equilibria (that is, with the fixed phase-status) in your POP file and the optimizing values lack appropriate starting values (such as the default value of 0 for example), then Thermo-Calc may not be able to compute the equilibria for the experiments. In these cases, a common tangent cannot be found, that is, a state where the chemical potentials for all components are the same in all phases cannot be found. A common tangent may not exist or it be found at the wrong composition or temperature given the initial set of model parameters.

If you are not able to estimate reasonable starting values for the optimizing variables, then this problem can be overcome by initially running your optimization in alternate mode. The alternate mode in PARROT module should help you find reasonable starting values for the optimizing variables. Note that you are only supposed to use alternate mode in the beginning of the optimization. Once you have achieved a reasonable fit between calculated results and experimental data, turn off alternate mode and calculate all equilibria again in the normal mode.

In alternate mode, PARROT modifies multi-phase equilibria so that the chemical potentials for each stable phases is calculated separately. For example, consider the following experimental equilibrium:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ FCC=FIX 1
SET_CONDITION T=1000 P=1E5
EXPERIMENT X(LIQ,B)=.2:.01 X(FCC,B)=.1
```

When PARROT optimizes in alternate mode, the computation of this equilibrium is done by way of the following two calculations:

```
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1000 P=1E5 X(LIQ,B)=.2
CHANGE_STATUS PHASE FCC=FIX 1
SET_CONDITION T=1000 P=1E5 X(FCC,B)=.1
```

The difference between the chemical potentials in every pair of phases is calculated and PARROT tries to adjust the parameters of the phases so that these differences are minimized. In other words, PARROT tries to make the chemical potentials equal in all phases. For PARROT to be able to do this, some additional information about the experimental multi-phase equilibria is required, at least for all invariant equilibria.

Optimizing in Alternate Mode

When you are optimizing in the alternate mode, you usually do not need to enter the ED_EXP module and manually change the weights of experiments that the computed results have not been fitted well with. Instead, after using OPTIMIZE_VARIABLES initially with no iterations, and listing the result with LIST_RESULT, simply run OPTIMIZE_VARIABLES again specifying, say, thirty iterations. Continue to optimize until your optimization seems to be going in the right direction, then set the optimizing variables' starting values to their current values use RESCALE_VARIABLES before you turn alternate mode off by answering N at the SET_ALTERNATE_MODE prompt.

Preparing the POP File for Alternate Mode

Information in your POP file that concerns equilibria with ENTERED or DORMANT phases is ignored when you optimize in alternate mode.

To use the alternate mode, ensure that there is enough information about each phase in a given equilibrium. In addition to the temperature and pressure of the system, you should specify the composition of all phases in a given equilibrium. This is done with, SET_CONDITION, EXPERIMENT, or SET_ALTERNATE_CONDITION.

If both compositions of a binary tie-line have been measured, then you could specify this in the POP file in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01 X(FCC,B)=.3:.01
```

This equilibrium could be calculated with alternate mode without any modification. The compositions specified with the experiment command is used as condition when the thermodynamic properties of each phase are calculated.

Examples of SET_ALTERNATE_CONDITION

The following topics demonstrate how SET_ALTERNATE_CONDITION is used to prepare different kinds of equilibria for optimization in alternate mode.

How to Specify the Composition of One Side of a Binary Tie-Line

If only one side of the tie-line has been measured, then you must provide an estimate of the composition of the other phase. You can make such an estimate with SET_ALTERNATE_ CONDITION. This command has no effect unless alternate mode is turned on. The equilibrium described could thus be specified in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01
SET_ALTERNATE_CONDITION X(FCC,B)=.3
```

When the alternate mode is turned on, the composition given by the SET_ALTERNATE_ CONDITION command is used for the FCC phase. The properties of the BCC phase is calculated using the composition specified by experiment as a condition.

How to Specify the Compositions of a Three-Phase Equilibrium

If you have a three-phase equilibrium in your POP file, then one of its compositions can be specified as experimentally determined, while two can be provided as alternate conditions:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=912:5 X(LIQ,B)=0.2:.02
SET_ALTERNATE_CONDITION X(FCC,B)=0.1 X(BCC,B)=.4
```

How to Specify the Composition of a Stoichiometric Phase

When you specify the composition of stoichiometric phase with SET_ALTERNATE_ CONDITION, the value must be given with at least seven decimal digits, as in the following example:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ A2B=FIX 1
```

```
SET_CONDITION P=1E5 X(LIQ,B)=0.2
EXPERIMENT T=992:5
SET_ALTERNATE_CONDITION X(A2B,B)=.6666667
```

Entering Other Experiments in the POP with Alternate Mode

The following table shows some additional examples of how to enter different kinds of experiments in the POP file when you are using the alternate mode.

Example	ED_EXP commands
Two-phase equilibrium: The melting temperature of an Au-Cu alloy	`CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X(FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2 SET_ALTERNATE_CONDITION X(LIQUID,CU)=0.16`
Invariant equilibrium experiment: A three-phase equilibrium in a binary system	`CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5` `EXPERIMENT T=912:5 SET_ALTERNATE_CONDITION X(FCC,B)=0.1SET_ALTERNATE_CONDITION X(BCC,B)=0.4SET_ALTERNATE_CONDITION X(LIQ,B)=0.2`
Ternary system, with two compositions measured (both with uncertainty 0.02)	`CREATE_NEW_EQUILIBRUM 1 1 CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 SET_CONDITION X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02 SET_ALTERNATE_CONDITION X(BCC,B)=0.17 SET_ALTERNATE_CONDITION X (BCC,C)=0.07`

Troubleshooting

During an optimization, you are likely to run into many different problems and challenges. This topic gives some general guidelines that can help avoid common mistakes and problems.

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Excluding and Including the Correct Equilibria 75

Conflicting Data 76

Useful Guidelines

The following rules of thumb are generally good to adhere to when you are planning and executing an optimization:

- Do not use data from thermochemical tables of unknown origin.
- Use experimentally determined properties; avoid converted quantities.
- Carefully estimate the accuracy of the experiments.
- Correct systematic errors (by adjusting a temperature scale for example).
- Use negative information such as, for example, the information that a phase should not be stable in a composition or temperature region.
- With a hundred activity measurements in a system but only ten composition points from the phase diagram, it is often appropriate to decrease the weights on the activity experiments.
- If you initially exclude any intermediate phases to only optimize the liquid and the terminal or end-member phases for the pure components, then it is often useful to compute a metastable phase diagram with just these phases. In the metastable phase diagram, the metastable solubility lines should not have any strange kinks or turns. Such a diagram is often also useful to compute at later stages in the optimization.
- When you have fitted the liquid phase and some solution phases reasonably well, then you can fix the optimizing variables that characterise these phases. You can then go on and optimize the variables for the intermediate phases.
- Phases with miscibility gaps are always difficult to optimize. Try to keep control of the miscibility gaps by using real or estimated experimental information. (Note that it is not possible to calculate the top of a miscibility gap as a single equilibrium.)
- Phases with order/disorder transformation are often difficult to optimize. It may be difficult to find the right start values on the optimizing variables. The TABULATION module can be useful sometimes. Properties for specified site fractions can be calculated in the TABULATION module. This is not possible in the POLY module since this module only calculates for equilibrium site fractions. The ordered state may also disappear during the optimization of these phases. If this happens, you may be able to add an experiment that controls the state of order.
- Only use the alternate mode to find an initial set of model parameters that can then be make it possible to calculate the experimental equilibria in the normal mode.
- When you have achieved a satisfactory fit between calculated results and experimental data with an appropriate number of optimization variables, perform a couple of final optimization runs to make sure that your results are stable.

- Make sure that the values of the optimizing variables keep within a reasonable range. If a variable starts to change several orders of magnitudes, then you must consider whether you have the right weights on the experiments and whether you are using too many optimizing variables.

Excluding and Including the Correct Equilibria

Use as few experiments as possible initially to get a reasonable overall fit. It is generally best to first focus on the invariant equilibria, as well as metastable states that can be estimated by excluding some phases. Crucially, any experiments for which the computed results are clearly faulty should be excluded from the final critical set, while all important invariant equilibria are calculated and included in this critical set.

If you cannot compute some invariant equilibria with intermediate phases, then it may be best to first exclude those phases from the optimization and only optimize the liquid and the most important solution phases. After you have obtained reasonable results for these phases, you can enter the intermediate phases back in again. With the variables for the optimized liquid and solid phases set fixed, you can finally optimize the intermediate phases.

Conflicting Data

It is important that you do not include conflicting sets of data at the same time during an optimization. After all, if they are genuinely conflicting, then at least one of the sets must be incorrect. If you have conflicting sets of data, then only use one of these sets at a time together with the rest of the data. Often, the optimization makes it clear which dataset coheres best with the other information that is available about the system.

Sometimes, conflicting data cannot be detected directly. For example, you may have activity data which is inconsistent with solubility data from the phase diagram. This would be indicated by large errors in the fit when both the activity data and the solubility data are included. To find these inconsistencies, let alone correct the errors, you may thus have to optimize with some datasets excluded.

Experiments and Experimental Data

These topics contain examples of different kinds of equilibria in different kinds of systems. They are intended to help you figure out how to use various kinds of experimental data when creating POP files. The topics that follow contain examples how to enter various kinds of experimental data into a POP file.

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Phase Diagram Data 78

Data for Individual Compounds 79

Single Phase Mixing Enthalpies or Partial Enthalpies 81

Enthalpies of Formation and Enthalpies of Reactions 82

Chemical Potentials via EMF Measurements 83

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Pressure-Temperature-Volume EOS Data 85

Crystal Structure, Lattice Parameters, and Site-Occupancy 86

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Phase Diagram Data

P-T-X phase diagram data for binary and ternary systems, or systems of even higher order can be used in the POP file. This includes data of the following types:

- Data about the temperature- and composition-dependence of various properties (obtained from differential thermal analysis (DTA) measurements for example), including enthalpy, lattice parameter, dilatometric length, electronic conductivity and magnetic susceptibility;
- Data about reaction types (invariant/monovariant) and phase relations obtained from qualitative or quantitative metallographic studies;
- Data about phase amounts or compositions obtained from microprobe measurements (using X-ray spectroscopy or transmission electron microscopy (TEM));
- Data about the positions or directions of two-phase tie-lines and three-phase equilibria for ternary systems.

The following table shows a POP file excerpt that demonstrates how some kinds of phase diagram data can be entered.

Example	ED_EXP commands

Solidus (melting temperature) of an Au-Cu alloy	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE LIQUID FCC=FIX 1`
	`SET_CONDITION X(FCC,CU)=0.14 P=1E5`
	`EXPERIMENT T=970:2`

Three-phase equilibrium in a binary A-B system	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1`
	`SET_CONDITION P=1E5`
	`EXPERIMENT T=912:5`

Congruent transformation in a binary A-B system	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE BCC LIQUID=FIX 1`
	`SET_CONDITION P=1E5 X(BCC,B)-X(LIQ,B)=0`
	`EXPERIMENT T=1213:10`

Tie-line in a ternary A-B-C system	An uncertainty factor is set not only for the experimental measurement, but also for the X(FCC,B) condition. The factor is 0.02.
	`CREATE_NEW_EQUILIBRUM 1 1`
	`CHANGE_STATUS PHASE FCC BCC=FIX 1`
	`SET_CONDITION T=1273 P=1E5 X(FCC,B)=0.1:0.02`
	`EXPERIMENT X(FCC,C)=0.12:.02`

Data for Individual Compounds

You can use data about individual components in the POP file. Such data includes activity, heat capacity, heat content, entropy, Gibbs energy of phase transformations, heat of transition, and heat of melting.

Example	ED_EXP commands
Carbon activity data in the fcc phase	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=FIX 1 CHANGE_STATUS PHASE GRAPHITE=D SET_REFERENCE_STATE C GRAPHITE,,,, SET_CONDITION P=101325 T=1273 X(MN)=0.03 SET_CONDITION X(C)=0.03 EXPERIMENT ACR(C)=0.29:5%
Ln(activity coefficient for O)	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE IONIC_LIQ=FIX 1 CHANGE_STATUS PHASE GAS=D SET_CONDITION X(O)=0.02 T=1523 P=101325 SET_REFERENCE_STATE O GAS,,,, ENTER_SYMBOL FUNCTION LNFO=LOG(ACR(O)/X(O)); EXPERIMENT LNFO=-1.5:0.01
Entropy at 298.15 K of Cu2O	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CU2O=FIX 1 CHANGE_STATUS PHASE CUO=FIX 0 SET_CONDITION P=101325 T=298.15 EXPERIMENT S=92.36:1
Gibbs energy of formation of NiAl2O4	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 CHANGE_STATUS PHASE FCC O2GAS=DORM SET_REFERENCE_STATE NI FCC,,,, SET_REFERENCE_STATE AL FCC,,,, SET_REFERENCE_STATE O O2GAS,,,, SET_CONDITION P=101325 T=1000 N(NI)=1 N(AL)=2 SET_CONDITION N(O)=4 EXPERIMENT GM=-298911:5%
Heat capacity of MgFe2O4	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(FE)=2 N(MG)=1 N(O)=4 SET_CONDITION T=800

Example	ED_EXP commands
	ENTER_SYMBOL FUNCTION CP=H.T; EXPERIMENT CP=207:5%
Heat content (H-H298) for MnFe2O4	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 T=298.15 N(MN)=1 N(FE)=2 SET_CONDITION N(O)=4 ENTER_SYMBOL VAR H298=H; ENTER_SYMBOL FUN HMNFE2O4=H-H298; CREATE_NEW_EQUILIBRIUM 2 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(MN)=1 N(FE)=2 N(O)=4 SET_CONDITION T=400 EXPERIMENT HMNFE2O4=16610:5%

Single Phase Mixing Enthalpies or Partial Enthalpies

You can use calorimetric data for mixing in the POP file. This data could be the result of, for example, drop calorimetry or scanning calorimetry. This includes data about, for example, enthalpy of mixing of liquids, series of mixing-enthalpy and about partial enthalpy. Information about enthalpies of mixing can also be derived from theoretical principles using special quasi-random structures (SQSs).

Example	ED_EXP commands
Enthalpy of mixing in the liquid state of an Au-Cu alloy	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=FIX 1 SET_CONDITION T=1379 P=1E5 SET_CONDITION X(LIQUID,AU)=0.0563 SET_REFERENCE_STATE AU LIQ * 1E5 SET_REFERENCE_STATE CU LIQ * 1E5 EXPERIMENT HMR=-1520:200

Enthalpies of Formation and Enthalpies of Reactions

You can use calorimetric data for phase transformations in the POP file. This data could be the result of, for example, direct-reaction calorimetry, solution calorimetry or combustion calorimetry. Information about enthalpies of formation can also be derived from theoretical principles.

Example	ED_EXP commands
Enthalpy of melting of the eutectic in the Al2O3-ZrO2 binary (J/g)	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CORUNDUM ZRO2_TETR=FIX 0 CHANGE_STATUS PHASE IONIC_LIQ=ENT 1 SET_CONDITION P=101325 N=1 LNAC(O)=-80 SET_REFERENCE_STATE ZRO2 TETR,,,,,, SET_REFERENCE_STATE AL2O3 CORUND,,,,,, EXPERIMENT HWR=1080:90
Enthalpy of formation of o-CaZrO3 from the component oxides	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE ZRO2_MONO HALITE CAZRO3_O=ENT 1 SET_CONDITION T=298.15 P=101325 N(CAO)=.5 SET_CONDITION N(ZRO2)=.5 LNAC(O)=-20 SET_REFERENCE_STATE CAO HALITE,,,, SET_REFERENCE_STATE ZRO2 ZRO2_MONO,,,, EXPERIMENT HMR(CAZRO3_O)=-15960:5%

Chemical Potentials via EMF Measurements

You can use chemical potentials and activities/activity coefficients from electromagnetic field (EMF) measurements in the POP file.

Example	ED_EXP commands
Emf data on Cu(s)/Cu2O(s)	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC CU2O=FIX 1 CHANGE_STATUS PHASE O2GAS=DORM SET_CONDITION P=101325 T=1000 SET_REFERENCE_STATE O O2GAS,, 100000 EXPERIMENT MUR(O)=-95387:1000

Driving Force for Metastable Phases

You can use chemical driving forces for metastable phases in the POP file.

Example	ED_EXP commands
To prevent BCC_A2 to be stable	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1 M7C3 M23C6=FIX 1 CHANGE_STATUS PHASE BCC_A2=D SET_CONDITION P=101325 T=1473 EXPERIMENT DGM(BCC)<-0.1:0.1
To promote CEMENTITE to be stable	CHANGE_STATUS PHASE BCC M7C3 GRAPHITE=FIX 1 CHANGE_STATUS PHASE CEMENTITE=DORMANT SET_CONDITION P=P0 T=973 EXPERIMENT DGM(CEM)>0.1:0.01

Pressure-Temperature-Volume EOS Data

You can use Pressure-Temperature-Volume Equation of State (EOS) data in the POP file. Such data includes, for example, molar volume, density, thermal expansion and bulk modulus/compressibility.

Example	ED_EXP commands
Volume of liquid Pt	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=ENT 1 SET_CONDITION P=101325 N=1 T=1873 EXPERIMENT VM=1.00758E-5:5%
Thermal expansion	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 SET_CONDITION P=101325 N=1 T=400 ENTER_SYMBOL FUNCTION ALPHA=VM.T/VM/3; EXPERIMENT ALPHA=2.35E-5:5%

Crystal Structure, Lattice Parameters, and Site-Occupancy

You use information about defects, ordering or site occupancy, as well as information about crystal structures in the form of lattice parameter values. This information may come from measurements made by X-ray, neutron diffraction, Mössbauer spectroscopy or perturbed angular-correlation.

Example	ED_EXP commands
Lattice parameter for fcc	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 SET_CONDITION P=101325 N=1 T=298.15 SET_CONDITION X(CR)=0.05 ENTER_SYMBOL FUNCTION LPFCC=((4*VM/6.02214179E23)**(1/3))*1E10; EXPERIMENT LPFCC=4.02:5%
Lattice parameter for bcc	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE BCC_A2=ENT 1 SET_CONDITION P=101325 N=1 T=298.15 SET_CONDITION X(AL)=0.08 ENTER_SYMBOL FUNCTION LPBCC=((2*VM/6.02214179E23)**(1/3))*1E10; EXPERIMENT LPBCC=2.90:5%
Site-occupancy, degree of inversion for spinel	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(MG)=1 N(AL)=2 N(O)=4 SET_CONDITION T=1073 EXPERIMENT Y(SPINEL,AL+3#1)=0.31:5%

Magnetism and Other Atomistic Properties

You can use data about atomistic properties such as magnetism and Curie temperatures in the POP file.

Example	ED_EXP commands
Curie temperature of MnxFe3-xO4, x=1.26	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION T=520 P=101325 N(O)=4 SET_CONDITION N(FE)+N(MN)=3 N(MN)=1.26 EXPERIMENT TC(SPINEL)=520:5

Data About Systems of Different Orders

You might want to use data about systems of different orders in the same optimization, such as data about a binary equilibrium with components A and B in a ternary system with components A, B and C, together with data about equilibria in the binary system with components A and B. To do this, you must first suspend all components in the ternary system (A, B and C), and then set the two components you want binary information on (A and B) to status `ENTERED`.

Suspending all components is done by giving the initialization code 0 to the CREATE_NEW_EQUILIBRIUM command. The components about which you want to use binary information must then be entered again using the CHANGE_STATUS command.

Example	ED_EXP commands

A binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C)	`CREATE_NEW_EQUILIBRIUM 1 0`
	`CHANGE_STATUS COMPONENT A B = ENTERED`
	`CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1`
	`SET_CONDITION P=1E5`
	`EXPERIMENT T=1177:10`

Thermodynamic Models

The most common models used in assessments are described briefly in these topics. Examples of how to write the phase definitions in the setup-file are also given for each of these models. In addition to the models described here, a large number of thermodynamic models for various phases in different states have been implemented.

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Gas

The gaseous mixture phase is usually treated as a substitutional phase without sublattice. In the gaseous mixture phase, there are usually molecules formed, and the number of constituents of the gas phase is often much larger than the number of elements. These complex constituents have to be defined as species. The ideal gas model may handle a gas phase under low pressures (and low temperatures). This implies that the P-V-T relations and thermodynamic properties of pure gaseous species are calculated as for ideal gas, and that there is interaction between gaseous species in the mixture. In a defined system, there may only exist one gaseous mixture phase. Type code `G` is used for the gas phase:

```
ENTER_PHASE GAS G, 1 H,H1O1,H1O2,H2,H2O1,H2O2,O,O2,O3; N N
```

Compound Energy Formalism

If the atoms are sufficiently different in size, electronegativity or charge, they may prefer different types of sites in the lattice of crystalline solids. In some cases, a solute atom may even occupy interstitial sites between the normal lattice sites. All such phenomena are treated in Thermo-Calc by the sublattice concept. The Compound Energy Formalism (CEF) has proved to be the most general formalism for many different types of solution phases. It is therefore by default applied to various solid solution phases in the Thermo-Calc software package. CEF can also take ionic constraints (charged cation/anion species) into account. For a comprehensive description on the CEF, please see Hillert (2001), Frisk and Selleby (2001), Sundman and Ågren (1981).

Since the CEF is used by default, no special notation is needed in the phase definition, except for ionic phases, where type code `I` is given.

Examples of phase definitions in a setup-file using the CEF:

```
ENTER_PHASE SPINEL I, 4 1 2 2 4
     FE+2,FE+3; FE+2,FE+3,VA; FE+2,VA; O-2; N N
ENTER_PHASE SIGMA, 3 10 4 16
     AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; N N
ENTER_PHASE FCC_A1, 2 1 1
     CR,FE,MN; C,N,VA; N N
ENTER_PHASE BCC_A2, 2 1 3
     CR,FE,MN,VA; C,N,VA; N N
```

Substitutional Liquid

The liquid phase is normally (but not always) modeled as a substitutional phase with no sublattice, which is occupied by two or more constituents. The constituents are normally the elements, but molecules or associates can also be used. Type code `L` is used for the liquid phase.

```
ENTER_PHASE LIQUID L, 1
     AL,C,CR,FE,MO,NI,SI ;  N N
ENTER_PHASE LIQUID L, 1
     C,FE,FEO,FEO3/2,NI,NIO ;  N N
```

Ionic Two-Sublattice Liquid Model

Within the framework of the CEF, the ionic two-sublattice liquid (I2SL) model was developed to be used when there is a tendency for ionization in the liquid, which happens in liquid oxides and sulphides for example. The same model can be used both for metallic and oxide melts. At low levels of oxygen, the model becomes equivalent to a substitutional solution model between metallic atoms. Two sublattices are assumed, one containing charged cations and one containing charged anions, neutrals and vacancies. The complication for an ionic liquid is that the numbers of sites on the cation sublattice and anion sublattice vary with the composition to preserve electroneutrality. For a comprehensive description on the I2SL model, see Hillert et al. (1985), Sundman (1991). In these references, the possible excess parameters are also discussed. Type code `Y` is used for the I2SL model.

Examples of phase definitions in a setup-file:

```
ENTER_PHASE LIQUID Y,
     AL+3,CR+2,FE+2,NI+2; VA; N N
ENTER_PHASE IONIC_LIQ Y,
     CA+2,MG+2; O-2; N N
ENTER_PHASE IONIC_LIQ Y,
     AL+3,CA+2,FE+2,MG+2,SI+4;
     ALO2-1,O-2,SIO4-4,VA,FEO3/2,SIO2; N N
```

Models for Ordered Phases

Some solution phases have chemical order-disorder transformations: for example, the disordered FCC_A1 phase can transform to the ordered $L1_2$ or $L1_0$ structure where the atoms of different kinds occupy different sublattices. In some cases, it may be advantageous and easy to describe such ordered structures as completely different phases; but in some other cases, like the B2-ordered BCC structure in Al-Fe, the disordered and ordered structures must be described as one singe phase because the transformation is of second order along a line in temperature and composition.

The ordering can easily be described by the CEF. For instance, an ordered FCC phase with only $L1_2$ or $L1_0$ ordering can be efficiently handled by the so-called Two Substitutional-Sublattice Ordering Model (2SL model), while an ordered FCC with both $L1_2$ and $L1_0$ ordering must be described with four sublattices using the so-called Four Substitutional-Sublattice Ordering Model (4SL model). Please note that in both these models, all the substitutional constituents must enter into these sublattices. In addition, you may also have one sublattice for interstitials.

Thermo-Calc supports a feature of splitting the parameters of a chemically ordered phase onto two different phase descriptions. This is very convenient. In this way, you can have one phase for all parameters describing the disordered state (the configuration independent state) and in the other phase only those parameters needed to describe the remaining part (the configuration dependent part), that is, the Gibbs energy contribution due to the ordering transformation. This has been implemented in such a way that the contribution from the configuration dependent part is zero when the solution phase is disordered. The optimization of the disordered phase is independent of the order-disorder transformation; the ordering energy is an add-on to the disordered part. This is particularly useful in higher order systems, as an ordered phase can dissolve several elements that have no particular contribution to the actual ordering. The phases Gibbs energy add together by giving this command in the setup-file: AMEND_PHASE_DESCRIPTION `<ordered phase> disordered_part <disordered phase>`

Since PARROT does not automatically create new composition sets, it is necessary to create composition sets for both the ordered and disordered phases in the setup-file: `Amend_phase_description <phase> composition_sets <new highest set number>,,,,`

Example of phase definitions for the corresponding disordered and ordered parts in a setup-file:

```
ENTER_PHASE FCC_A1, 2 1 1
     AL,CR,FE,NI; VA; N N
ENTER_PHASE FCC_L12, 3 .75 .25 1
     AL,CR,FE,NI ; AL,CR,FE,NI; VA; N N
AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_A1
```

4SL Model for FCC, HCP, and BCC

Ordered FCC, HCP and BCC solution phases handled by the 4SL model requires four sublattices for substitutional ordering and can additionally have an interstitial sublattice. A 4SL model is especially useful for modelling different kinds of ordered phases that are based on the same disordered phase, such as $L1_0$ and $L1_2$ based on FCC_A1, and B2, $D0_3$, $L2_1$ and B32 based on BCC_A2 etc.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours. These corners are equivalent lattice points, thus all G parameters for each end-member with the same elements, but distributed on different sites, must be identical. It should be emphasized that the end-member energy here represents the ordering energy rather than the formation energy of the compound.

The constraints on the parameters in the 4SL model can be derived based on the symmetry of the lattice:

$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$

$G_{A:A:B:B}=G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}=G_{B:B:A:A}$

$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$

$L_{A,B:*:*:*}=L_{*:A,B:*:*}=L_{*:*:A,B:*}=L_{*:*:*:A,B}$

The asterisk * means that the interaction parameter is independent of the occupation of that sublattice. For the disordered phase to be completely disordered, i.e. that all site fractions are equal on all four sublattices, all constraints must be correct.

For ordered BCC phases, the situation is a bit more complicated, as the four sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase, with A located on two sublattice sites and B on the other two, the end-member described by $G_{A:A:B:B}$ has four nearest neighbour bonds between A and B atoms, whereas the end-member described by $G_{A:B:A:B}$ has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds. Many parameters thus have a relation:

$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$

$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$

$G_{A:A:B:B}=G_{B:B:A:A}$

$G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}$

$L_{A,B:*:*:*}=L_{*:A,B:*:*}=L_{*:*:A,B:*}=L_{*:*:*:A,B}$

The $G_{A:B:B:B}$ term represents $D0_3$, $G_{A:A:B:B}$ B2 and the $G_{A:B:A:B}$ B32 ordering. There are also two kinds of reciprocal interaction parameters:

$L_{A,B:A,B:*:*;0…9}$

$L_{A,B:*:A,B:*;0…9}$

Kusoffsky et al. (2001) have shown the influence of different parameters available in the 4SL model applied to fcc ordering. The possibility to use the 4SL model to BCC ordering has been studied by Sundman et al. (2009) in the Al-Fe system.

2SL Model for FCC, HCP, and BCC

The reason for using a 2SL model instead of a 4SL model is that the calculations are faster, but on the other hand it can only model one kind of ordered phase(s). For instance, it is not possible to model FCC with both $L1_0$ and $L2_1$, or BCC with $D0_3$ and B2, etc.

In order to get the fully disordered phase to form, constraints are needed as for the 4SL model. For the symmetric phases, e.g. B2 and $L1_0$, the relation between parameters are:

$G_{A:B}=G_{B:A}$

$L_{A,B:*}=L_{*:A,B}$

For a 2SL asymmetric model including, but not limited to, $L1_2$, more constraints are needed. This model has many complicated relations between the parameters. The relation between the parameters for the 2SL $L1_2$ model can be derived from a 4SL model. The conversion from 4SL model parameters to 2SL parameters for $L1_2$ can be found in Dupin et al. (2001) and for $L1_0$ in Yuan et al. (2012). Higher-order systems with an $L1_2$ phase modeled with two sublattices require a lot of ternary and some quaternary interaction parameters in order to make the disordered state stable. These parameters have been derived by e.g. Dupin (1995), also found in Kusoffsky et al. (2001).

Many publications exist on how to model order/disorder transformations using a two-sublattice model, see e.g. Dupin, Ansara (1999), De Keyzer et al. (2009).

Magnetic Ordering

The magnetic contribution to the Gibbs energy is given by a model proposed by Inden (1975) and adapted by Hillert and Jarl (1978), and is described by:

```
G=RTln(b+1)f(t)
```

where $t=T/T_C$.

The values of the Curie temperature, T_C, and Bohr magneton number, b, at a certain composition are then used in an optimization procedure to calculate the contribution to Gibbs energy due to magnetic ordering. Curie temperature and Bohr magneton number are given in the command ENTER_PARAMETER for phases that undergo a magnetic transition:

```
AMEND_PHASE_DESCRIPTION BCC_A2 MAGNETIC -1.0 0.4
ENTER_PARAMETER TC(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N
ENTER_PARAMETER BMAGN(BCC_A2,FE:VA;0) 298.15 +V2; 6000 N
```

The arguments -1 and 0.4 specify the values of parameters in the magnetic model: -1 is the antiferromagnetic factor and 0.4 is the structure factor. Usually the antiferromagnetic factor =-1 for bcc and =-3 for fcc (and other non-bcc phases). The structure factor corresponds to the short range order fraction of the enthalpy. This factor is 0.4 for bcc and 0.28 for non-bcc phases.

Molar Volumes and High Pressure

Including volumes in a thermodynamic database enable calculations of volume changes, volume fraction, lattice mismatch in cubic structures and phase diagrams at increased pressure. Pressure independent volumes can be used up to about 1 GPa. At pressures above 1 GPa the pressure dependence of the volumes must be included by using a proper equation of state (EOS). An EOS has been developed by Lu et al. (2005), based on the EOS from Jacobs and Oonk (2000). Four parameters are used in the implementation of the model in Thermo-Calc:

- `V0`: Volume at 1 bar and at reference temperature T_0
- `VA`: Integrated thermal expansivity
- `VK`: Isothermal compressibility at 1 bar
- `VC`: Parameter to fit high pressure data

All parameters can be composition dependent in the same way as all other model parameters in Thermo-Calc. Experimental information about the temperature, pressure and composition dependence of the volume can be assessed using these model parameters. To evaluate V0, VA and VK experimental data at 1 bar only are needed.

Examples on modeling molar volume in a setup-file:

```
ENTER_PARAMETER V0(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N
ENTER_PARAMETER VA(BCC_A2,FE:VA;0) 298.15 +V2*T+V3*T**2; 6000 N
ENTER_PARAMETER VC(BCC_A2,FE:VA;0) 298.15 +V4+V5*T; 6000 N
ENTER_PARAMETER VK(BCC_A2,FE:VA;0) 298.15 +V6+V7*T; 6000 N
ENTER_PARAMETER V0(FCC_A1,CR,FE:VA;0) 298.15 +V8; 6000 N
ENTER_PARAMETER VA(FCC_A1,CR,FE:VA;0) 298.15 +V9*(T-298.15); 6000 N
```

Excess Models

Unless specifically amended, the excess Gibbs energy terms are modeled by the Redlich-Kister-Muggianu Model. Other excess models for the Gibbs energy are also implemented in Thermo-Calc, such as e.g. Kohler and Toop-Kohler extrapolation models.

Thermo-Calc is not restricted to binary interaction parameters. Ternary, quaternary and higher-order interaction parameters can also be used if there is enough information to evaluate these from experimental data. The ternary interaction parameters are identified by the degrees of the so-called ternary L parameter (i.e. 0, 1 and 2) in the command ENTER_PARAMETER. If the parameter is composition-independent, you only need a single interaction parameter with a degree of zero, i.e. only the ^{0}L term. If there is a ternary composition-dependent interaction parameter, you must enter all three parameters (0,1 and 2). If such a ternary interaction parameter should be zero, then assign it a function which is zero. If the three interaction parameters have the same value, then that is identical to having a composition-independent ternary parameter.

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +1000; 6000 N
ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +1000; 6000 N
```

is identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

This also means that

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +ZERO#; 6000 N
ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +ZERO#; 6000 N
```

is NOT identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

Database Manager User Guide

Thermo-Calc Version 2021b



Introduction to the Database Manager Guide

In this section:

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Thermodynamic and Kinetic/Mobility Databases

This guide describes how to define and construct a thermodynamic or kinetic database. It includes details about the data structures and formats of the Thermo-Calc databases as well as the Diffusion Module (DICTRA) database-extensions.

The Thermo-Calc databases are created and maintained in the Thermo-Calc Database Format (TDB) which is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations. This document gives a full description of the TDB format (with the Diffusion Module (DICTRA) database extension) and is a comprehensive guide about how to create and manage a Thermo-Calc (and Diffusion Module (DICTRA)) database.

Usually, a Thermo-Calc or Diffusion Module (DICTRA) database is constructed as a single text file with an extension of TDB, for example, `PAQ2setup.TDB`. For some databases (especially large databases used with older versions of Thermo-Calc or Diffusion Module (DICTRA)) a database may consist of one primary-definition file (`***setup.TDB`) and several additional-definition TDB files (such as `***param.TDB`, `***funct.TDB`, `***refer.TDB`, etc. These are built for a variety of defined parameters, functions, references and so forth, and are linked to the `***setup.TDB` file through the correct use of the TYPE_DEFINITION and/or FTP_FILE commands inside the `***setup.TDB` file.



With Thermo-Calc, the Add-on Modules and Thermo-Calc Software Development Kits (SDKs), you can code everything into a single *****setup.TDB** file for a database at any scale.

Initialization of the TDB Module

The following explains how a database initialization file is constructed to work with the so-called TDB (database) module. When you start, the TDB module looks for a file that has information about the available standard databases. The database initialization file is called `tc_initd.tdb`. By default it is located in the `data` subdirectory of the Thermo-Calc installation directory.

See Database Installation Folder in the *Thermo-Calc User Guide*.

The location can be overridden by:

- A command line parameter `-t` followed by the path to the directory containing the `tc_initd.tdb` file.
- The environment variable `TC_DATABASE_DIRECTORY` pointing to the directory containing the `tc_initd.tdb` file. This overrides both the default value and a directory given with the `-t` command line argument.

Each database defined in `tc_initd.tdb` represents a database that can be used within Thermo-Calc. Each entry has three parts:

- the database short-name (e.g. `FEDEMO`, maximum seven characters),
- the path to the database setup file (max 78 characters), and
- a short description of the database (max 60 characters). The entry must end with an exclamation mark (`!`), the first two parts must not contain white space, and it can span over two lines.

The paths can be relative to the `tc_initd.tdb` file or absolute. For platform independence, the recommendation is to always use forward slashes (`/`) in the paths, but on Windows backslash (`\`) also works.

You can add comment lines in the database initialization file. Comments must start with a `$` sign.



Each entry record (i.e. for a single database) must finish with an exclamation mark `!`. There should be no spaces or commas within the first and second fields since these characters are taken as field separators, while spaces or commas can be used in the third field.

Example

The following are examples of an initialization file defining two databases:

```
SSOL7 SSOL7\SSOL7SETUP.TDC  SGTE Solutions Database version 7.0 !
MYDB1 ../../../MYDATABASES/ABC.TDB My database 1.0 !
```

The Database Definition File and Keywords

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Database Definition File Syntax

The database definition (*.TDB) file (normally named `***setup.TDB`) consists of a set of keyword codes each followed by one or several parameters (arguments).

- A complete keyword entry must end with an exclamation mark (!).
- A single keyword entry can be up to 2000 characters long. However, the maximum length of a line in an *.TDB file is 78 characters--it may be necessary to continue the keyword parameter (arguments) on several lines. The ! must be at the end of the last line.
- It is recommended to always have at least one empty space at the beginning of each continuation line for the keyword parameters (arguments); otherwise, the DATA module can misunderstand the parameters (or arguments), or issue an error message.
- The keyword and its various parameters (arguments) are separated by a space or a comma.
- A dollar sign ($) in the first position of the line indicates that the line is a comment line, which is ignored by the DATA module.

When the database is selected the DATA module only reads the database definition file (***setup.TDB) once, from beginning to end. The DATA module checks continuously when reading the definition file. This implies that (nearly) everything must be declared or defined before it is used in any other way.

For example, if the GRAPHITE phase is to be included in the database definition, the element C (carbon) and the phase GRAPHITE must be defined before declaring that carbon dissolves in graphite. This definition order is necessary to build the internal data structure acceptable by the DATA module (during its consistency checking).

This topic gives a description of the available keywords and the appropriate arguments. A basic knowledge of the Gibbs Energy System (GIBBS) module is assumed.

This syntax is used:

```
KEYWORD [arg.1]*# [arg.2]*## {optional arg.3}!
```

The keywords are written in full length but can be abbreviated as long as the abbreviation is unique. A keyword may have syntax consisting of several arguments and optional arguments. The number, # or ##, in the notation, [...]*# or [...]*##, indicates an argument with a maximum length of # ASCII characters.



Arguments within square brackets `[...]` must always be given, but are optional when enclosed in curly brackets `{...}`.

ELEMENT

```
ELEMENT [element name]*2 [ref. state]*24 [mass] [H298] [S298] !
```

The *element name* (maximum two characters) is the one found in the periodic chart but there are no naming restrictions. However, the GIBBS module only recognizes UPPER-case element names (if the `Upper Case Mode` is selected by the GIBBS command REINITIATE), which means that lower-case (if defined in a database) is automatically converted to UPPER-case by the DATA/GIBBS module.

The elements are automatically entered as species using the same names of the elements. If, for example, the species corresponding to FE needs to be named FE1, you can define the species as FE1, which results in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase), need to be entered as special elements for correct handling by the DATA module.

The *reference (ref.) state* (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and be used as the reference state for all element thermodynamic data. The *mass*, given in gram per mole, is used in various calculation programs and should always be given the correct value. *H298* and *S298* denote the enthalpy and entropy difference between 0 and 298.15 K for the element in SI units. If these are unknown, the values can be set to zero. All this information (reference state, H298 and S298) define the SER (Stable Element Reference state).

Examples

```
ELEMENT /- ELECTRON_GAS       0.0  0.0  0.0 !
ELEMENT VA VACUUM             0.0  0.0  0.0 !
ELEMENT ZE UNIT_CHARGE        0.0000000001  0.0  0.0 !
ELEMENT AL FCC_A1             26.98154 4577.296 28.3215 !
ELEMENT C  GRAPHITE           12.011  1054.0    5.74 !
ELEMENT FE BCC_A2             55.847  4489     27.28 !
ELEMENT O  1/2_MOLE_O2(G)     15.9994 4341    102.5158 !
ELEMENT TI HCP_A3             47.88   4810     30.648 !
ELEMENT ZR HCP_A3             91.224  5566.27  39.181 !
ELEMENT ZY DUMMY               1         1         1 !
```

SPECIES

```
SPECIES [species name]*24 [stoichiometric formula] !
```

This keyword defines species in the data structure. Every *species name* (maximum 24 characters) must be unique. The species are built from the predefined set of elements in the stoichiometric formula. If an undefined element is referenced, DATA displays an error message and the data structure is probably damaged.

The species names do not have to be the same as the stoichiometry formula, although in general this is recommended. The elements are automatically entered as species using the same names of the elements.



You can define a species name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case species names.

When naming the species in a database, use special characters (such as +, -, _, / and .) in species names. Avoid using other special characters (such as (and)).

The *stoichiometric formula* is written with a simplified chemical notation, in which the chemical elements should always be given in UPPER-case and in any preferred order, and the stoichiometric coefficients are written in either real numerical factors or integer digits.



It is important that the numerical factor of 1 is not left out. Subgroups are not allowed in a stoichiometry formula; however, while specifying the stoichiometry formula for a specific species in a database, you can specify it in a way that some elements (always together with the corresponding partial stoichiometric coefficients) are repeated (as in the examples below).

Examples

```
SPECIES AL2O3      AL2O3 !
SPECIES Silica     SI1O2 !
SPECIES NaSb_6OH   NA1SB1O6H6 !
SPECIES FE+2        FE/+2 !
SPECIES SB-3        SB/-3 !
SPECIES AlCl2/3            AL.33333CL.666667 !
```

```
SPECIES AL1CL1H2O2         AL1CL1H2O2 !
SPECIES AlCl3_3H2O         AL1CL3H6O3 !
SPECIES AlO2H2Cl.H6O3      AL1O2H2CL1H6O3 !
SPECIES AlCl2-OH.3H2O      AL1CL2O1H1H6O3 !
SPECIES AlCl2OH.3Water     AL1O1H1CL2H6O3 !
```

PHASE

```
PHASE [phase name]*24 [data-type code]*8 [numb. subl.] [sites in
subl. 1] [sites in subl. 2] etc... {auxiliary text string} !
```

This keyword defines a phase and its properties (except for what species are allowed to enter it and for its parameters).

The *phase name* (maximum 24 characters) must be unique; otherwise the DATA module sees it as an attempt to redefine a previously defined phase. This causes DATA to display an error message and ignore the rest of the line. A phase name can be suffixed by an underscore (_and letters to identify the physical state(s) or structure type(s) of the phase.

Examples of Recommended Suffixes

Suffix	Definition
ABC_S	The ABC phase in solid state.
ABC_S2	The ABC phase in solid state 2.
ABC_S3	The ABC phase in solid state 3.
ABC_LT	The ABC phase in solid state at low temperatures.
ABC_HT	The ABC phase in solid state at high temperatures.
ABC_L	The ABC phase in liquid state.
ABC_LIQ	The ABC phase in liquid state.
FCC_A1	The FCC phase in disordered structure type A1.
FCC_L12	The FCC phase in ordered structure type L12.

The *phase name* can also be attached with a colon sign (:) and a letter for a legal GIBBS phase-type code (e.g. IONIC_LIQ:Y and GAS:G).

GIBBS Phase-type Codes

Code	Definition
G	Bit set for a gaseous mixture phase.
A	Bit set for an aqueous solution phase.

Code	Definition
Y	Bit set for an ionic liquid solution phase (specially treated by the Ionic Two-Sublattice Liquid Model).
L	Bit set for a liquid solution phase (but not A (aqueous) or Y (ionic liquid)).
I	Bit set for a phase with charged species (but not G (gaseous), A (aqueous) or Y (ionic liquid)).
F	Bit set for an ordered FCC or HCP solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).
B	Bit set for an ordered BCC solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).



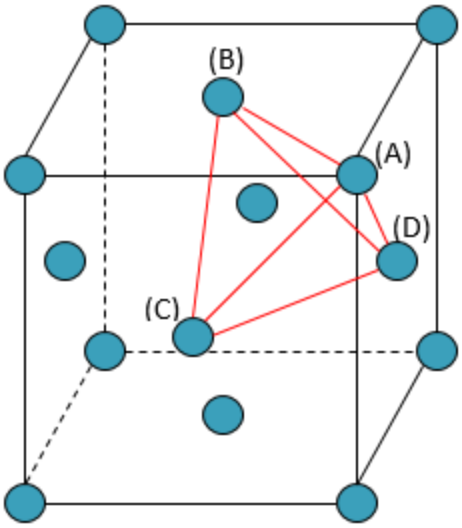
Other invalid characters (e.g. M or P) are eventually treated, together with the colon (:) as a part of a phase name.

A G phase (gaseous mixture) or an A phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and an L phase (ordinary liquid solution) is normally (but not always) modeled as a substitutional phase without sublattice, too.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours, as shown.

FCC Unit Cell Example

An FCC unit cell with the lattice positions indicated that correspond to the G (FCC,A:B:C:D) end member. All lattice positions are equivalent for a four substitutional-sublattice ordering model.



A *Normal 4-Sublattice Model* requires that all the G parameters for each of the end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically.

Additional Clarification

An A-B binary solution phase (with the element A located on one sublattice site and B on the other three sublattice sites) treated by the Normal 4-Sublattice Model has to have four G parameters for four end-members, i.e.

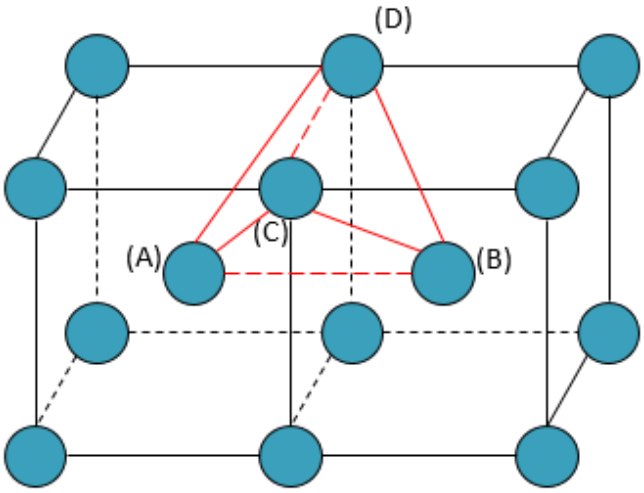
- G(phase,A:B:B:B)
- G(phase,B:A:B:B)
- G(phase,B:B:A:B, and
- G(phase,B:B:B:A)

This is because in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, they are identical and thus all G parameters of such end-members need to be given only once, and the possible permutations are then automatically handled by the GIBBS module. Also, only one of the identical permutations is listed; in this example, G(phase,A:B:B:B) where it is alphabetically the first in the list of permutations. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

For ordered BCC phases, the phase-type option B means the same thing but it is more complicated since the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours as shown:

BCC Unit Cell Example

Two BCC unit cells with the lattice positions indicated that correspond to the G (BCC,A:B:C:D,0) end member. Lattice positions (A) and (B) are equivalent, as are lattice positions (C) and (B) for a four substitutional-sublattice ordering model.



For an end member described by the parameter `G (phase,A:B:C:D)` A and B are next nearest neighbours, as are C and D. And the nearest neighbours of A (or B) are C and D. Thus, for an `A-B` binary solution phase (with the element A located on two sublattice sites and `B` on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the `G(phase,A:A:B:B)` term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the `G(phase,A:B:A:B)` term has two nearest neighbour bonds between A and B atoms and three next nearest neighbour bonds.

The first end-member (described by the `G(phase,A:A:B:B)` term) represents B2-ordering and the second (described by the `G(phase,A:B:A:B)` term) stands for B32-ordering. There are two permutations of the `G(phase,A:A:B:B)` term and four permutations of the `G (phase,A:B:A:B)` term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. If you enter the unary, binary, ternary and quaternary parameters you are dealing with 1, 6, 21, 55 parameters for BCC:B, 1, 5, 15, 35 parameters for FCC:F and 1, 16, 81, 256 parameters for phases without F/B.

An additional feature with the phase-type options `F` and `B` is that a composition set that represents the solution phase has a suffix (indicating what ordering the phase has) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams).

Such suffix indications can be:

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
FCC PHASE	FCC_A1	FCC_L12
		FCC_L10
BCC PHASE	BCC_A2	BCC_B2
		BCC_B32
		BCC_D03
		BCC_L21
HCP PHASE	HCP_A3	HCP_D019
		HCP_B19



If you want to convert an existing database TDB file to use the F/B feature, add the phase-type code to the corresponding phase name in the PHASE and CONSTITUENT commands in the TDB-file, then when running the LIST_DATA command in the Gibbs (GES) module. The created database file is in this less verbose format.

The *data-type code* consists of 1 to 8 characters where each character must stand for an action, which is to be coupled to this phase. The keyword TYPE_DEFINITION, described below, must be used in the current database to specify what action should be taken by DATA for each character code.

The data entries `[numb. subl.] [sites in subl. 1] [sites in subl. 2]` etc., specify the total number of sublattices (always as an integer digit) and the sites (i.e. stoichiometric coefficients) of each of the sublattices (given in either integer digits or real numerical factors) for the phase.

Optionally, an *auxiliary text string* (maximum 78 characters) can be given after the last [sites in sublattice #] but before the exclamation mark `!`. This string displays in connection with the phase name in some listings within the DATA module.

Examples

```
PHASE GAS:G  % 1 1.0 !
PHASE LIQUID:L %ZCDQ  2  1.0  1.0
> Metallic liquid solution, modeled by CEF Model. !
```

```
PHASE IONIC-LIQ:Y %ZCDQ  2  1.0  1.0
> Ionic liquid solution, modeled by Ionic Two-Sublattice Model. !
PHASE SPINEL:I    %ZA   4   1  2  2  4
> Complex Spinel Solution, by CEF model with ionic constraints. !
PHASE M23C6  % 3 20.0 3.0 6.0 !
PHASE FCC_A1    %&A  2  1 1
> Disordered FCC phase; also as MX carbides/nitrides. !
PHASE FCC_L10   %&AX  3  0.75 0.25 1
> Ordered FCC phase, modeled by 2-Sublattice Model for Ordering. !
PHASE FCC_L12:F %&AX  5  0.25 0.25 0.25 0.25 1.0
> Ordered FCC phase, modeled by 4-Sublattice Model for Ordering. !
PHASE AQUEOUS:A %HIJMR 1 1.0
> Aqueous Solution: using the Complete Revised HKF Model. !
```

CONSTITUENT

```
CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword (and the ADD_CONSTITUENT keyword for large solution phase) defines the phase-constitution as a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase).

The *phase name* (maximum 24 characters) must be a predefined phase (i.e. already through the PHASE keyword).



It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, SLAG:L, LIQUID:L, IONIC_LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code must also always be attached to the phase name in the CONSTITUENT keyword (and the ADD_CONSTITUENT keyword).



Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent description* (maximum 2000 characters) is a list of the species that enter a phase. The list starts with a colon (`:`), indicating the start of the sub-list of species for the first sublattice, and different sublattices are separated by colons. The complete sequence ends with a final colon.

Optionally, each sublattice may specify which species are considered to be major constituents. This is done by adding a percent sign (`%`) directly to the species name. The start values on the site fractions of the major constituents should sum to 0.99 on a specific sublattice. Thus, the minor constituents (i.e. those without a `%`) add up to 0.01. A maximum of 2000 characters can be coded in the constituent description, continuing in sequent lines. If the phase has a constituent description longer than 2000 characters, the rest can be coded in one or several ADD_CONSTITUENT keywords.

Examples

```
CONSTITUENT BCC_A2 :FE
CONSTITUENT IONIC-LIQ:Y :FE+2 : SB-3: !
```

```
CONSTITUENT M23C6 :CR FE :FE CR W MO : C: !

CONSTITUENT AQUEOUS:A :H2O% AG+1 AGF AGCL AGCL2-1 AGI3-2 AGSO4-1
AGC2H4+1

   AGN2H6+1 AGC2N2-1 AGC2H4NO2 AL+3 ALF3 ALO2-1, ... : !

CONSTITUENT SPINEL:I  : AL+3% CR+3 FE+2% FE+3 MG+2% NI+2

                      : AL+3% CA+2 CR+3 FE+2 FE+3 MG+2% NI+2 VA

                      : FE+2 MG+2 VA%

                      : N-3 O-2% :!
```

ADD_CONSTITUENT

```
ADD_CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword adds more constituents to a phase that already has some constituents. Its syntax is the same as for the CONSTITUENT keyword. This keyword can be used several times, if the phase is very large, e.g. a gaseous mixture or a complex aqueous solution. This is useful when there are so many constituents in a phase that the 2000 characters available for the constituent description list is not enough.



Constituents are not necessary on all sublattices. In the second example below, no addition is made to the first sublattice.

Examples

```
ADD_CONSTITUENT GAS :S1 S2 S3 ... : !

ADD_CONSTITUENT IM-PHASE : :CR:W ... : !

ADD_CONSTITUENT AQUEOUS:A :CUCL+1 CUCL2 CUCL2-1 CUCL3-2 CUOH+1 CUO2H2
CUO3H3-1

    CUO4H4-2 CU2OH+3 CU2O2H2+2 CU3O4H4+2 NIO2H2 NIO3H3-1 NIO4H4-2
NI2OH+3

    NI4O4H4+4 ZNOH+1 ZNO2H2 ZNO3H3-1 ZNO4H4-2 ... : !
```

COMPOUND_PHASE

```
COMPOUND_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

The keyword is a compact way to simultaneously define a species, a *compound phase* (maximum 24 characters) and its phase-constituent. It is useful for stoichiometric phases with constant compositions. The species name and stoichiometric formula must be identical, i.e. being the given *constituent*. The phase has this species as its only constituent. This keyword allows the database definition file for a large substance database to be more compact; it is a combination of the SPECIES, PHASE and CONSTITUENT keywords.

Examples

```
COMPOUND_PHASE AL2O3 % AL2O3 !
COMPOUND_PHASE MAGNETITE %MF FE3O4 !
COMPOUND_PHASE QUARTZ % SIO2 !
```

ALLOTROPIC_PHASE

```
ALLOTROPIC_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

This keyword does the same as the COMPOUND_PHASE keyword for entering an allotropic phase (maximum 24 characters), but does not enter the constituent as a species to the data structure. Use this if the species is already defined.

Examples

```
ALLOTROPIC_PHASE BETHA-AL2O3 % AL2O3 !
ALLOTROPIC_PHASE CRISTOBALITE % SIO2 !
ALLOTROPIC_PHASE TRIDYMITE % SIO2 !
```

TEMPERATURE_LIMITS

```
TEMPERATURE_LIMITS [lower limit] [upper limit] !
```

This keyword sets the default upper and lower temperature limits used by the GIBBS module for Gibbs energy parameters and functions. It can be used only once in one database definition file and all its sequential files.

Example

```
TEMPERATURE_LIMITS 500.0 1800.0 !
```

DEFINE_SYSTEM_DEFAULT

```
DEFINE_SYSTEM_DEFAULT [keyword] {G-ref. type index} !
```

This keyword sets the default value to ELEMENT or SPECIES in the DATA command DEFINE_SYSTEM.

For a substance database, it can be appropriate to have ELEMENT as a default value whereas a large solution database can benefit from having SPECIES as a default value. A proper default value is useful for beginners. An advanced user is more likely to use the DATA commands DEFINE_ELEMENT and DEFINE_SPECIES to override the default value.

{G-ref. type index} is an integer indicating the reference state type for an element when entering and listing data in the GIBBS module. The following lists legal numbers and the corresponding meaning (the reference state type for an element):

Number	Definition
1	symbol: G
2	symbol: H298
3	symbol: H0

For example:

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

DEFAULT_COMMAND

```
DEFAULT_COMMAND [secondary keyword and parameters] !
```

This keyword specifies commands to be executed by the DATA module at database initialization. The syntax of the available command is currently not the same as the user available DATA commands but the actions are similar. The available *secondary keyword and parameters* in syntax are:

```
DEFINE_SYSTEM_ELEMENT [element names]
DEFINE_SYSTEM_SPECIES [species names]
DEFINE_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_SYSTEM_ELEMENT [element names]
REJECT_SYSTEM_SPECIES [species names]
REJECT_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_PHASE [phase names]
RESTORE_PHASE [phase names]
```

Examples

```
DEFAULT_COMMAND DEFINE_SYSTEM_ELEMENT FE VA !
DEFAULT_COMMAND REJECT_SYSTEM_CONSTITUENT LIQUID 2 C !
DEFAULT_COMMAND REJECT_PHASE LIQUID !
DEFAULT_COMMAND RESTOR_PHASE GAS !
```

DATABASE_INFORMATION

```
DATABASE_INFORMATION [text]*10000 !
```

This keyword defines a text for the detailed description of the current database. The text can be listed with the DATA command DATBASE_INFORMATION. An apostrophe (') can be used in the text to indicate a new line; and two apostrophes, ('') can be used in the text to indicate a new line plus an empty line.



The continuous *text* length (each line with max 78 characters) is 10,000 characters.

Example

```
DATABASE_INFORMATION This is the XXX-Alloy Solution Database '
      in the A-B-C-D-..... System. '
   Developed by TCS, released in May 2001. ''
... more ... !
```

TYPE_DEFINITION

```
TYPE_DEFINITION [data-type code]*1 [secondary keyword with
parameters] !
```

This keyword couples phases to an action performed by the DATA module when the DATA command GET_DATA is executed.

Secondary Keywords

The secondary keywords and associated parameters in syntax are:

```
SEQ [filename]

RND# [filename]

GES [valid GIBBS command with parameters]

POLY3 [valid POLY command with parameters]

TDB [valid DATA command with parameters]

IF [conditional statement] THEN [keyword with parameters]

AFTER [valid GIBBS command with parameters]
```

The secondary keyword `SEQ` specifies a sequential file that stores parameters belonging to the phases using the associated data type code (which is defined by this keyword). A special case where the filename is given as an asterisk (`*`) implies that the database definition file also acts as a sequential data storage file. This case makes it possible to have a single file for a small database, which is especially suited for personal databases.

The secondary keyword `RND` should be concatenated with a positive integer `#` to indicate the type of the random file. Currently, there are these types of random files:

- `RND0`, the default, is used for complete Gibbs energy expressions (G0 parameters), where the search field is the unabbreviated parameter name.
- `RND1` is designated for functions, where the function name is used as the search field.
- `RND2` is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation.



Ternary and higher order interaction parameters must be specified on a sequential file. Moreover, the internal structures of these random files are subject to changes with different versions of DATA, and with implementations of DATA on various computer systems. For more information, see the FORTRAN program TDBSORT, which is available from Thermo-Calc Software AB.

The secondary keywords `GES`, `POLY3`, or `TDB` specifies a modification of, or addition to, phases having the associated data type code, such as magnetic contribution, another excess model, or any other valid GIBBS/POLY/DATA command that applies to a certain phase. By implementing this as a call to the interactive GIBBS/POLY/DATA module, flexibility is achieved. If a new type of addition is implemented in a GIBBS/POLY/DATA module, it can be immediately used in the database definition file without reprogramming the DATA module.



In several examples below, the use of the at (`@`) sign indicates any phase to which the relevant type definition (e.g. `A`, `B`, `4`, or `E`) applies.

The secondary keywords `IF` and `THEN` allow specification of a conditional statement structured with respect to the phase constitution that controls the execution of a following type-definition (keyword with parameters) string. See the last four examples.

The secondary keyword `AFTER` is similar to the GES keyword except the defined GIBBS command is executed after all parameters are entered. The reason for this is that the command has no effect unless there is a parameter. Following the `AFTER` keyword, a GIBBS command must be given and it is executed after entering the parameters of the phase.

The data-type code (always as one string) can be any normal or special character, e.g. `0`, `5`, `A`, `F`, `M`, `%`, `&`, and so forth, and is referred in the definition keywords PHASE, COMPOUND_PHASE and ALLOTROPIC_PHASE for various phases.

A phase can have several ADDITIONAL parts of different types (that are enforced by certain TYPE_DEFINITIONS which call the GIBBS command AMEND_PHASE_DESCRIPTION for describing various contributions to Gibbs energy). However, the DATA/GIBBS module automatically deletes any early-defined ADDITIONAL part(s) of the same type.

The DATA module can selectively retrieve functions that are necessary for a defined system from a database that has functions stored in its `setup` file or `SEQ` sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces.

Examples

```
TYPE_DEF % SEQ  TCPATH\DATA\[DATABASE]\PARAMETERS.TDB !
```

```
TYPE_DEF I SEQ  TCPATH\DATA\[DATABASE]\INTERACTION-PARAMS.TDB !
TYPE_DEF G RND0 TCPATH\DATA\[DATABASE]\GZERO-PARAMS.TDB !
TYPE_DEF F RND1 TCPATH\DATA\[DATABASE]\FUNCTIONS.TDB !
TYPE_DEF & RND2 TCPATH\DATA\[DATABASE]\BINARY-INTERACTIONS.TDB !
TYPE_DEF A GES AM_PH_DES @ MAGNETIC -1 0.40 !
TYPE_DEF B GES AM_PH_DES @ MAGNETIC -3 0.28 !
TYPE_DEF 4 GES AM_PH_DES @ EXCESS_MODEL REDLICH-KISTER_KOHLER !
TYPE_DEF 5 GES AM_PH_DES AQUEOUS EXCESS_MODEL HKF !
TYPE_DEF 6 GES AM_PH_DES AQUEOUS HKF_ELECTROSTATIC !
TYPE_DEF 7 GES AM_PH_DES AQUEOUS STATUS 02084000,,, !
TYPE_DEF 8 GES AM_PH_DES AQUEOUS MAJOR_CONST 1 H2O !
TYPE_DEF E AFTER AM_PH_DES LIQUID EXCESS MIXED-EXCESS
                        A B LEGENDRE   C A POLYNOM ,,,, !
TYPE_DEF T AFTER AM_PH_DES LIQUID TERN-EXT TOOP-KOHLER  B A C ,,,, !
TYPE_DEF Q AFTER AM_PH_DES LIQUID TERN-EXT KOHLER FE CR NI !
TYPE_DEF C IF (PD AND PT AND SN)  THEN TDB RESTORE_PHASE BCT_A5 !
TYPE_DEF D IF (PD AND (PT OR SN)) THEN TDB REJECT_PHASE BCC_A2 !
TYPE_DEF E IF ((NB OR TI OR V) AND (C OR N)) THEN
          GES AM_PH_DES @ COMP_SET ,, CR NB TI V: C N: !
TYPE_DEF F IF (ALO3/2 OR CRO3/2 OR FEO OR MNO OR SIO2) THEN
          GES AM_PH_DES LIQUID COMP_SET ,, ALN%,ALO3/2%,CRO3/2%,
             FEO%,FEO3/2,MNO3/2%,MNS%,SIO2%,TIO2% : !
TYPE_DEF R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS  Fe 0 0.6
         Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
         Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
         Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
         U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
         B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
         P  0 0.01  S  0 0.01  !
```

Ordered Phase Restores Disorder Contribution

When an ordered phase with disordered contribution is restored, the disordered contribution is automatically restored as well. You can also restore the disordered phase *without* restoring the ordered phase.



However the DIS_PART TYPE_DEFINITION must always be set on the ordered phase. It is important that the disordered phase is declared *before* the ordered phase. Otherwise it causes an error when DIS_PART TYPE_DEFINITION is executed and then either the ordered or disordered phase is rejected.

Example

```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_A1  %&  2 1   1 !
    CONSTITUENT FCC_A1  :CR,NI% : C%,VA :  !
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
TYPE_DEFINITION ' GES AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_
A1,,,!
TYPE_DEFINITION ( GES A_P_D FCC_L12 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_L12  %'(  3 .75   .25   1 !
    CONSTITUENT FCC_L12  :CR,NI% : CR,NI% : C,VA% :  !
```

For example a GES command such as the following only affects phases defined above or at the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( GES A_P_D FCC_L12 DIS_PART FCC_A1,,, !
```

For example a TDB command such as the following only affects phases defined *below* the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( TDB RESTORE_PHASE FCC_A1 !
```

FTP_FILE

```
FTP_FILE [filename] !
```

FTP_FILE is a special function random file and the function names correspond to the record numbers where these record names and the functions are stored. The FTP_FILE decreases search time for the associated database in the DATA module. The file is used for large substance databases along with a SEQ sequential or RND0 random file for storage of G0 parameters referring the functions named `FxxxxT` that are stored in the FTP file. The integer number `xxxx` is a search code used by DATA when such files are processed.



No modification of this file type is allowed.

Example

```
FTP_FILE TCPATH\DATA\[DATABASE]\FTP-FILE.DATA !
```

FUNCTION

```
FUNCTION [function name]*8 [lowest temp. limit]
[expression 2]; [upper temp. limit 2] Y
[expression 1]; [upper temp. limit 1] Y
[expression 3]; [upper temp. limit 2] Y
   ..... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

GIBBS can use predefined functions in the expression (TP-Function) of a Gibbs energy parameter or in other functions. This is often used when several parameters (or functions) have a common sub-expression, such as for metastable modifications of elements. This keyword can appear in both files for database definition and sequential storage, but not in FTP files. A valid *function name* can have up to 8 characters.

A function always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and other entered functions (normally with a `#` suffix, e.g. `+3*GHSERAL#`).

- ENTER_PARAMETER

The expression is a FORTRAN-like expression and operators `+`, `-`, `*`, `=` and `**` can be used (`**` only with integer powers). Unary-functions `LN` or `LOG` (both for natural logarithm) and `EXP` (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon (`;`), and be followed by its upper applicable temperature limit and a continuation indicator (`Y` to continue with the next expression or `N` to end the function's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the `N` indicator.

A complete/valid function entry can be written in several continuation lines if the function's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.



It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may misunderstand the expression or issue some error messages when reading the function entry. Avoid entering functions like the one below.

```
FUNCTION GHSERXY  298.15
```

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Such a function is read by the DATA module as

```
1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

rather than

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

This is because the DATA module concatenates all lines and removes extra spaces before trying to enter the function in the GIBBS workspace. Thus, the - sign is taken as a delimiter between 298.15 and 1000, and the function incorrectly becomes:

```
FUNCTION GHSERXY 298.15 1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```



Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
FUNCTION GHSERXY  298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

which is read correctly as

```
FUNCTION GHSERXY  298.15 -1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a function is normally set by default as 298.15 K, in most cases. However, you can set another limit when it is applicable (according to experimental data and assessments).

An upper-temperature limit (in Kelvin; followed by a `Y` or `N` sign) for the applicability of each TP-Function in a function must be given after the semicolon (`;`) immediately following the specific TP-Function. The highest-temperature limit (in Kelvin) for the applicability of the current function is always followed by the `N` sign. If a negative number is given as the lowest-temperature limit, it assumes there are breakpoints in pressure for this function. In these cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function is also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular function in a special reference file. The references are listed when doing the GET_ DATA command in the DATA module. They can also be listed in the GIBBS module with the command LIST_DATA with the option `R`.



For accounting for the reference indices, also see the keyword REFERENCE_FILE.

The reference index field can also be an abbreviation (such as `REF:250`, `REF_002`, or `REF-SGTE`) which denotes the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `R`).

However, the references directly coded in the database definition file (`***setup.TDB`) starting with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `N` or `R`). Normally, such references must be located after the `LIST_OF_REFERENCE` keyword. It is recommended to use reference code names such as `REF001`, `REF018`, etc. The reference list, which is generated by the GIBBS command LIST_DATA `<file>` with the `N` or `R` option, is also possible to be directly read by the DATA module.

The DATA module can selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its setup file or SEQ sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces. Previously, this can only be done for large databases that have functions stored in `RND1` random or `FTP` function files.

Examples

```
FUNCTION GFREE  298.15  1000+GFUNXY#; 6000 N !
FUNCTION GFUNXY 298.15 -1000+200*T+30*T*LOG(T); 6000 N 505 !
FUNCTION G0_CAO 298.15 -663538.11+352.67749*T-57.7533*T*LN(T)
        +5.3895E-03*T**2-8.879385E-07*T**3+575530*T**(-1);
     1400.00 Y -625196.99+78.896993*T-20.40145*T*LN(T)
        -1.112923E-02*T**2+5.1896733E-07*T**3-6917350*T**(-1);
     2900.00 Y -499226.55-490.37695*T+51.95912*T*LN(T)
       -2.961051E-02*T**2+1.4033905E-06*T**3-48114685*T**(-1);
     3172.00 Y -587711.89+375.04117-62.76*T*LN(T);
     6000.00 N REF020 !
```

PARAMETER

```
PARAMETER <parameter name> [lowest temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
   .......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. After the keyword, a valid < *parameter name*> in some cases should be given.

It is used to define standard Gibbs energies (i.e. the `G` parameters for Gibbs energy of formations) of all valid end-members of various stoichiometric and solution phases, and excess Gibbs energies (i.e. the `L` parameters for Gibbs energy of interactions) of all binary, ternary, quaternary or higher-order interactions in various solution phases; both standard Gibbs energies and excess energies can also have parameters for contributions from PT-depended volume variations (i.e. the `V0`, `VA`, `VC` and `VK` parameters for molar volume, thermal expansivity, bulk modulus, isothermal compressibility and high-pressure fitting parameter), magnetic ordering (i.e. the `TC` and `BM` parameters for Curie temperature and Bohr magneton number) and hypothetical electrostatic interactions (i.e. `BM` parameter for Born functions ωPr,Tr of aqueous solute species).

The general form of a parameter is:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx>
<expression> <yyy> <keyword Y or N> <zzz> !
```

General Form

Name	Description
identifier	The parameter type.
phase	The phase name (maximum 24 characters).
constituent array	The specific constituent array in the phase.

Name	Description
digit	The degree of composition-dependent interaction contribution (an integer number from 0 to 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted.
expression	The mathematical relation to describe the parameter.
xxx and yyy	The low and high temperature limits respectively for the applicable temperature range of the parameter expression
keyword Y or N	The indicator on if there is continuation for the parameter expression or not
zzz	The reference index/number for the assessment of this parameter;
!	The exclamation mark is used to indicate that the current parameter definition is ended

GIBBS Parameter Name

The GIBBS parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Type-Identifier and Definition

The GIBBS parameter name consists of several parts. The first is a *type-identifier*. The following type-identifiers are legal:

Type-Identifier	Definition
G	Standard energy parameter (Gibbs energy of formation)
L	Excess energy parameter (Gibbs energy of interaction)
TC	Curie temperature for magnetic ordering
BMAGN or BM	Bohr magneton number for magnetic ordering (or Born function ω Pr,Tr for aqueous solute species).
V0	Molar volume at 298.15 K and 1 bar (a numeric value only)

Type-Identifier	Definition
VA	Integrated thermal expansivity $\int_{298.15}^{T} \alpha(T)dT$
VC	High-pressure fitting parameter
VK	Isothermal compressibility
VISC	RT*ln(η) where η is the dynamic viscosity
ELRS	Electric resistivity
THCD	Thermal conductivity
SIGM	Surface tension of a liquid end-member
XI	Surface tension dampening factor/interaction for one constituent in a two-constituent combination. See the examples for how to use these parameters

Examples

Parameter	Definition
G(GAS,C1O2)	The Gibbs energy of formation of a CO2 molecule in gas.
G(FCC,FE:VA)	The Gibbs energy of formation of fcc Fe with interstitials.
L(LIQ,Fe,Cr;0)	The regular solution parameter for Fe and Cr in liquid.
L(LIQ,Fe,Cr;1)	The sub-regular solution parameter.
TC(BCC,Fe:Va)	The Curie temperature of bcc Fe.
BMAGN(BCC,Fe:Va)	The Bohr magneton number parameter of bcc Fe.
SIGM(LIQUID,AL;0)	Surface tension of Al in LIQUID. Constant value or linear temperature dependence.
XI(LIQUID,AL,CU;0)	Surface tension dampening factor for Al in the Al-Cu combination in LIQUID. Constant value.
XI(LIQUID,AL,CU;1)	Surface tension dampening factor for Cu in the Al-Cu combination in LIQUID. Constant value.

You can also use G for interaction parameters; and on output list (performed by the GIBBS command LIST_PARAMETER or LIST_PHASE_DATA) the type-identifier L is always used for interaction parameters. Note that the type-identifier BM is also used for Born functions ωPr,Tr of aqueous solute species.

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.



It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, LIQUID:L, SLAG:L, IONIC_LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name in the PARAMETER keyword.



Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent array* consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The exception is if the phase is ionic liquid (specified with the "phase bit" `:Y`), then neutral endmember and interaction parameters are written as if the first sublattice does not exist, e.g. `PARAM G (IONIC_LIQ,FEO3/2;0)`, i.e. the constituent array does not contain any constituents from the first (cation) sublattice.

For more ionic liquid specific parameters, see Parameters for the Two Sublattice Ionic Liquid Model.

The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents.

Be careful about the sign of odd terms, for example, `L(BCC, B, A:VA;1)` is treated as `L(BCC,A,B:VA;1)`, i.e. it is always put into alphabetical order.

Solution phases with sublattices may have interacting constituents in each sublattice.

You can use an asterisk (`*`) to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12,AL,NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC_L12 solution phase, while it is independent of all constituents on the second sublattice. A interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk (`*`) is calculated with the term of [`1-∑y(specified constituents)`], which implies that in an A-B binary system the following three `L` parameters are identical (but in higher-order systems, they are different):

- `L(phase,A,B)` is multiplied with `X(A)*X(B)`
- `L(phase,A,*)` is multiplied with `X(A)*(1-X(A))`

- `L(phase,B,*)` is multiplied with `X(B)*(1-X(B))`

A parameter always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) coded as mathematical relations of constants, functions of stable variables (`T` and `P`) and entered functions (normally with a `#` suffix, e.g. `+3*GSERAL#`).

The expression is a FORTRAN-like expression and operators `+`, `-`, `*`, `=` and `**` can be used (`**` only with integer powers). Unary-functions `LN` or `LOG` (both for natural logarithm) and `EXP` (for exponential) can also be used. Each expression (`TP-Function`) should ends with a semicolon (`;`) and be followed by its upper applicable temperature limit and a continuation indicator (`Y` to continue with the next expression, or `N` to end the parameter's expression). If there is no continuation after a specific expression (TP-Function), the reference index can be optionally given after the `N` indicator.

A complete/valid parameter entry can be written in several continuation lines if the parameter's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.



It is recommended to always have at least one empty space at the beginning of each continuation line. Avoid entering parameters such as:

```
PARAMETR G(LIQUID,A,B) 298.15
-2000+4568*T+2*GFUNAB#; 6000 N !
```

Such a parameter is read by the DATA module as `2000+4568*T+2*GFUNAB#`, rather than as `-2000 +4568*T+2*GFUNAB#`.



Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
PARAMETR G(LIQUID,A,B) 298.15
-2000+4568*T+2*GFUNAB#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a parameter is normally set by default as 298.15 K, in most cases; however, you can set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by a `Y` or `N` sign) for the applicability of each TP-Function in a parameter must be given after the semicolon (`;`) immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current parameter is always followed by the `N` sign. If a negative number is given as the

lowest-temperature limit, it is assumed that there are breakpoints in pressure for this parameter. In such cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter are also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular parameter in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. These can also be listed in the GIBBS module with the command LIST_DATA and the option `R` or `N`.



For accounting the reference indices, also see the keyword REFERENCE_FILE.

The reference index field can also be an abbreviation (such as `REF:250`, `REF_002`, or `REF-SGTE`) denoting the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `R` or `N`).

However, the references directly coded in the database definition file (`***setup.TDB`) that starts with a letter can be shown when issuing the DATA command `GET_DATA` or the GIBBS command LIST_DATA (with the option `R` or `N`). Normally, such references must be located after the `LIST_OF_REFERENCE` keyword. It is recommended to use reference code names such as `REF001`, `REF018`, etc. The reference list, which is generated by the GIBBS command LIST_DATA `<file>` with the `N` option, is thus also possible to be directly read by the DATA module.

Examples

```
PARAMETER G(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N 91DIN !
PARAMETER TC(BCC,FE:VA)    298.15 +1043; 6000 N 91DIN !
PARAMETER BMAGN(BCC,FE:VA) 298.15 +2.22; 6000 N 91DIN !
PARAMETER G(SIGMA,FE:CR:CR;0) 298.15 1000+200*T+...; 6000 N 101 !
PARAMETER G(LIQUID,AL;0)  298.15  +11005.553-11.840873*T
        +7.9401E-20*T**7+GHSERAL#;
933.60 Y +10481.974-11.252014*T+1.234264E+28*T**(-9)+GHSERAL#;
   2900.00 N  REF:283 !
```

```
PARAMETER G(BCC_A2,PB:C)   298.15 UN_ASS#; 300 N REF:0 !
PARAMETER G(BCC_A2,NI:C;0) 298.15 +GHSERNI#+3*GHSERCC#
                                  +400000-100*T; 6000 N REF071 !
PARAMETER G(BCC_A2,MN:VA)  298.15 +GMNBCC#; 6000 N REF285 !
PARAMETER BM(AQUEOUS,OH-1) 298.15 +Z0002PW0#; 1600 N 155 !
PARAMETER L(BCC,FE,CO:VA;0) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;1) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;2) 298.15 1000+200*T+...; 6000 N !
PARAM    TC(BCC_A2,CO,MO:VA;0) 298.15  -3700;    6000 N R454 !
PARAM    TC(BCC_A2,CO,MO:VA;1) 298.15  +2300;    6000 N R454 !
PARAM BMAGN(BCC_A2,CO,MO:VA;0) 298.15 -3.445;    6000 N R454 !
PARAM V0(BCC_A2,CR,FE:VA;0) 298.15 +ZERO#; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;1) 298.15 -1.10524097E-7; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;2) 298.15 +1.40024130E-7; 6000 N REF06V !
PARAM VA(BCC_A2,CR,FE:VA;0) 298.15 -6.49444634E-6*DELTAT#; 6000 N
REF06V !
PARAM VA(BCC_A2,CR,FE:VA;1) 298.15 +2.91269321E-5*DELTAT#; 6000 N
REF06V !
```

Parameters for the Two Sublattice Ionic Liquid Model

For the two sublattice ionic liquid model (specified with the "phase bit" `:Y` in the phase declaration), there are some additional requirements on the allowed parameters. While in the regular case all combinations of a phase's constituents are allowed as end-members, there are some constraints on the allowed parameters for ionic liquid.

In the ionic liquid model, the vacancy has been given an "induced" charge `-Q`, where `Q` is the average charge of the first (cation) sublattice.

All allowed parameters are listed below. The following notations are used:

- `C` = Cation
- `C1` = Cation 1 if more than one. Similar for anions and neutrals.
- `A` = Anion
- `VA` = Vacancy
- `N` = Neutral
- `D` = Anion or vacancy or neutral (i.e. anything on the second sublattice)

The phase description is:

```
(C1,C2…Ci)P(A1,A2...Ai,VA,N1, N2...Ni)Q
```

In the ionic liquid model,the `Vacancy` has been given an "induced" charge `-Q`, where `Q` is the average charge of the first (cation) sublattice.

Allowed end-members, assuming the phase name is IONIC_LIQ:

```
G(IONIC_LIQ,C:A;0)
G(IONIC_LIQ,C:VA;0)
G(IONIC_LIQ,N;0)
```

(The last line is an exception to the case that the constituent array must contain constituents from all sublattices)

This leaves one not allowed end-member:

```
G(IONIC_LIQ,C:N;0)
```

Allowed binary interaction parameters, where `i` is the interaction order in a Redlich-Kister expansion.

```
G(IONIC_LIQ,C1,C2:A;i)
G(IONIC_LIQ,C1,C2:VA;i)
G(IONIC_LIQ,C:VA,N;i)
G(IONIC_LIQ,N1,N2;i)
G(IONIC_LIQ,C:A1,A2;i)
G(IONIC_LIQ,C:A,VA;i)
G(IONIC_LIQ,C:A,N;i)
```

No other binary interactions are allowed.

Allowed ternary interaction parameters. The interaction is composition independent if there is one parameter with `i = 0`. It is composition dependent if there are three parameters with `i = 0`, `1` and `2`. There can only be one or three parameters for one combination of constituents

```
G(IONIC_LIQ,C1,C2,C3:A;i)
G(IONIC_LIQ,C1,C2,C3:VA;i)
G(IONIC_LIQ,N1,N2,N3;i)
G(IONIC_LIQ,C1,C2:VA,N;i)
G(IONIC_LIQ,C:VA,N1,N2;i)
G(IONIC_LIQ,C:A,D1,D2;i)
G(IONIC_LIQ,C1,C2:A,D;i)
```

No other ternary interactions are allowed.

OPTIONS

```
OPTIONS /[alloy name]([composition limitations for all alloying
elements]) !
```

This keyword defines an alloy in a database. An alloy has a name, a major component and a number of alloying elements. The purpose for defining an alloy is to be able to tell you about applicable composition limits of the current database in applications to that particular type of alloy. It is possible to have several alloys in the same database. The alloys are given after the keyword in the database.

The alloy name must be proceeded by a slash (/) and terminated by the opening parenthesis, with no spaces are allowed in between.

- The alloy name is maximum 8 characters.
- After the parenthesis, follows the major element and a parenthesis with its minimum mass and minimum mole percent given inside.
- Then, the alloying element names, each with its maximum mass and mole percent are given within parenthesis.
- There must a space between definitions for each alloying element.
- The alloy definition is terminated by a closing parenthesis, and the whole OPTIONS keyword by the exclamation mark (!).

Example

```
OPTIONS /SSteel(Fe(60,60) CR(30,30) NI(15,15) SI(1,1) N(.1,1)) !
```

TABLE



It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may issue some error messages when reading the table entry.

```
TABLE [name]*8 [start temp] [end temp] [delta temp] [table values] !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. It makes a table of Gibbs energy as a function of temperature where the values are given from the start temperature to the end temperature, at a step of the delta temperature.

Example

```
TABLE DEMTAB 1000.0 1500.0 100.0 -2912.9008 -2834.2416 -2755.5824
             -2677.7600 -2600.7744 -2524.2072 !
```

ASSESSED_SYSTEMS

```
ASSESSED_SYSTEM [descriptions on special treatments for specific
assessed systems]*8000 !
```

This keyword can be included in the database definition file (the `***setup.TDB` file). A maximum of 8000 characters after the keyword (to describe some special options when the DATA, GIBBS and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark (`!`).

Several ASSESSED_SYSTEMS keywords can be used in the same TDB file in order to have more lists of assessed systems. There is no limit to the number of the entries in the same TDB file.

The assessed systems in the database, and the special treatment options, are typed after the keyword. The elements (always in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, such as `C-FE` for the Fe-C binary system, and `C-CR-FE` for the Fe-Cr-C ternary system. A space must be between each assessed system. Information on assessed binary, ternary or higher-order systems may also be given in this way.



A ternary system like C-CR-FE does not imply that the binary C-CR, C-FE and CR-FE are assessed. There is no way to indicate partially assessed systems.

- There is a field to give some descriptive information for a specific system, with various options about how to:
- Reject or restore phase(s) from the current database in the DATA module;
- Set major constituent(s) in the first composition set and to set a second composition set for a specific phase available in the current database in the GIBBS module; *and*
- Calculate this specific system in the POLY module.
- This is the facility used by the BIN (binary phase diagrams) and TERN (ternary phase diagrams) modules in the Thermo-Calc software/database package.

The descriptive information must immediately follow the specific system name, and must be enclosed within parenthesis `(` and `)`, and the left parenthesis must follow directly after the system, such as :

```
AL-NI(TDB +L12 ;G5 C—S:L12/NI:AL:VA ;P3 STP:.8/1200/1 STP:.2/600/1)
```

The syntax TDB means that the commands to the DATA module proceed, and +L12 in the example means that the phase called L12 should be restored (it has been rejected by default).

The directive ;G5 means that the following are commands to the GIBBS module. C_S: means creating a second composition set, after the colon follows the phase name and after the slash the major constituents.

After the directive ;P3 follows commands to the POLY module. STP: means setting a start point with the value of the X-axis first (composition for the second element in a binary system), the slash separates the Y-axis value (temperature), and possibly one or more directions (-1, 1, -2 or 2).

A summary of the allowed syntax is:

TDB accepts

- +phase and -phase for restore/reject.
- ;G5 accepts
- MAJ:phase/constituent-array for major constituents of the first composition set.
- C_S:phase/constituent-array for a second composition set.
- ;P3 accepts
- TMM:lt/ht for the low-/high-temperature limits (lt and ht; for instance TMM:500/4000) suitable for calculating phase diagrams and property diagrams of a binary system.
- * for a default start point which is set as:
- for a binary system: at the composition X(2nd element)=.1234, temperature T=1100 K and with the default directions; or
- for a ternary system: at the compositions X(2nd element)=.1234 and X(3rd element)=.1234 and with the default directions.
- STP:x/t/d1/d2/d3 for a specific start point in a binary system which is set as at the composition X(2nd element)=x and temperature T=t (in K), and with the directions d1, d2 and/or d3.
- STP:x1/x2/d1/d2/d3 for a specific start point in a ternary system which is set as at the compositions X(2nd element)=x1 and X(3rd element)=x2 and with the directions d1, d2 and/or d3.
- The direction(s) can be defined as -1, 1, -2 or 2. If no direction is specified, all default directions are used (meaning no ADD command is enforced in the POLY module).
- If only one start point is specified, the direction(s) may be omitted; if more than one start points are specified, at least one direction for each start point must be given for all start points.

Each entry for a specific binary or ternary sub-system can be written in one or several lines (each line with 78 characters).

Other Examples

```
ASSESSED_SYSTEMS
AL-NI(TDB +L12 +BCC_B2 ;G5 C_S:L12/NI:AL:VA
       ;P3 STP:.8/1000/1 STP:.45/700/1 STP:.7/700/1)
AL-PB(TDB -HCP -BCC
       ;G5 MAJ:LIQ/AL MAJ:FCC/AL:VA C—S:LIQ/PB C—S:FCC/PB:VA ;P3 *)
CR-FE(;G5 C—S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
AG-CU(;G5 MAJ:FCC/AG:VA C_S:FCC/CU:VA ;P3 STP:.3/1000)
C-NB(;P3 STP:.9/1100/1)
C-SI(;P3 *)
CO-CR(;G5 MAJ:FCC/CO:VA C_S:FCC/CR:VA ;P3 STP:.1/1100)
CR-FE(TDB -HCP ;G5 C_S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
CR-NI(;P3 *)
CR-W(;G5 MAJ:BCC/W:VA C_S:BCC/CR:VA
       ;P3 TMM:500/4000 STP:.3/700/1 STP:.3/1800/2 )
CU-FE(TDB -HCP ;G5 MAJ:LIQ/CU MAJ:FCC/FE:VA C_S:FCC/CU:VA
       ;P3 STP:.9/1400)
FE-N(TDB +FE4N ;P3 *)
FE-O(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:O-2 MAJ:ION_LIQ/FE+2:VA
      ;P3 STP:.2/2000/1 )
FE-S(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:S MAJ:ION_LIQ/FE+2:S-2
;P3 *)
AL-MG-SI(;P3 *)
C-CR-FE ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA ;P3 *) !
```



The semicolon (`;`) is a part of the `;G5` and `;P3` directives. A long descriptive information can be written in more than one line, such as for the `AL-NI`, `AL-PB`, `CU-FE` and `FE-O` systems shown above.

The directive `;P3 *` is needed if the default start point should be used. If there is no `P3` directive, the BIN or TERN module generates some 20 different start points in order to cover all possible compositions and temperatures (for a binary system) or all possible compositions (for a ternary system under any specific temperature).

REFERENCE_FILE

```
REFERENCE_FILE [file name] !
```

This keyword takes a reference file name as its argument. This reference file (that must be edited in a restrictive way and be saved as a blocked file with a fixed line-length for each line in the file, as described below) contains a complete list of the references for the various parameters (and sometimes functions) in the database. The file must have a fixed record structure: each reference entry with one or several records, and each record with exactly 78 characters written in one single blocked line; and no empty space is allowed at the beginning of all lines in the file. If there are more than one record entered for a reference entry, all the continuation lines must start with an ampersand (&). The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which is referred when a parameter or function calls this integer as the optional *{Ref. Index}*.

- Keywords PARAMETER or FUNCTION have information about specifying a reference index.

Example

```
/-1<G>            T.C.R.A.S. Class 1
AG1.64TE1         THERMODATA 01/93
&28/01/93
&SILVER 1.64-TELLURIDE. Solid Standard State.
AG1               HULTGREN SELECTED VAL.        SGTE **
&AT.WEIGHT 107.870,STANDARD STATE:CODATA KEY VALUE.MPT=1234.93K. &--
U.D. 30/10/85.
AG1<G>            T.C.R.A.S  Class: 1
AG1/+1<G>         T.C.R.A.S  Class: 1
AG1BR1            N.P.L.                        SGTE **
&Tfusion uncertain and heat vaporization estimated.
AG1BR1<G>         THERMODATA 01/93
&28/01/93
&Gaseous Standard State.
AG1BR1O3          BARIN & KNACKE.SUPPL.REF:62,* SGTE **
&AGO3BR   SILVER OXYTRIBROMIDE
```

In the example, the unique integers of related references (for assessed elements, species, phases, interactions, etc.) are:

```
1/-1<G>
```

```
2AG1.64TE1
5 AG1
8AG1<G>
9AG1/+1<G>
10AG1BR1
12AG1BR1<G>
15AG1BR1O3
```

LIST_OF_REFERENCE

```
LIST_OF_REFERENCE
NUMBER SOURCE
  [REFxxx]  '[Detailed reference]'
..........
.......... !
```

This keyword starts a reference list that is directly coded in the database definition file (`***setup.TDB`). Its argument begins on the following line, and normally has an explanation line (NUMBER SOURCE) that is followed by various reference codes. Each reference code may occupy one or more lines (each line with maximum 78 characters), but must have a reference code name (that starts with a letter) and the detailed reference information (that is written within two single-quotation marks, `''`). It is recommended to use reference code names such as `REF001`, `REF018`, etc. A maximum of 400,000 characters after the keyword is allowed until the exclamation mark (`!`).

Such a reference list can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the `R` option). The reference list, which is generated by the GIBBS command LIST_DATA `<file>` with the `N` option, has this structure, and is thus possible to be directly read by the DATA module.

Example

```
LIST_OF_REFERENCES
NUMBER  SOURCE
REF283 'Alan Dinsdale, SGTE Data for Pure Elements,
          Calphad Vol 15(1991) p 317-425,
          also in NPL Report DMA(A)195 Rev. August 1990'
REF224 'P-Y Chevalier, Thermochimica Acta, 130 (1988) p 33-41; AG-SI'
!
```

ADD_REFERENCE

```
ADD_REFERENCE
  [REFxxx]  '[Detailed reference]'
.........
......... !
```

Use this keyword to have an unlimited number of references. The use of this is the same as that of LIST_OF_REFERENCE, and is used after it. Several ADD_REFERENCES sections can be used in a single database if there are too many references.

It is recommended to always start with a so-called *empty reference* (such as the DUMP0 reference in the following example) as the first entry in each of the ADD_REFERENCE sections to make sure that all references are listed appropriately as retrieving data by issuing the GET_DATA command.

Example

```
ADD_REFERENCE
   DUMP0  'Empty reference 0'
   REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
          TRITA 0270 (1986); CR-FE'
   REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
          TRITA 0207 (1986); C-CR-FE'
   REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys
Database,
          v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
          at high temperatures.'
   ... ...
!
ADD_REFERENCE
   DUMP1  'Empty reference 1'
   REF275 'A. Fernandez Guillermet, Z. Metallkde. Vol 79(1988) p.524-
536,
          TRITA-MAC 362 (1988); C-CO-NI AND C-CO-FE-NI'
   REF393   'K. Frisk, Metall. Trans. Vol 21A (1990) p 2477-2488,
          TRITA 0409 (1989); CR-FE-N'
   REF1096  'P. Gustafson, Metall. Trans. 19A(1988) p 2547-2554,
```

```
            TRITA-MAC 348, (1987); C-CR-FE-W'
      ... ...
   !
```

CASE and ENDCASE

```
CASE [ELEMENT/SPECIE/PHASE] !
  IF (boolean algebra on element, species or phase names) THEN
       [GIBBS/POLY/DATA command] !
ENDCASE !
```

This keyword takes as its argument, a definition on which type of the following Boolean algebra operates. A simple Boolean algebra using AND and OR with a maximum of four levels of parentheses works. The CASE construction must end with the ENDCASE keyword. This makes it possible to have additional GIBBS or POLY commands executed depending on the user selection of elements, species or phases. The DATA commands that can be given as secondary keyword to DEFAULT_COMMAND can also be executed.

Example 1

```
CASE ELEMENT !
   IF((CR OR TI OR V) AND N)
   THEN GES AM_PH_DES @ C_S ,, CR MO TI V:C N: !
ENDCASE !
```

Example 2

```
CASE ELEMENT !
   IF(O) THEN TDB DEFINE_SYSTEM_ELEMENT /- !
ENDCASE !
```

Example 3

```
CASE ELEMENT !
   IF(AL AND FE)
   THEN TDB DEF_SYS_ELEMENT VA !
ENDCASE !
```

VERSION_DATA

```
VERSION_DATE [string]*78 !
```

The string is denoted as the version/revision date and database manager of the database. Nowadays, this directive is used mainly for the purpose of keeping the development and revision history mostly updated.

Example

```
VERSION_DATE Last update and adjustment: Database Manager, 2015-09-25
!
```

Working with the Mobility Databases

In this section:

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PARAMETER 59
DIFFUSION 60
ZEROVOLUME_SPECIES 61

Extensions to Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), need both thermodynamic data and kinetic data (i.e. diffusivities or mobilities). Naturally, the handling and storage of kinetic data also benefits from the use of some kind of database management. Thus, the TDB database definition file syntax has been extended to incorporate some new keywords needed for storing kinetic data - PARAMETER, DIFFUSION, and ZEROVOLUME_SPECIES .

PARAMETER

```
PARAMETER [special GIBBS parameter name] [low temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
   ......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword allows you to enter all types of normal GIBBS parameters for thermodynamic data as well as five special extensions suitable for kinetic data used in the Diffusion Module (DICTRA).

Valid extensions to special GIBBS parameter names are:

- `MQ`: Activation enthalpy for mobility equation.
- `MF`: Pre-exponential factor for mobility equation.
- `DQ`: Activation enthalpy for diffusivity equation.
- `DF`: Pre-exponential factor for diffusivity equation.
- `VS`: Volume counted per mole of volume carrying species.

Example



See the TDB file for DICTRA example *exa4: Carburization of binary Fe-C alloy: Comparison to an analytical erf solution*. Press F1 in Thermo-Calc to search the help for more information.

```
$============== D I F F U S I O N   D A T A ====================
$
 ZEROVOLUME_SPECIES C VA !


PARA DQ(FCC_A1&C,*:*),,  -148000+32.8*T+R*T*LOG(4.53E-7);,,N!
PARA DQ(FCC_A1&FE,*:*),, -286000+R*T*LOG(0.700E-4);,,N!
```

DIFFUSION

```
DIFFUSION [model keyword] [phase name] [additional parameter(s)] !
```

This keyword specifies the type of diffusion model to use for a phase if the default model is not desired. The default model calculates the full diffusion matrix. A diffusivity is calculated from the different mobilities and the thermodynamic factors. The former ones are calculated as:

```
M = exp (∑MF/RT) exp (∑MQ/RT) / RT
```

where ∑ stands for a weighted summation of the different MF's and MQ's plus possibly a Redlich-Kister term.

Valid Model Keywords

Keyword	Description
NONE	No diffusion in this phase
DILUTE	Constitution list of dependent species in each sublattice must be given as an additional parameter. Only the diagonal terms in the diffusion matrix are calculated. D = exp (∑ DF/RT) exp (∑DQ/RT).
SIMPLE	Constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms in the diffusion matrix are calculated. D = ∑ DF + ∑ DQ.
MAGNETIC	The so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an & sign and a species name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated.

Examples

```
DIFFUSION NONE SIGMA !
DIFFUSION DILUTE CEMENTITE : FE : C : !
DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
```

ZEROVOLUME_SPECIES

```
ZEROVOLUME_SPECIES [list of species] !
```

In the Diffusion Module (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes. This keyword uses a list of which species are to be considered as zero volume ones for an argument.



There is no underscore (_) between *Zero* and *Volume*.

Example

```
ZEROVOLUME_SPECIES VA C N !
```

Database Definition File Examples

In this section:

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Example 2: A Custom Database for the Sb-Sn Binary System 65

Example 3: A Public Database for the Fe-Cr-C Ternary System 69

Example 1: A Steel Database

```
TEMP-LIM 500.0 2000.0 !
$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
ELEMENT VA VACUUM            0.0    0.0 0.0 !
ELEMENT C  GRAPHITE         12.011  0.0 0.0 !
ELEMENT V  BCC              50.9415 0.0 0.0 !
ELEMENT CR BCC-PARAMAGNETIC 51.996  0.0 0.0 !
ELEMENT FE FCC-PARAMAGNETIC 55.847  0.0 0.0 !
ELEMENT NI FCC-PARAMAGNETIC 58.69   0.0 0.0 !
ELEMENT MO BCC              95.94   0.0 0.0 !
ELEMENT W  BCC             183.85   0.0 0.0 !
$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
PHASE BCC       B1M  2 1.0 3.0 !
PHASE FCC       F2M  2 1.0 1.0 !
PHASE HCP       0    2 2.0 1.0 !
PHASE LIQUID    3    2 1.0 1.0 !
PHASE CEMENTITE 4    2 3.0 1.0 !
PHASE M23C6     4    2 23.0 6.0 !
PHASE M7C3      4    2 7.0 3.0 !
PHASE M6C       4    4 2.0 2.0 2.0 1.0 !
PHASE SIGMA     0    3 10.0 4.0 16.0 !
PHASE MU-PHASE  0    3 7.0 2.0 4.0 !
PHASE R-PHASE   0    3 27.0 14.0 12.0 !
PHASE GRAPHITE  4    1 1.0 !
$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
CONSTITUENT BCC :V CR FE NI MO W:VA C: !
CONSTITUENT FCC :V CR FE NI MO W:VA C: !
CONSTITUENT HCP :CR FE NI:VA C N: !
CONSTITUENT LIQUID :C V CR FE NI MO W VA:VA C: !
CONSTITUENT CEMENTITE :CR FE:C: !
CONSTITUENT M23C6 :CR FE:C: !
CONSTITUENT M7C3 :CR FE:C: !
```

```
CONSTITUENT M6C :FE:W:FE W:C: !
CONSTITUENT SIGMA :FE:V CR MO:FE V CR MO: !
CONSTITUENT MU-PHASE :FE:MO W:FE MO W: !
CONSTITUENT R-PHASE :FE:MO :FE MO: !
CONSTITUENT GRAPHITE :C: !
$
$TYPE_DEFINITIIONS:
TYPE-DEFINITION 0 SEQ TCPATH\DATA\METDATA\TC-THEREST.TDB !
TYPE-DEFINITION 1 SEQ TCPATH\DATA\METDATA\TC-BCC.TDB !
TYPE-DEFINITION 2 SEQ TCPATH\DATA\METDATA\TC-FCC.TDB !
TYPE-DEFINITION 3 SEQ TCPATH\DATA\METDATA\TC-LIQUID.TDB !
TYPE-DEFINITION 4 SEQ TCPATH\DATA\METDATA\TC-CARBIDES.TDB !
TYPE-DEFINITION M SEQ TCPATH\DATA\METDATA\TC-CURIE-BOHR.TDB !
TYPE-DEFINITION B GES AM-PH BCC MAGNETIC -1 .4 !
TYPE-DEFINITION F GES AM-PH FCC MAGNETIC -3 .28 !
$
$DEFAULT_COMMANDS:
DEFAULT-COMMAND DEF_ELEMENT VA !
DEFAULT-COMMAND REJ_SYS-CONST LIQUID 1 VA !
$DATABASE_INFORMATION:
DATABASE-INFO The following binary and ternary systems are available: '
  FE-CR-NI by Hertzman'
  FE-MO       Fernandez'
  FE-CR-C     Andersson'
  FE-W-C      Gustafson'
  FE-W        Andersson & Gustafson' !
```

Example 2: A Custom Database for the Sb-Sn Binary System

```
$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
ELEM VA VACUUM              0.0    0.0 0.0 !
ELEM MG HCP(A3)            24.305 0.0 0.0 !
ELEM SB RHOMBOHEDRAL(A7) 121.75   0.0 0.0 !
ELEM SN BCT(A5)          118.69   0.0 0.0 !
ELEM /- ELECTRON-GAS        0      0    0 !
$
$SPECIES, NAME, STOICHIOMETRIC-FORMULA !
SPECIE MG1 MG1!
SPECIE MG2 MG2!
SPECIE MG2+ MG/+2!
SPECIE SB1 SB1!
SPECIE SB2 SB2!
SPECIE SB4 SB4!
SPECIE SB3- SB/-3!
SPECIE SB5- SB/-5!
SPECIE SN1 SN1!
SPECIE SN4- SN/-4!
$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
PHASE BCT         Z 1 1.0!
PHASE HCP         Z 1 1.0!
PHASE RHOMBO      Z 1 1.0!
PHASE GAS:G       Z 1 1.0!
PHASE LIQUID:L    Z 1 1.0!
PHASE IONICLIQ:Y Z 2 1 1!
PHASE SPLIQ:Y     Z 2 1 1!
PHASE BMG3SB2:I   Z 2 3 2!
PHASE AMG3SB2:I   Z 2 3 2!
PHASE MG2SN:I     Z 2 2 1!
PHASE SBSN        Z 2 1 1!
PHASE SB2SN3      Z 2 2 3!
```

```
$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
CONSTITUENT RHOMBO :SB SN:!
CONSTITUENT HCP :MG SN:!
CONSTITUENT BCT :SB SN:!
CONSTITUENT GAS:G :MG1 MG2 SB1 SB2 SB4 SN1:
  > Gas phase, using the Ideal EOS and Mixing Model. !
CONSTITUENT LIQUID:L :SB SN:!
CONSTITUENT IONICLIQ:Y :MG2+:SB SB3- SN SN4- VA:
  > This is the Ionic Liquid Solution Phase. !
CONSTITUENT SPLIQ:Y :MG2+:SB SB3- SN SN4- VA:!
CONSTITUENT BMG3SB2:I :MG2+:SB3- SB5- VA SN4-:!
CONSTITUENT AMG3SB2:I :MG2+:SB3- VA SN4-:!
CONSTITUENT MG2SN:I :MG2+ VA:SB3- SN4-:!
CONSTITUENT SBSN :SB SN:SB SN:!
CONSTITUENT SB2SN3 :SB:SN:!
$
$DEFAULT_COMMANDS:
DEFAULT-COM DEF-ELEM VA /-!
DEFAULT-COM REJ-PHASE LIQUID!
DEFAULT-COM REJ-PHASE SPLIQ!
$
$TYPE_DEFINITIIONS:
TYPE-DEFINITION Z SEQ * !
$
$DATABASE_INFORMATION:
DATABASE_INFO The Sb-Sn system with isentropic temperatures!
$
$VERSION_DATE:
VERSION_DATE Last update 1986-05-18 11:39:49 !
$
$
$ HERE COMES THE THERMODYNAMIC DATA (expressed in functions &
parameters):
$
FUNCTION MGLIQUID 298.15 -4630.90976+192.994374*T-34.0888057*T*LOG(T)
   -36544605.6*T**(-2); 6000 N!
```

```
$
FUNCTION MGSOLID 298.15 -8367.34+143.677876*T-26.1849785*T*LOG(T)
   +4.858E-4*T**2-1.393669E-6*T**3+78950*T**(-1);
    923.00 Y -13804.4772 +202.909445*T-34.0888057*T*LOG(T)
   -3.65446056E7*T**(-2) +1.06753982E28*T**(-9); 6000 N!
$
FUNCTION SBLIQUID 298.15 9071.98+146.800*T-31.38*T*LOG(T)
   -2.441646E8*T**(-2); 6000 N!
$
.....
..... <more>
$
FUNCTION LFCT 298.15 -17325.6+5.03600*T; 6000 N!
FUNCTION GFCTSBSN 298.15 LFCT+SBSOLID+SNSOLID+2948.291+3721.286;
   6000 N!
FUNCTION ISB 298.15 15000; 6000 N!
FUNCTION ISN 298.15 47199.9-95.6270*T; 6000 N!
$
.....
..... <more>
$
PARAMETER G(RHOMBO,SB;0) 298.15 SBSOLID; 6000 N!
PARAMETER G(RHOMBO,SN;0) 298.15 2035+SNSOLID; 6000 N!
$
PARAMETER G(HCP,MG;0) 298.15 MGSOLID; 6000 N!
PARAMETER G(HCP,SN;0) 298.15 32000+SNSOLID; 6000 N!
PARAMETER G(HCP,MG,SN;0) 298.15 -69566-9.23183*T; 6000 N!
$
PARAMETER G(BCT,SN;0) 298.15 SNSOLID; 6000 N!
PARAMETER G(BCT,SB;0) 298.15 1000+SBSOLID; 6000 N!
PARAMETER G(BCT,SB,SN;0) 298.15 0.5*ISB+0.5*ISN; 6000 N!
PARAMETER G(BCT,SB,SN;1) 298.15 0.5*ISB-0.5*ISN; 6000 N!
$
PARAMETER G(IONICLIQ,MG2+:SB3-;0) 298.15 -204389-4.98506*T
   -2.75637E9*T**(-2)+3*MGLIQUID+2*SBLIQUID; 6000 N!
PARAMETER G(IONICLIQ,MG2+:SN4-;0) 298.15 -98639.5+881.073*T
   -174.523*T*LOG(T)-1.79808E9*T**(-2); 6000 N!
```

```
PARAMETER G(IONICLIQ,MG2+:SB;0) 298.15 SBLIQUID; 6000 N!
$
......
...... <more>
$
```

Example 3: A Public Database for the Fe-Cr-C Ternary System

```
$
$   Revision history:
$       Created as PDEMO  by Pingfang Shi  on 2004-10-05
$       Renamed to DFeCrC by Pingfang Shi  on 2006-10-25
$
$ FURTHER MODIFICATIONS:
$ ======================
$ pfs: /20041005 (PDEMO)
$       * Retrieved all definitions from PTERN for the Fe-Cr-C ternary !
$
$ pfs: /20061025 (DFeCrC)
$       * Ignore ELEMENT /- definition.
$       * Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parameters, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$           $L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
$            L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REF1 !
$           $L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
$            L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REF3 !
$       * Add Cr into HCP_A3 phase, and
$         add all necessary G0/L parameters (according to SSOL2/TCFE3):
$           G(HCP_A3,CR:VA;0)
$           TC(HCP_A3,CR:VA;0)
$           BMAGN(HCP_A3,CR:VA;0)
$           G(HCP_A3,FE:C;0)
$           G(HCP_A3,CR:C;0)
$           L(HCP_A3,CR:C,VA;0)
$           L(HCP_A3,CR,FE:VA;0)
$       * Add "TMM:300/3000" limits to all three binary joins in the
$           ASSESSED_SYSTEM section.
$       * Change the reference indices, e.g., 101 to REF1, in order to
$           always get the reference list correctly.
$       * Re-arrange database format slightly.
```

```
$       * Updated the DATABASE_INFO section.
$-----------------------------------------------------------------------
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ DATABASE INFORMATION:
$***********************************************************************
$
DATABASE_INFO                                      DFeCrC '
                TCS Demo Fe-Cr-C Alloy Solutions Database'
          (only for demonstration purposes in TCC-Demo/TCW-Demo)'
       ********************************************************** '
                         (Version 1.2, Oct. 2006) ''
          Copyright @ 2004-2012: Thermo-Calc Software AB, Sweden ''
The DFeCrC database (previously called PDEMO) is the TCS Demo Fe-Cr-C '
Alloy Solutions Database, which is especially designed for primarily '
demonstrating the uses of: '
  * TCC-Demo software: BIN, TERN, SCHEIL and some other modules; '
  * TCW-Demo software: '
     "Binary" module calculations of phase diagrams and property
diagrams'
                 in available binary systems; '
     "Ternary" module calculations of phase diagrams (e.g., isothermal'
                 sections, monovariant lines involving liquid, liquidus'
                 surface projections) and property diagrams in available'
                 ternary systems; '
     "Scheil" module simulations of alloy solidifications; and/or '
     "Equilibrium" calculation routines for phase diagrams and property'
                 diagrams in available binary or ternary systems. '
It can also be used for other types of calculations/simulations in both'
TCC and TCW software, and in their application programming interfaces.''
It includes critically-assessed data for all possible three binary joins'
(i.e. Cr-C, Fe-Cr and Fe-Cr) and one complete ternary alloy solutions '
within the Fe-Cr-C system. However, due to the fact that experimental'
data for the Fe-C and Cr-C binary joins and Fe-Cr-C ternary system at '
extremely-high temperatures are not sufficient, the available assessed'
data can not be applied to temperature conditions higher than 4000 K.''
Included thermodynamic data are available for various stoichiometric '
```

```
and solution phases, e.g. liquid mixture, various alloy solutions and '
intermetallic phases. But the gaseous mixture phase is excluded in this'
DEMO version.''
The DFeCrC database can be used not only in calculating various types '
of phase diagrams (binary phase diagrams, ternary isothermal sections,'
ternary monovariant lines involving liquid, ternary liquidus surface '
projections, ternary isopleth sections, etc.) and property diagrams '
(the easiest ways are through the BIN and TERN modules), but also in '
simulating alloy solidification processes (with the SCHEIL module) of'
Fe-based or Cr-based alloys (but limited within the Fe-Cr-C ternary '
system in this DEMO version). Many unique features of the TCC/TCW '
software can be demonstrated using this and other specially-designed '
DEMO databases. ''
However, this DFeCrC database (similar to other DEMO and/or PUBLIC TC '
databases) is provided within the TCC-Demo/TCW-Demo software only for '
the purposes of demonstration, testing and evaluation. For R&D projects'
and teaching activities, you are highly encouraged to only use the FULL'
versions of the TCC and/or TCW software together with some commercial '
databases that are appropriate for your specific applications. Please '
contact us for all kinds of details. ''
Release History: Version 1.1 with minor improvements,  Oct. 2004 '
                 Version 1.2 with minor modifications, Oct. 2006 ''
Edited by: Dr. Pingfang Shi (Thermo-Calc Software, Oct. 2006). ''
!

$ ----------------------------------------------------------------------
$VERSION_DATE Last update and adjustment: Pingfang Shi, 2004-10-05 !
VERSION_DATE Last update and adjustment: Pingfang Shi, 2006-10-25 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Definition of Elements in the Database System:
$----------------------------------------------------------------------
$ELEM NAME STABLE_ELEMENT_REF         ATOMIC MASS  H298-H0     S298 !
$----------------------------------------------------------------------
$ELEMENT /-   ELECTRON_GAS            0.0000E+00  0.0000E+00  0.0000E+00!
ELEMENT VA   VACUUM                  0.0000E+00  0.0000E+00  0.0000E+00!
```

```
ELEMENT C    GRAPHITE                1.2011E+01  1.0540E+03  5.7400E+00!
ELEMENT CR   BCC_A2                  5.1996E+01  4.0500E+03  2.3560E+01!
ELEMENT FE   BCC_A2                  5.5847E+01  4.4890E+03  2.7280E+01!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ TYPE_DEFINITIONS for data inclusions:
$-----------------------------------------------------------------------
TYPE_DEFINITION % SEQ *!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$  TYPE_DEFINITIONS for phase descriptions:
$-----------------------------------------------------------------------
$... For magnetic contributions:
TYPE_DEFINITION A GES AMEND_PHASE_DES @ MAGNETIC  -1.0  4.00000E-01 !
TYPE_DEFINITION B GES AMEND_PHASE_DES @ MAGNETIC  -3.0  2.80000E-01 !

$... For Cr/Fe-C in FCC phase and Cr/Fe-C in HCP phase:
TYPE_DEFINITION C IF(C) THEN GES AMEND_PHASE_DES @ C_S ,, :C: !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Default Commands:
$-----------------------------------------------------------------------
$DEFINE_SYSTEM_DEFAULT SPECIES 2 !
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !

DEFAULT_COMMAND DEF_SYS_ELEMENT VA !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ FUNCTIONS for various phases:
$-----------------------------------------------------------------------
$
FUNCT GHSERCC  298.15 -17368.441+170.73*T-24.3*T*LN(T)
     -4.723E-04*T**2+2562600*T**(-1)-2.643E+08*T**(-2)
```

```
     +1.2E+10*T**(-3); 6000 N!
FUNCT GHSERCR  298.15 -8856.94+157.48*T-26.908*T*LN(T)
     +.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);  2180 Y
      -34869.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9); 6000 N!
FUNCT GHSERFE  298.15 +1225.7+124.134*T-23.5143*T*LN(T)
     -.00439752*T**2-5.8927E-08*T**3+77359*T**(-1);  1811.00 Y
     -25383.581+299.31255*T-46*T*LN(T)+2.29603E+31*T**(-9); 6000 N!

FUNCT GFELIQ   298.15 +GHSERFE#+12040.17-6.55843*T
     -3.6751551E-21*T**7;  1811 Y
      -10839.7+291.302*T-46*T*LN(T);  6000 N!
FUNCT GFEFCC   298.15 +GHSERFE#-1462.4+8.282*T
     -1.15*T*LN(T)+6.4E-04*T**2;  1811 Y
      -27098.266+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9);  6000 N!
FUNCT GFECEM   298.15 +GPCEM1#-10745+706.04*T-120.6*T*LN(T); 6000 N!
FUNCT GFEM23C6  298.15 +7.666667*GFECEM#-1.666667*GHSERCC#
     +66920-40*T; 6000 N!

FUNCT GCRFCC   298.15 +GHSERCR#+7284+.163*T;  6000 N!
FUNCT GCRM23C6 298.15 -521983+3622.24*T-620.965*T*LN(T)
     -.126431*T**2;   6000 N!
FUNCT GCRM3C2  298.15 -100823.8+530.66989*T-89.6694*T*LN(T)
     -.0301188*T**2;  6000 N!
FUNCT GCRM7C3  298.15 -201690+1103.128*T-190.177*T*LN(T)
     -.0578207*T**2;  6000 N!

FUNCT GPCLIQ   298.15 +YCLIQ#*EXP(ZCLIQ#);    6000 N!
FUNCT ACLIQ    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCLIQ    298.15 +1+3.2E-10*P;               6000 N!
FUNCT CCLIQ    298.15 1.6E-10;                    6000 N!
FUNCT DCLIQ    298.15 +1*LN(BCLIQ#);              6000 N!
FUNCT ECLIQ    298.15 +1*LN(CCLIQ#);              6000 N!
FUNCT VCLIQ    298.15 +7.626E-06*EXP(ACLIQ#);     6000 N!
FUNCT XCLIQ    298.15 +1*EXP(.5*DCLIQ#)-1;        6000 N!
FUNCT YCLIQ    298.15 +VCLIQ#*EXP(-ECLIQ#);       6000 N!
FUNCT ZCLIQ    298.15 +1*LN(XCLIQ#);              6000 N!
```

```
FUNCT GPCGRA   298.15 +YCGRA#*EXP(ZCGRA#);    6000 N!
FUNCT ACGRA    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCGRA    298.15 +1+3.6E-10*P;               6000 N!
FUNCT CCGRA    298.15 3.3E-10;                    6000 N!
FUNCT DCGRA    298.15 +1*LN(BCGRA#);              6000 N!
FUNCT ECGRA    298.15 +1*LN(CCGRA#);              6000 N!
FUNCT VCGRA    298.15 +5.259E-06*EXP(ACGRA#);     6000 N!
FUNCT XCGRA    298.15 +1*EXP(.9166667*DCGRA#)-1;  6000 N!
FUNCT YCGRA    298.15 +VCGRA#*EXP(-ECGRA#);       6000 N!
FUNCT ZCGRA    298.15 +1*LN(XCGRA#);              6000 N!

FUNCT GPCFCC   298.15 +YCFCC#*EXP(ZFEFCC#);   6000 N!
FUNCT ACFCC    298.15 +1.44E-04*T;              6000 N!
FUNCT VCFCC    298.15 +1.031E-05*EXP(ACFCC#);   6000 N!
FUNCT YCFCC    298.15 +VCFCC#*EXP(-EFEFCC#);    6000 N!

FUNCT GPCRLIQ  298.15 +YCRLIQ#*EXP(ZCRLIQ#);    6000 N!
FUNCT ACRLIQ   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRLIQ   298.15 +1+4.65E-11*P;            6000 N!
FUNCT CCRLIQ   298.15 3.72E-11;                 6000 N!
FUNCT DCRLIQ   298.15 +1*LN(BCRLIQ#);           6000 N!
FUNCT ECRLIQ   298.15 +1*LN(CCRLIQ#);           6000 N!
FUNCT VCRLIQ   298.15 +7.653E-06*EXP(ACRLIQ#);  6000 N!
FUNCT XCRLIQ   298.15 +1*EXP(.8*DCRLIQ#)-1;     6000 N!
FUNCT YCRLIQ   298.15 +VCRLIQ#*EXP(-ECRLIQ#);   6000 N!
FUNCT ZCRLIQ   298.15 +1*LN(XCRLIQ#);           6000 N!

FUNCT GPCRBCC  298.15 +YCRBCC#*EXP(ZCRBCC#);  6000 N!
FUNCT ACRBCC   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRBCC   298.15 +1+2.6E-11*P;             6000 N!
FUNCT CCRBCC   298.15 2.08E-11;                 6000 N!
FUNCT DCRBCC   298.15 +1*LN(BCRBCC#);           6000 N!
FUNCT ECRBCC   298.15 +1*LN(CCRBCC#);           6000 N!
FUNCT VCRBCC   298.15 +7.188E-06*EXP(ACRBCC#);  6000 N!
FUNCT XCRBCC   298.15 +1*EXP(.8*DCRBCC#)-1;     6000 N!
FUNCT YCRBCC   298.15 +VCRBCC#*EXP(-ECRBCC#);   6000 N!
FUNCT ZCRBCC   298.15 +1*LN(XCRBCC#);           6000 N!
```

```
FUNCT GPFELIQ  298.15 +YFELIQ#*EXP(ZFELIQ#);  6000 N!
FUNCT AFELIQ   298.15 +1.135E-04*T;                              6000 N!
FUNCT BFELIQ   298.15 +1+4.98009787E-12*P+3.20078924E-14*T*P; 6000 N!
FUNCT CFELIQ   298.15 +4.22534787E-12+2.71569924E-14*T;        6000 N!
FUNCT DFELIQ   298.15 +1*LN(BFELIQ#);                            6000 N!
FUNCT EFELIQ   298.15 +1*LN(CFELIQ#);                            6000 N!
FUNCT VFELIQ   298.15 +6.46677E-06*EXP(AFELIQ#);                 6000 N!
FUNCT XFELIQ   298.15 +1*EXP(.8484467*DFELIQ#)-1;                6000 N!
FUNCT YFELIQ   298.15 +VFELIQ#*EXP(-EFELIQ#);                    6000 N!
FUNCT ZFELIQ   298.15 +1*LN(XFELIQ#);                            6000 N!

FUNCT GPFEFCC  298.15 +YFEFCC#*EXP(ZFEFCC#);  6000 N!
FUNCT AFEFCC   298.15 +7.3097E-05*T;                             6000 N!
FUNCT BFEFCC   298.15 +1+3.25236341E-11*P+3.36607808E-16*T*P; 6000 N!
FUNCT CFEFCC   298.15 +2.62285341E-11+2.71455808E-16*T;        6000 N!
FUNCT DFEFCC   298.15 +1*LN(BFEFCC#);                            6000 N!
FUNCT EFEFCC   298.15 +1*LN(CFEFCC#);                            6000 N!
FUNCT VFEFCC   298.15 +6.688726E-06*EXP(AFEFCC#);                6000 N!
FUNCT XFEFCC   298.15 +1*EXP(.8064454*DFEFCC#)-1;                6000 N!
FUNCT YFEFCC   298.15 +VFEFCC#*EXP(-EFEFCC#);                    6000 N!
FUNCT ZFEFCC   298.15 +1*LN(XFEFCC#);                            6000 N!

FUNCT GPFEBCC  298.15 +YFEBCC#*EXP(ZFEBCC#);  6000 N!
FUNCT AFEBCC   298.15 +2.3987E-05*T+1.2845E-08*T**2;             6000 N!
FUNCT BFEBCC   298.15 +1+2.80599565E-11*P+3.06481523E-16*T*P; 6000 N!
FUNCT CFEBCC   298.15 +2.20949565E-11+2.41329523E-16*T;        6000 N!
FUNCT DFEBCC   298.15 +1*LN(BFEBCC#);                            6000 N!
FUNCT EFEBCC   298.15 +1*LN(CFEBCC#);                            6000 N!
FUNCT VFEBCC   298.15 +7.042095E-06*EXP(AFEBCC#);                6000 N!
FUNCT XFEBCC   298.15 +1*EXP(.7874195*DFEBCC#)-1;                6000 N!
FUNCT YFEBCC   298.15 +VFEBCC#*EXP(-EFEBCC#);                    6000 N!
FUNCT ZFEBCC   298.15 +1*LN(XFEBCC#);                            6000 N!

FUNCT GPFEHCP  298.15 +YFEHCP#*EXP(ZFEHCP#);  6000 N!
FUNCT AFEHCP 298.15 +7.3646E-5*T;                              6000 N!
FUNCT BFEHCP 298.15 +1+32.5236341E-12*P+3.36607808E-16*P*T; 6000 N!
```

```
FUNCT CFEHCP 298.15 +26.2285341E-12+2.71455808E-16*T;       6000 N!
FUNCT DFEHCP 298.15 +LOG(BFEHCP#);                          6000 N!
FUNCT EFEHCP 298.15 +LOG(CFEHCP#);                          6000 N!
FUNCT VFEHCP 298.15 +6.59121E-6*EXP(AFEHCP#);               6000 N!
FUNCT XFEHCP 298.15 +EXP(0.8064454*DFEHCP#)-1;              6000 N!
FUNCT YFEHCP 298.15 +VFEHCP#*EXP(-1*EFEHCP#);               6000 N!
FUNCT ZFEHCP 298.15 +LOG(XFEHCP#);                          6000 N!

FUNCT GPCEM1   298.15 +VCEM1#*P;     6000 N!
FUNCT ACEM1    298.15 -1.36E-05*T+4E-08*T**2;    6000 N!
FUNCT VCEM1    298.15 +2.339E-05*EXP(ACEM1#);    6000 N!

FUNCT GPSIG1   298.15 +1.09E-04*P;        6000 N!
FUNCT GPSIG2   298.15 +1.117E-04*P;       6000 N!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Define the various Phase and their Constituents, and
$ Assign parameters to phases:
$---------------------------------------------------------------------
$PHASE  NAME:TYPE  MARKCODE  #SUBL  SITES_IN_EACH_SUBL. !
$---------------------------------------------------------------------

$***** LIQUID (Solution) ********************************************
PHASE LIQUID:L %  1  1.0
  > This is metallic liquid solution phase, with C species !
CONST LIQUID:L  : C,CR,FE :  !

PARAM G(LIQUID,C;0)  298.15 +GHSERCC#+GPCLIQ#
                              +117369-24.63*T; 6000 N REF0 !
PARAM G(LIQUID,CR;0)  298.15 +GHSERCR#+GPCRLIQ#
                 +24339.955-11.420225*T+2.37615E-21*T**7;  2180 Y
                           +GHSERCR#+GPCRLIQ#
                 +18409.36-8.563683*T+2.88526E+32*T**(-9); 6000 N REF0 !
PARAM G(LIQUID,FE;0)  298.15 +GFELIQ#+GPFELIQ#;  6000 N REF0 !

PARAM L(LIQUID,C,CR;0)  298.15 -90526-25.9116*T; 6000 N REF1 !
```

```
PARAM L(LIQUID,C,CR;1)  298.15 +80000;           6000 N REF1 !
PARAM L(LIQUID,C,CR;2)  298.15 +80000;           6000 N REF1 !
PARAM L(LIQUID,C,FE;0)  298.15 -124320+28.5*T;  6000 N REF3 !
PARAM L(LIQUID,C,FE;1)  298.15  +19300;         6000 N REF3 !
PARAM L(LIQUID,C,FE;2)  298.15  +49260-19*T;    6000 N REF3 !
PARAM L(LIQUID,CR,FE;0)  298.15 -14550+6.65*T;   6000 N REF4 !
PARAM L(LIQUID,C,CR,FE;0)  298.15 -496063;  6000 N REF2 !
PARAM L(LIQUID,C,CR,FE;1)  298.15  +57990;  6000 N REF2 !
PARAM L(LIQUID,C,CR,FE;2)  298.15  +61404;  6000 N REF2 !

$***** FCC_A1 (Solution) ********************************************
$PHASE FCC_A1  %BC  2 1   1 !
$ Note the C TYPE_DEF for 2nd FCC composition-set (MC) is not necessary
$    for the (Fe,Cr)-C system.
PHASE FCC_A1  %B   2 1   1 !
CONST FCC_A1  : CR,FE%
              : C,VA% :  !

PARAM G(FCC_A1,CR:VA;0)  298.15 +GCRFCC#+GPCRBCC#;  6000 N REF0 !
PARAM TC(FCC_A1,CR:VA;0)     298.15 -1109;  6000 N REF0 !
PARAM BMAGN(FCC_A1,CR:VA;0)  298.15 -2.46;  6000 N REF0 !
PARAM G(FCC_A1,FE:VA;0)  298.15 +GFEFCC#+GPFEFCC#;  6000 N REF0 !
PARAM TC(FCC_A1,FE:VA;0)     298.15 -201;  6000 N REF0 !
PARAM BMAGN(FCC_A1,FE:VA;0)  298.15 -2.1;  6000 N REF0 !

PARAM G(FCC_A1,CR:C;0)  298.15 +GHSERCR#+GHSERCC#
                                +1200-1.94*T;     6000 N REF2 !
PARAM G(FCC_A1,FE:C;0)  298.15 +GFEFCC#+GHSERCC#+GPCFCC#
                                +77207-15.877*T;  6000 N REF3 !
PARAM TC(FCC_A1,FE:C;0)     298.15 -201;  6000 N REF3 !
PARAM BMAGN(FCC_A1,FE:C;0)  298.15 -2.1;  6000 N REF3 !

PARAM L(FCC_A1,CR:C,VA;0)  298.15 -11977+6.8194*T; 6000 N REF2 !
PARAM L(FCC_A1,FE:C,VA;0)  298.15 -34671;          6000 N REF3 !
PARAM L(FCC_A1,CR,FE:VA;0) 298.15 +10833-7.477*T;  6000 N REF4 !
PARAM L(FCC_A1,CR,FE:VA;1) 298.15  +1410;          6000 N REF4 !
PARAM L(FCC_A1,CR,FE:C;0)  298.15 -74319+3.2353*T; 6000 N REF2 !
```

```
$***** BCC_A2 (Solution) ********************************************
PHASE BCC_A2  %A  2 1   3 !
CONST BCC_A2  : CR%,FE%
              : C,VA% :  !

PARAM G(BCC_A2,CR:VA;0)  298.15 +GHSERCR#+GPCRBCC#;  6000 N REF0 !
PARAM TC(BCC_A2,CR:VA;0)     298.15 -311.5;  6000 N REF0 !
PARAM BMAGN(BCC_A2,CR:VA;0)  298.15   -.01;  6000 N REF0 !
PARAM G(BCC_A2,FE:VA;0)  298.15 +GHSERFE#+GPFEBCC#;  6000 N REF0 !
PARAM TC(BCC_A2,FE:VA;0)     298.15 1043;  6000 N REF0 !
PARAM BMAGN(BCC_A2,FE:VA;0)  298.15 2.22;  6000 N REF0 !

PARAM G(BCC_A2,CR:C;0)  298.15 +GHSERCR#+3*GHSERCC#+GPCRBCC#+3*GPCGRA#
                                +416000;            6000 N REF1 !
PARAM TC(BCC_A2,CR:C;0)     298.15 -311.5;  6000 N REF1 !
PARAM BMAGN(BCC_A2,CR:C;0)  298.15  -.008;  6000 N REF1 !
PARAM G(BCC_A2,FE:C;0)  298.15 +GHSERFE#+3*GHSERCC#+GPFEBCC#+3*GPCGRA#
                                +322050+75.667*T;   6000 N REF3 !
PARAM TC(BCC_A2,FE:C;0)     298.15 1043;  6000 N REF3 !
PARAM BMAGN(BCC_A2,FE:C;0)  298.15 2.22;  6000 N REF3 !

$ PF-20061025: Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parametera, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REFS !
$PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REFS !
$
PARAM L(BCC_A2,CR,FE:VA;0) 298.15 +20500-9.68*T;   6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;0)     298.15 1650;  6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;1)     298.15  550;  6000 N REF4 !
PARAM BMAGN(BCC_A2,CR,FE:VA;0)  298.15 -.85;  6000 N REF4 !

PARAM L(BCC_A2,CR,FE:C;0)  298.15 -1250000+667.7*T; 6000 N REF2 !
```

```
PARAM TC(BCC_A2,CR,FE:C;0)    298.15 1650;  6000 N REF5 !
PARAM TC(BCC_A2,CR,FE:C;1)    298.15  550;  6000 N REF5 !
PARAM BMAGN(BCC_A2,CR,FE:C;0) 298.15 -.85;  6000 N REF5 !

$***** HCP_A3 (Solution) ********************************************
$PHASE HCP_A3  %BC  2 1   .5 !
$ Note the C TYPE_DEF for 2nd HCP composition-set (M2C) is not necessary
$    for the (Fe,Cr)-C system.
PHASE HCP_A3  %B   2 1   .5 !
CONST HCP_A3  : CR,FE,
              : VA%,C :  !

PARAM G(HCP_A3,CR:VA;0) 298.15 +GHSERCR#+4438;           6000 N REF1 !
PARAM TC(HCP_A3,CR:VA;0)    298.15 -1109;  6000 N REF1 !
PARAM BMAGN(HCP_A3,CR:VA;0) 298.15 -2.46;  6000 N REF1 !
PARAM G(HCP_A3,FE:VA;0) 298.15 +GHSERFE#+GPFEHCP#
              -3705.78+12.591*T-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
                           +GHSERFE#+GPFEHCP#
              -3957.199+5.24951*T+4.9251E+30*T**(-9);      6000 N REF0 !
PARAM G(HCP_A3,CR:C;0) 298.15 +GHSERCR#+.5*GHSERCC#
              -18504+9.4173*T-2.4997*T*LN(T)+.001386*T**2; 6000 N REF1 !
PARAM G(HCP_A3,FE:C;0) 298.15 +GFEFCC#+.5*GHSERCC#+GPCFCC#
                              +52905-11.9075*T;          6000 N REF3 !

PARAM L(HCP_A3,CR:C,VA;0)  298.15  +4165;  6000 N REF1 !
PARAM L(HCP_A3,FE:C,VA;0)  298.15 -22126;  6000 N REF3 !
$PARAM L(HCP_A3,FE:C,VA;0)  298.15 -17335;  6000 N TCFE3 !
PARAM L(HCP_A3,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !

$***** SIGMA (Solution) *********************************************
PHASE SIGMA  %  3 8   4   18 !
CONST SIGMA  : FE
             : CR
             : CR,FE :  !

PARAM G(SIGMA,FE:CR:CR;0)  298.15 +8*GFEFCC#+22*GHSERCR#
                              +92300-95.96*T+GPSIG1#;   6000 N REF4 !
```

```
PARAM G(SIGMA,FE:CR:FE;0)  298.15 +8*GFEFCC#+4*GHSERCR#+18*GHSERFE#
                                +117300-95.96*T+GPSIG2#;  6000 N REF4 !

$***** CEMENTITE (Solution) ******************************************
PHASE CEMENTITE  %  2 3   1 !
CONST CEMENTITE  : CR,FE%
                 : C :  !

PARAM G(CEMENTITE,CR:C;0)  298.15 +3*GHSERCR#+GHSERCC#
                                   -48000-9.2888*T; 6000 N REF2 !
PARAM G(CEMENTITE,FE:C;0)  298.15 +GFECEM#;          6000 N REF3 !

PARAM L(CEMENTITE,CR,FE:C;0)  298.15 +25278-17.5*T;  6000 N REF2 !

$***** M3C2 (Compound) ***********************************************
PHASE M3C2  %  2 3   2 !
CONST M3C2  : CR
            : C :  !

PARAM G(M3C2,CR:C;0)  298.15 +GCRM3C2#;  6000 N REF2 !

$***** M7C3 (Solution) ************************************************
PHASE M7C3  %  2 7   3 !
CONST M7C3  : CR%,FE
            : C :  !

PARAM G(M7C3,CR:C;0)  298.15 +GCRM7C3#;          6000 N REF2 !
PARAM G(M7C3,FE:C;0)  298.15 +7*GHSERFE#+3*GHSERCC#
                                +75000-48.2168*T; 6000 N REF2 !

PARAM L(M7C3,CR,FE:C;0)  298.15 -4520-10*T;  6000 N REF2 !

$***** M23C6 (Solution) **********************************************
PHASE M23C6  %  3 20   3   6 !
CONST M23C6  : CR%,FE%
             : CR%,FE%
             : C :  !
```

```
PARAM G(M23C6,CR:CR:C;0)  298.15 +GCRM23C6#;           6000 N REF5 !
PARAM G(M23C6,FE:CR:C;0)  298.15 +.1304348*GCRM23C6#
                                  +.8695652*GFEM23C6#; 6000 N REF5 !
PARAM G(M23C6,CR:FE:C;0)  298.15 +.8695652*GCRM23C6#
                                  +.1304348*GFEM23C6#; 6000 N REF5 !
PARAM G(M23C6,FE:FE:C;0)  298.15 +GFEM23C6#;           6000 N REF5 !

PARAM L(M23C6,CR,FE:CR:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !
PARAM L(M23C6,CR,FE:FE:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !

$***** GRAPHITE (Compound) ****************************************
PHASE GRAPHITE  %  1  1.0  !
CONST GRAPHITE  : C :  !

PARAM G(GRAPHITE,C;0)  298.15 +GHSERCC#+GPCGRA#; 6000 N REF0 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ ASSESSED_SYSTEMS information:
$    *  necessary for the BIN and TERN modules in TCC
$                     the Binary Phase Diagram module in TCW
$                  and the Equilibrium calculation routine in TCW
$-----------------------------------------------------------------------
ASSESSED_SYSTEM
$... Binary ...
  C-FE(;P3 TMM:300/4000 *)
  C-CR(;P3 TMM:300/4000 *)
  CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
        ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$ CR-FE(TDB -HCP ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
$       ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$
$... Ternary ...
  C-CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
          ;P3 STP:.4/.5/1 STP:0.1/0.5/1)
!
```

```
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$
$ LIST OF REFERENCE:
$
$---------------------------------------------------------------------------
LIST_OF_REFERENCES
NUMBER  SOURCE
REF0 'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991)
       p 317-425, also in NPL Report DMA(A)195 Rev. August 1990'
REF1 'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
REF2 'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
REF3 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
       TRITA 0237 (1984); C-FE'
REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
       TRITA 0270 (1986); CR-FE'
REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
       TRITA 0207 (1986); C-CR-FE'
REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database,
       v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
       at high temperatures.'
!
```

Database Checker

In this section:

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About the Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.



Thermo-Calc accepts some deviations from these syntax rules. Although warnings can be ignored, errors must be corrected.

For example, a warning is reported if an abbreviated phase name is found and phase name abbreviations are accepted by Thermo-Calc and its Add-on Modules. However, reported errors must be corrected in the TDB file before the database can be loaded by the application.

With respect to using this tool, the executable `DatabaseChecker` file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu in Thermo-Calc.



Large amounts of RAM can be required when checking large databases.

The Database Checker application is standalone and available as indicated from the **Tools** menu in Thermo-Calc. However, as required, you can run the `DatabaseChecker.exe` file as a stand-alone program from the file Thermo-Calc installation directory.

- Installation Default Directory: Windows, Installation Default Directory: macOS, or Installation Default Directory: Linux
- Using the Database Checker

Custom Databases: GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For custom database users, you may sometimes see messages in the log indicating that additional preparation is being done by Thermo-Calc prior to a calculation. The preparation is carried out automatically; it is usually fast and only needed the first time a custom database is used after a modification. While databases with warnings are tolerated, databases that contain errors can only be loaded by GES6 after the errors are corrected.

The Database Checker tool uses the same parser as GES6 and can be used to verify the consistency and correctness of databases during development, before the databases are actually used.

- Database Checker



To globally set the default from GES6 back to GES5, go to the **Tools → Options → General** tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The SET_GES_VERSION Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Using the Database Checker

About the Database Checker

Once you have installed the Thermo-Calc and are familiar with the TDB database file concept you can start working with the file to ensure it does not contain errors that prevent it from working with Thermo-Calc.

Example of Working with the Database Checker

The following shows a couple of the features available when using an unencrypted TDB database file included with Thermo-Calc Console Mode example *tcex11 - Oxidation of Cu_2S with an H_2O/O_2 Gas Mixture*.

Thermo-Calc Console Mode Examples

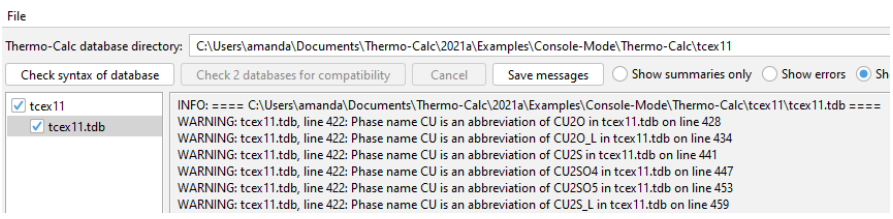
Open a TDB file. This example uses `tcex11.TDB`, which is the user-defined database referred to from the Thermo-Calc macro file `tcex11.TCM`.

1. In Thermo-Calc, from the menu select **Tools→Database Checker**.

2. In the Thermo-Calc Database Checker window, click the **File** button and navigate to a directory with TDB files or a file with a `.TDB` extension.

   If two databases are selected at the same time, these can be tested for compatibility i.e., whether the databases can be appended. The tool generates error messages for database entities e.g., phases, that are not compatible but this does not necessarily mean that the databases cannot be appended, only that the erroneous phases cannot be appended and must be rejected from the system.

3. Click **Select directory or file**.With the file loaded, click **Check syntax of database**. Choose how to show the information: **Show summaries only**, **Show errors**, **Show errors and warnings**, or **Show all messages**. The Database Checker lists the information in the window.



4. Click **Save messages** as needed to save a `.txt` file and use this to help improve your database.

TDB Editor

In this section:

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Using the TDB Editor 93

About the TDB Editor

In order to use this tool, it is important to understand how to work with the standard TDB database format. For example, see Thermodynamic and Kinetic/Mobility Databases in the *Database Manager User Guide*, which is part of the *Thermo-Calc Documentation Set*, or press F1 in Thermo-Calc and search for *TDB file* in the help.

The TDB Editor is an editing tool for those who develop their own custom databases for use with Thermo-Calc or other applications. The tool speeds up the database editing process by providing immediate feedback through syntax coloring, syntax checking, and by allowing formatting and easy navigation to items of interest in the TDB file.

The advantage to using the TDB Editor compared to a basic text editor includes features such as syntax coloring and checking, formatting of TDB files, and generally easier navigation.

The TDB Editor has two components (see Installing VSCode and the TDB Editor for details):

- As an installed extension to the open source code editor Microsoft Visual Studio Code (VSCode), which has the user interface for the TDB Editor. VSCode is available for free.

- A server application that runs invisibly in the background and provides the VSCode extension with services specific to the TDB format, such as syntax checking, formatting and the location within the document of various items, such as functions and references.

The syntax checker uses the same text parsing engine as the Database Checker tool and the Thermo-Calc application itself. This means that an edited TDB file with no errors shown in the TDB Editor, is also accepted by the Thermo-Calc application. For more information see About the Database Checker.

Installing VSCode and the TDB Editor

The TDB Editor is not available for macOS.

About the TDB Editor

To use the TDB Editor, you install the Visual Studio Code (VSCode) and then in VSCode you install the TDB Editor extension, which is included with your Thermo-Calc installation.

In order to access the most-up-to-date version of the VSCode plugin, it must be updated every time a *new* version of Thermo-Calc is installed.

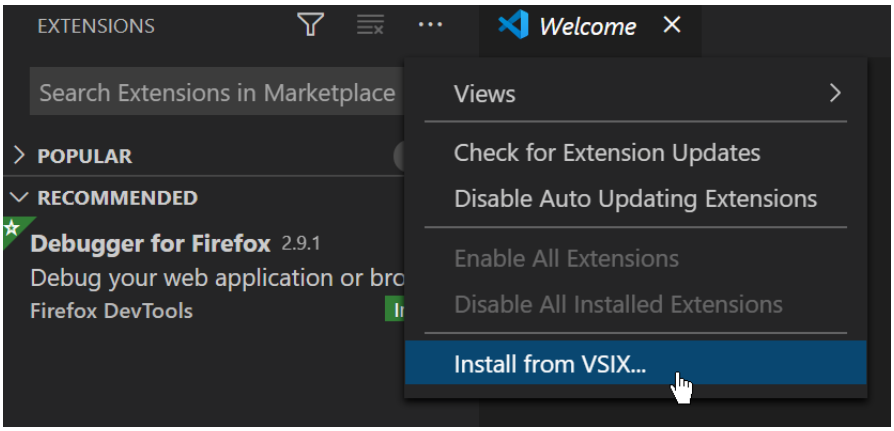
System Requirements

The same system requirements apply to the TDB Editor as to the Thermo-Calc installation but the TDB Editor is only available for Windows and Linux platforms.

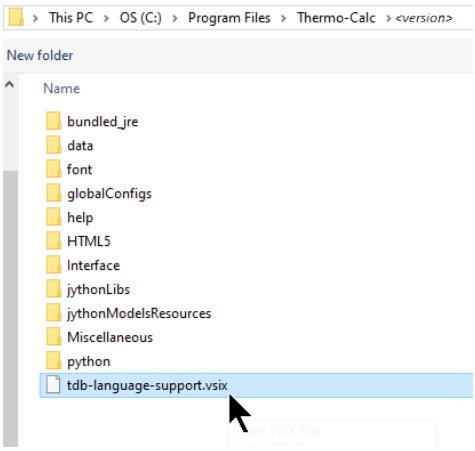
A full list of system requirements and program availability is found on the Thermo-Calc website. You can also see the roadmap for platform support to use for planning purposes.

How to Install the TDB Editor Extension

1. Install VSCode for Windows or Linux from https://code.visualstudio.com/download.
2. In VSCode, press Ctrl+Shift+X (or from the menu, select **View→Extensions**). The **Extensions** panel opens.
3. In the upper right corner of the **Extensions** panel, click the three dots (...) **Views and More Actions** button. Select **Install from VSIX**.

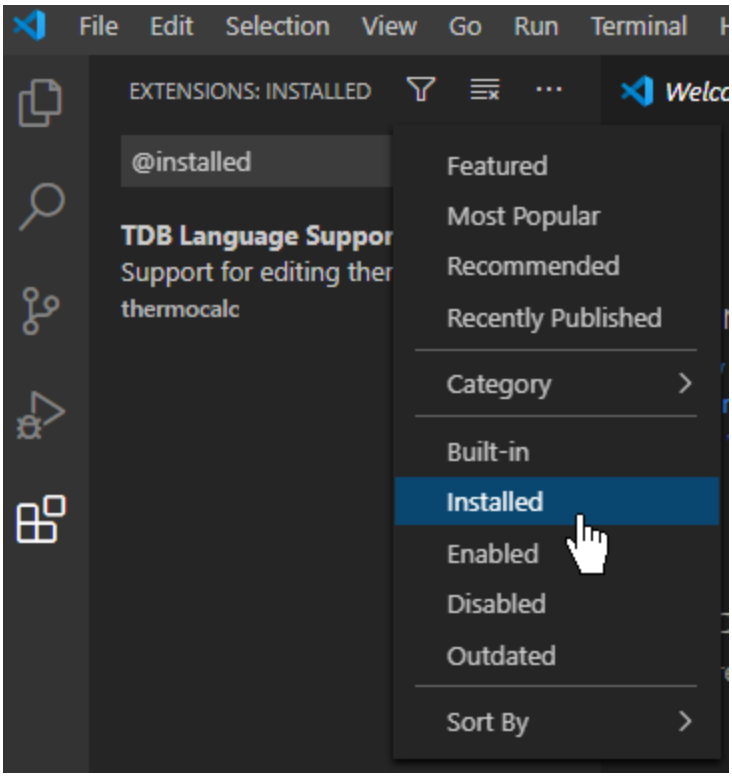


4. Navigate to the Thermo-Calc distribution directory based on your operating system. Select `tdb-language-support.vsix` and click **Install**. A message in VSCode confirms the extension is installed. If asked, confirm reloading of the interface.



   - Installation Default Directory: Windows or Installation Default Directory: Linux

5. Locate **TDB Language Support** in the Extensions panel. For example, click **Filter Extensions → Installed** and the file displays in the panel.



6. Click **TDB Language Support** to see the README file, which includes current version information, known bugs, and limitations.

READ ME Section Included with the Extension



After installing the TDB Editor, there is a READ ME section available on the front page of the extension in VSCode has the most recent information, some of which is listed below.

- The syntax checker cannot resolve references to TDB files with partial database information and gives errors in such cases. Only databases contained in single files can be handled. For syntax checking of multi-file databases, use the stand-alone Database Checker tool. See About the Database Checker.

- If you encounter warning messages that do not match the content in the TDB Editor, a possible solution is to save the file to disk (press Ctrl+S on the keyboard), which reloads the file and restarts the syntax checker.

- Very large files can sometimes cause issues with the language support functionality although the actual editing should be unaffected by this.

Using the TDB Editor

About the TDB Editor

Once you have installed the TDB Editor and are familiar with the TDB database file concept you can start working with it to edit an existing file or create a new TDB file.

How to Create a TDB File

To create a new TDB file, save an empty text file with a `.TDB` extension.

How to Open a TDB File

In VSCode, from the menu select **File→Open** and navigate to a file with a `.TDB` extension.

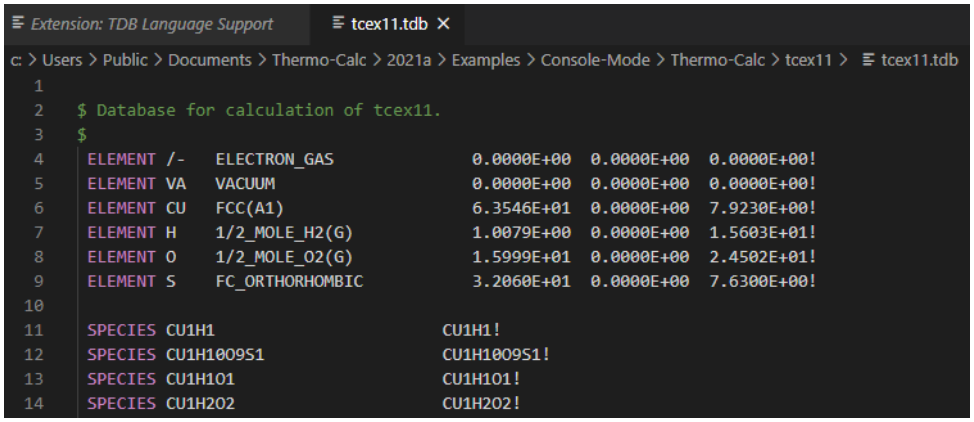
Example of Working with the TDB Editor

The following shows a couple of the features available when using an unencrypted TDB database file included with Thermo-Calc Console Mode example *tcex11 - Oxidation of Cu_2S with an H_2O/O_2 Gas Mixture*.

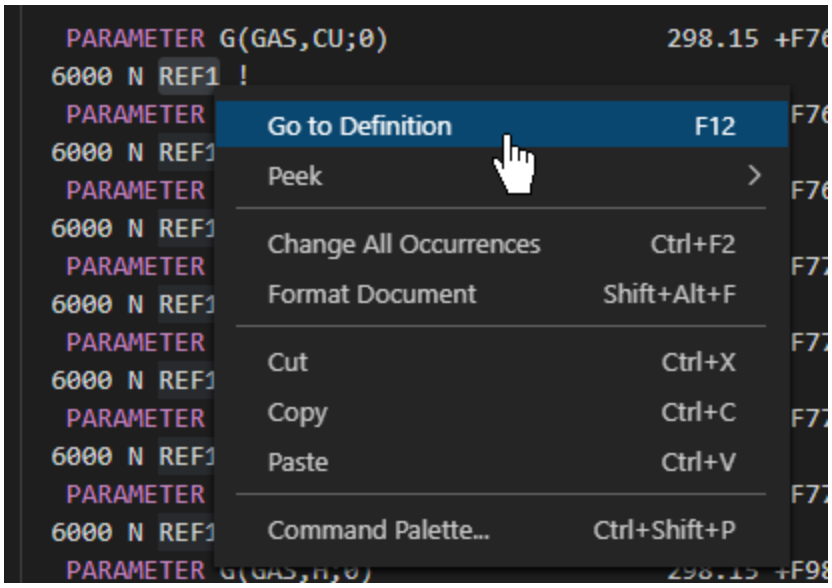
Thermo-Calc Console Mode Examples

Open a TDB file. This example uses `tcex11.TDB`, which is the user-defined database referred to from the Thermo-Calc macro file `tcex11.TCM`.

The unencrypted database opens in the TDB Editor where you can quickly see the color syntax of the commands making it easy to navigate.



Where there are definitions or references included with the file, you can also navigate quickly to these using **Go To Definition** (press F12 or right-click to select from the menu).

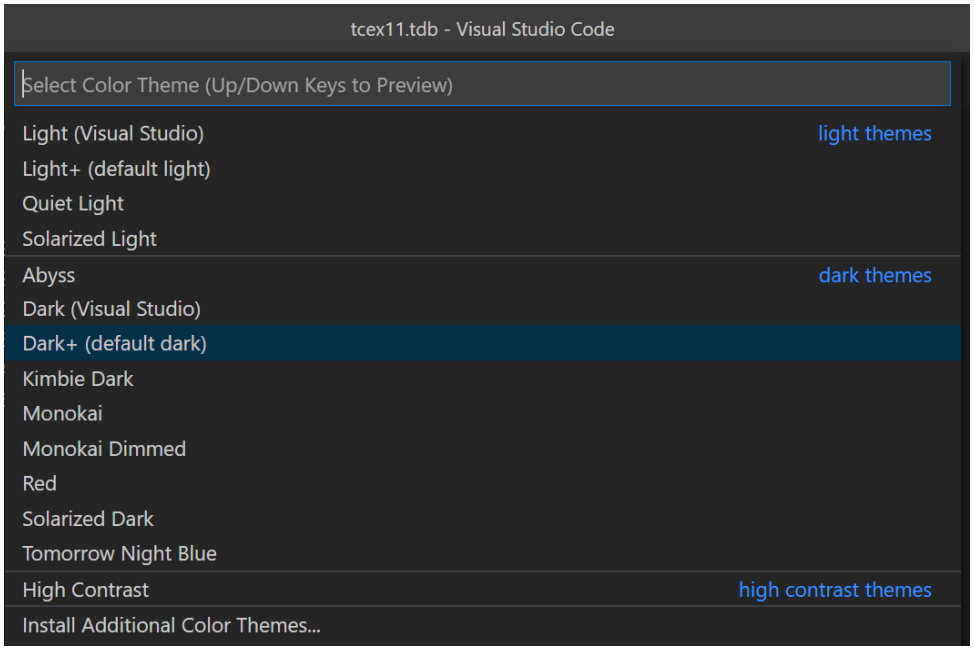


There are many other VSCode features available that you can learn more about from the Visual Studio Code Help menu. One such item of particular use is to be able to customize the color scheme.

Customize the Color

VSCode comes with a number of pre-defined color themes and additional themes can be downloaded as extensions.

To select a color theme, in VSCode press `Ctrl+K` then `Ctrl+T`.



A preview of each theme is shown. Use the arrow keys to try each and select the theme that best suits your preferences.

DATAPLOT User Guide

Thermo-Calc Version 2021b



Introduction to the DATAPLOT User Guide

In this section:

Using this Guide 3

About the DATAPLOT Graphical Language 4

Plotting Experimental Data Files 5

Using this Guide

The *DATAPLOT User Guide* gives all the details on the graphical language DATAPLOT that a phase diagram or property diagram calculated by Thermo-Calc or a kinetic profile simulated by the Diffusion Module (DICTRA) can be defined.

This guide

- Discusses the important features of the DATAPLOT language.
- Describes the commands to define PROLOGUE and DATASET.
- Several examples and the standard codes for formatting are provided.

One topic introduces the method of formatting DIGLIB symbols in LaTeX documents, for the purpose of necessarily/appropriately referring to the corresponding LaTeX symbols (closest to those DIGLIB symbols which have been plotted on a diagram using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

About the DATAPLOT Graphical Language

In order to obtain graphical output of any numerical data and informative strings, a graphical language called DATAPLOT was developed in connection with the graphical software DIGLIB. Using this graphical language, you can store information in a normal text file (*.EXP), which can be plotted as graphical symbols, lines, texts or Greek letters on any plot device support by DIGLIB.

You can generate and plot DATAPLOT (*.EXP) files together with various calculation and/or experimental results from, for example, phase and property diagrams calculated with the Thermo-Calc software composition profiles or other diagrams simulated by the Diffusion Module (DICTRA).

An EXP file automatically generated by the POST-processor (using the MAKE_EXPERIMENTAL_DATAFILE command) in the Thermo-Calc software is a DATAPLOT (*.EXP) file and may contain all types of legal DATAPLOT commands and parameters. With a text editor, you can modify or add some DATAPLOT commands and related parameters in an existing EXP file. This is useful when appending experimental information to calculated/simulated plots, and when specifying user-defined texts, symbols, colors, fonts, filled patterns, diagram types, diagram sizes, symbol/character sizes, titles, special characters, etc.



There is another type of experimental data file that is generated in Thermo-Calc when working with the PARROT module. For more information seeExperimental Data Files (*.POP, *.DOP).

DATAPLOT Examples

To help you prepare your EXP (experimental) files to use for your plotted diagrams generated by Thermo-Calc simulations, there are examples of EXP files using the DATAPLOT graphical language standard, which are normally independent of software versions.

Plotting Experimental Data Files

You can read and plot experimental data files in both Console Mode and Graphical Mode.

Graphical Mode

In Graphical Mode, the Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). This type of file has information specifying a plotted diagram, written in the DATAPLOT graphical language. From this activity node you can plot the EXP file or save a copy of the file to another location.

How to Plot an EXP file in Experimental File Reader

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the *EXP file* field, enter the name of the EXP file to plot. Or click the **Select Exp file** button to navigate to a location on the computer to add the dataset.
3. Once the .EXP file is added, under **Dataset Selection** you can choose to include or exclude specific datasets. Use the **Select/Deslect all datasets** check box as required.
4. Right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.

   If the source EXP file is changed, you can also click the **Reload the selected EXP file from disk** button to refresh the data. If you want to save or export the loaded file, click the **Save EXP file** button, then navigate to where you want to save it and give it a file name.

5. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

Console Mode

In Console Mode you use the QUICK EXPERIMENTAL PLOT command found in the POLY-3 POST module (as well as in the Diffusion Module (DICTRA) POST module) to plot the .EXP files. This command can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axes, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

How to Plot an EXP file in POST

1. Go to the POLY-3 Module: At the SYS prompt type `Go Poly`.
2. Go to the POST module: At the POLY_3 prompt type `Post`.
3. At the POST prompt, type `Quick`.
4. Enter Prologue and Dataset numbers (if applicable). See QUICK_EXPERIMENTAL_PLOT.
5. AT the POST prompt, type `Plot`.

Using DATAPLOT Graphical Language

In this section:

DATAPLOT File Structure 8
DATAPLOT Language Syntax 9
Coordinate Systems 10
Graphical Operation Codes 11
Tables or Blocks 13
Drawing a Polygon 14
Drawing an Analytical Function 15
Painting of an Enclosed Area 16
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DATAPLOT File Structure

A DATAPLOT file is a normal text file with the extension `EXP` that can be created with a text editor or by a program. The file must contain one or more `DATASETS` and possibly also one or more `PROLOGUES`. Each `PROLOGUE/DATASET` is an entity that can be individually selected for plotting.

A PROLOGUE/DATASET is identified by a unique positive number in the file. A PROLOGUE normally contains various DATASET commands for defining information about axis scaling, axis text, axis length, title and so on. A PROLOGUE is terminated by another PROLOGUE or by the first DATASET. This means that all PROLOGUES must be placed at the beginning of the file, before the first DATASET.

A DATASET normally contains DATASET commands that are associated to separate data points, as well as with one or more `BLOCKS` of data (calculated or experimental). A DATASET is terminated by another DATASET command or the end of file.

DATAPLOT Language Syntax

The DATAPLOT language consists of commands with or without parameters:

```
COMMAND {parameter(s)}
```

The basic graphical command consists of an X/Y coordinate pair and a Graphical Operation Code (GOC). With other commands, the interpretation of this basic command can be modified. There are separate commands to draw a polygon or a function and ways to get texts in different fonts.

To edit a DATAPLOT file, the graphical commands can be abbreviated.



A command (with parameters) must not exceed 80 characters. If it is too long (normally as writing necessary codes in a command's parameters for a complex expression), two or more lines can be edited.

Coordinate Systems

The DATAPLOT language accepts coordinates in three different coordinate systems, which are called *world*, *virtual* and *normalized*.

- The *world* coordinates are selected to represent any kind of data and be of “any” magnitude.
- The *virtual* coordinate system uses centimeters as units. However, the actual size of one unit is dependent on the implementation of the device driver in DIGLIB. It is not recommended to use this coordinate system if different output devices are used for preliminary and final plots.
- The *normalized* coordinate system goes from zero to one. When plotting, you interactively scale each axis by selecting the minimum and maximum word coordinates on the axis. In the normalized coordinate system, the minimum axis value is represented by zero and the maximum by one. DIGLIB draws a square between the four points (of the X and Y axes) that are determined by the coordinates zero and one in the normalized coordinates.



It is also possible to draw triangular plots as described below. However, in most places, it only references square diagrams. All data points within the minimum and maximum word coordinates are plotted inside this square. DIGLIB also writes tic marks and corresponding word values at such tic marks.

It may be convenient to use normalized coordinates to draw boxes and texts. You can give normalized coordinates outside zero and one if you want to write texts outside the area enclosed by the square. To ensure proper operation outside the normalized box, the clipping must be turned off.

Graphical Operation Codes

The Graphical Operation Code (GOC) determines how the coordinates are interpreted and what is done at the point determined by the coordinates. For an individual data point, its GOC codes must be given. For each data BLOCK, you define a default GOC that is used for the whole BLOCK, unless a GOC is explicitly defined for a specific point.

- If S is omitted, no symbol is plotted. A number selecting the symbol can optionally follow the character S. The DIGLIB software determines which symbol the number represents. See Plotting a Symbol.
- If any of the other characters are omitted, the default defined for the BLOCK is used. Absolute values imply the current coordinates; relative values mean that these are added to the current coordinates. The GOC must be written without any space between various characters, but the order for the characters is irrelevant.
- If no GOC is defined for a BLOCK, the system default is MWA, (Move Word Absolute), i.e., move to the given point that is interpreted as absolute word coordinates. GOC=DNA means draw a line from the current point to the new one interpreting the coordinates as normalized. After each draw or move operation, the so-called current point is the new point.
- The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor. To get PostScript outputs, the TEXT must be edited by the LaTeX Text Formatting Program instead (see LaTeX Formatting Codes).

GOC Character Definitions

The GOC is a combination of the following characters:

Character	Meaning
W, V or N	To use word (W), virtual (V) or normalized (N) coordinates. W is the default.
A or R	XY are absolute (A) or relative (R) values. A is the default.
M or D	To perform a move (M) or draw (D) operation to XY. M is the default.
B	To apply "soft" splines on a line drawn between the coordinate pairs (used only on BLOCK data).
S	To plot default symbol at XY.

Character	Meaning
S#	To change default symbol to No # symbol and plot it at XY.
'TEXT	To plot TEXT at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

Tables or Blocks

In many cases, you have (calculated or experimental) data in the form of tables, and want to plot one or several columns as X-axis and one or more columns as Y-axis. A single table can contain many sets of data records of the same kind of information for a specific data BLOCK. There can be many data BLOCKS in a DATASET.

By enclosing these tables in a data BLOCK, you can select which column(s) is the X-axis and which is the Y-axis. For example,

```
BLOCK X=C1; Y1=C3; Y2=C2; GOC=C4,DAW
```

Where the X-axis values are in column 1, the Y-axis values are in columns 2 and 3, and any GOC codes are in column 4. The default GOC for this BLOCK is Draw Absolute Word. The GOC code inside the table is only necessary if the default GOC is not applicable.

A more elaborate use of the table is shown in this example:

```
BLOCK X=C3; Y=1E3/(C3+273); GOC=C8,MAWS1
```

Where the X-axis values are in column 3, the Y-axis values are in column 1 with some additional calculations applied. Any GOC is in column 8, and the default GOC is Move Absolute Word and plot the symbol no. 1.

Columns in a table must be separated by one or more space characters and do not have to be justified.

It is possible to have tables with mixed text and numbers, but each word followed by a space is counted as one column. The columns used for plotting also must be numerical. An example of a legal line in a table is

```
298.15 This_is_the_second_column 11.5 This_is_the_fourth_column
```



A line in the table must not exceed 80 characters. A BLOCK must be terminated by a line with the BLOCKEND command.

Drawing a Polygon

Normally, each point is written on a separate line. But in order to draw a line in a more compact way, use the command DRAWLINE. DRAWLINE is followed by a couple of X/Y number pairs. The X/Y pairs must be separated by a space, and there must be a comma sign between the X and Y values. DRAWLINE makes a move operation to the first pair of X/Y coordinates, and then draws a line among all pairs up to the last one. All pairs must fit on one line of 80 characters, but there can be several consequent DRAWLINE commands.



Example 2 – Draw Polygons and Symbols

Drawing an Analytical Function

Use a BLOCK command to set an axis to a function. It is not necessary to use a value from any column in order to compute the function value to be plotted. Use the FUNCTION command to plot a function with an even increment of the independent variable.



Example 4 – Draw Curves Defined by Functions

Painting of an Enclosed Area

Use the PAINT command to paint or fill an area in a specified pattern in the plot. Available patterns are determined by the DIGLIB software. A related command to PAINT is PCFUNCTION.

Writing a Text

Use the TEXT command to write a text at the current point. You can write a text at any X/Y pair by appending a single quote followed by the text on the same line. For example:

```
1.1 1.0 NAM'This is a text
```

writes `This is a text` at the normalized coordinates (`1.1, 1.0`).

Use the command FONT to select the font used for the text, and CHARSIZE to select the size of the characters. Set this size of the symbols with SYMBOLSIZE.

If a text or a single character should be of a different font than all the other text, or to use subscripts or superscripts in a text, use the ^ operators or STRING command to create the text. The command STRING stores the text in a specified variable that includes all text-formatting information defined by the DIGLIB software.



Example 3 – Using Strings and Various Line Types and Example 5 – Use Included Files for Predefined Symbols.

However, if a graphical output is done on a PostScript device using the PostScript hardcopy fonts, special text formatting codes as LaTeX Formatting Codes should be used and the STRING formatting syntax is then not valid.

Plotting a Symbol

As described in Graphical Operation Codes, a GOC code in a data BLOCK may contain an `S` option to plot a symbol for an X/Y pair or the same symbols for the data BLOCK. A number selecting the symbol can optionally follow the character `S`. You can plot a symbol at any current X/Y position by appending a quote specified by the symbol number in the GOC code (e.g., `1.1 1.0 MANS5'This is a text`).

You can also insert DIGLIB symbols into LaTeX-edited documents.



Example 1 – Draw Lines and Symbols, Example 2 – Draw Polygons and Symbols and Example 8 - DIGLIB Symbols

Other Commands

General

- When plotting symbols representing various experimental data, it is important that the symbols are centered around the coordinate values.
- The dollar sign $ as the first character of a line stands for a comment character, which means the whole line is ignored when plotting.

ATTRIBUTE

Use the ATTRIBUTE command to change the coordinates where text is displayed. The default is the lower left corner of the first character in the text.

CLIP

Use the CLIP command to change the default where all data outside the normalized coordinates zero and one are not plotted.

COLOR

If you are using a color device, use the COLOR command to change color of the lines. On some black and white devices, colors are simulated with different width and dashing of the lines.

INCLUDE

Use the INCLUDE command to create libraries with texts and include these in similar plots.

LINETYPE

Use the LINETYPE command to define line types as solid, long dashed, short dashed or dotted.

Interactive Plotting

The DATAPLOT file is read into the POST module in the workspace with APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT. These commands ask for the name of the DATAPLOT file and also which PROLOGUE(S) and DATASET(S) are to be plotted.



Press F1 and search the Help for details.

By giving the PROLOGUE/DATASET number as `-1`, you get a list of the available PROLOGUES/DATASETS in the file. Note that if `DATASET 0` is in a DATAPLOT file, its data is always used even if other DATASETS are chosen.

Formatting DIGLAB Symbols in LaTeX Documents

When using the LaTeX editor, you can use the DIGLIB symbols in texts and in figures. This then refers to the corresponding LaTeX symbols (closest to those DIGLIB symbols which are plotted on a plot using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

This topic shows how to generate some DIGLIB symbols in texts, through the attached LaTeX source file and its converted jpg file.

 Example 8 - DIGLIB Symbols

DIGLIB_Sym.tex

```
\documentclass[dvips,12pt]{article}
\textwidth 165mm
\textheight 225mm
\oddsidemargin 1mm
\evensidemargin 1mm
\topmargin 1mm
%%\usepackage{amssymb}
%% next replace amssymb and to get udtimes
\usepackage[utopia]{mathdesign}
\usepackage{rotating}
\usepackage[latin1]{inputenc}
\usepackage{graphics}
\usepackage{graphicx,subfigure}% with figures
%\usepackage[draft]{graphicx}% without figures
\usepackage{subfigure}% with figures
\topmargin 1mm
\oddsidemargin 1mm
\evensidemargin 1mm
\begin{document}
{\Large \bf Diglib symbols and their corresponding LaTeX symbols}
\vspace{5mm}
```

The information below gives the closest corresponding LaTeX symbol. All symbols (except +) must be generated in math mode. Most of these require the package `amssymb`, i.e., you need a directive `usepackage{amssymb}` in the preamble. Two of the symbols require the more extensive `mathdesign` that can be included with `usepackage[utopia]{mathdesign}`.

```
\vspace{5mm}
{\Large
\begin{tabular}{llll}
Diglib & Latex & Latex name & Note\\
1& $\vartriangle$& $\backslash$vartriangle & amssymb \\
2& $\square$& $\backslash$square\\
3& {\Huge $\diamond$} & $\backslash$diamond & size $\backslash$Large \\
4& $\udtimes$& $\backslash$udtimes & mathdesign \\
5& $\triangledown$& $\backslash$triangledown & amssymb\\ 6 & +& normal + \\
7& $\ast$& $\backslash$ast & amssymb\\
8& $\times$& $\backslash$times \\
9& {\Huge $\circ$}& $\backslash$circ & size $\backslash$Large \\
10& {\Huge $\star$}& $\backslash$star & size $\backslash$Large, amssymb\\
11& $\curlyvee$& $\backslash$curlyvee & amssymb\\
12& $\Join$& $\backslash$Join\\
13&& - & nothing similar, overlapping $> <$\\
14&& - & nothing similar, 10-edged star \\
15& $\maltese$& $\backslash$maltese& mathdesign \\
16&& - & nothing similar, a pentagon \\
17& $\curlywedge$& $\backslash$curlywedge & amssymb\\
\end{tabular}}
\end{document}
```

LaTeX Formatting Codes



For a list of supported LaTeX commands, see: http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html.



By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.



As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

LTEXT vs LaTeX Commands for Labels

Symbol or text format	LTEXT	LaTeX
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al^DO2O^DO3	S-A-TEXT Y N \latex Mole-fraction Al_2O_3
Label with subscript	add .13 .15 n c-ZrO^DO2$	add .13 .15 n \latex c-ZrO_2
Greek symbol	ADD .05 .50 N ^GRd$	ADD .05 .50 N \latex \delta

PROLOGUE Commands

In this section:

PROLOG 25
DIAGRAM_TYPE 26
TIC_TYPE 27
TITLE 28
XLENGTH 29
XSCALE 30
XTEXT 31
XTYPE 32
YLENGTH 33
YSCALE 34
YTEXT 35
YTYPE 36

PROLOG

PROLOG is the beginning of a number of consequent lines of user-defined diagram layout commands. The lines are displayed with the `optional text` when using the `-1` option in the POST-processor as prompted for the PROLOG number with APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT.



Examples of DATAPLOT Files and Outputs

Syntax	`PROLOGUE # optional text`
	`#` is an unsigned integer identifying the PROLOG.

DIAGRAM_TYPE

DIAGRAM_TYPE sets the diagram type to square (the default) or triangular.

 Example 6 – Triangular Diagrams for Ternary Systems

Syntax	`DIAGRAM_TYPE type plot_3rd_axis clip_along_third-axis`
	`type` is a character string reading SQUARE (default) or TRIANGULAR. If `type` reads TRIANGULAR, then two additional parameters are given: `plot_3rd_axis` and `clip_along_third-axis` that are characters strings reading YES or NO.

TIC_TYPE

TIC_TYPE sets the relative length of the tic marks.

Syntax	`TIC_TYPE #`
	`#` is a real number. Default value is 1. Negative number gives tics on the inside of the diagram frame. 0 gives no tics.

TITLE

TITLE sets the title text string to be printed above the diagram.

Syntax	`TITLE text`
	`text` is an arbitrary text string that may contain text-formatting codes

XLENGTH

XLENGTH sets the X-axis length to approximately # centimeters.

Syntax	`XLENGTH #`
	`#` is a positive real number (the approximate X-axis length in centimeters).

XSCALE

XSCALE sets the scaling in word coordinates of the X-axis.

Syntax	`XSCALE min max`
	`min` and `max` are real numbers.

XTEXT

XTEXT sets the X-axis text.

Syntax	`XTEXT text`
	`text` is an arbitrary text string that may contain text-formatting codes.

XTYPE

XTYPE sets the X-axis type as linear (default), logarithmic or inverse.

Syntax	`XTYPE type`
	`type` is a character string reading LIN, LOG or INV.

YLENGTH

YLENGTH sets the Y-axis length to approximately # centimeters.

Syntax	`Y LENGTH #`
	`#` is a positive real number (the approximate Y-axis length in centimeters).

YSCALE

YSCALE sets the scaling in word coordinates of the Y-axis.

Syntax	`YSCALE min max`
	`min` and `max` are real numbers.

YTEXT

YTEXT sets the Y-axis text.

Syntax	`Y TEXT text`
	`text` is an arbitrary text string that may contain text-formatting codes.

YTYPE

YTYPE sets the Y-axis type as linear (default), logarithmic or inverse.

Syntax	`Y TYPE type`
	`type` is a character string reading LIN, LOG or INV.

DATASET Commands

In this section:

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BLOCK 39

BLOCKEND 40

CHARSIZE 41

CLIP 42

COLOR 43

DATASET 45

DATAPOINT 46

DRAWLINE 47

FONT 48

FUNCTION 49

GLOBALSIZE 50

INCLUDE 51

LINETYPE 52

PAINT 53

PCFUNCTION 54

SYMBOLSIZE 55

STRING 56

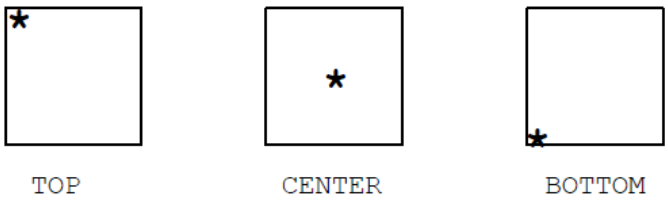
TEXT 58

ATTRIBUTE

ATTRIBUTE specifies where the current XY position is in the character or symbol plotbox.

Example 2 – Draw Polygons and Symbols, Example 3 – Using Strings and Various Line Types, and Example 5 – Use Included Files for Predefined Symbols

Syntax	ATTRIBUTE
Prompts	`attribute`
	`attribute` may be TOP, CENTER or BOTTOM. ATTRIBUTE CENTER is default for symbols; ATTRIBUTE BOTTOM is default for characters.



BLOCK

BLOCK defines how the following numeric data block shall be interpreted. The definitions of X and Y coordinates may also be expressed as a function of the column values, making it possible to perform transformations.

Syntax	`BLOCK X&=C#; ...; Y&=C#; ...; GOC=C#,@@@...`
	`&'` are optional unsigned integers that make it possible to plot several (maximum 9) X- or Y- axis columns. `#'` are unsigned integers identifying the column numbers. The column number # in "GOC=C#" is the location of any possible GOC codes in the current data BLOCK; @@@ stands for the default Graphical Operation Code (GOC) for the current BLOCK. The GOC code inside the current table is only necessary if the current default GOC is not applicable.

GOC Characters

The GOC is a combination of the following characters:

Character	Meaning
`W`, `V` or `N`	To use word (`W`), virtual (`V`) or normalized (`N`) coordinates. `W` is the default.
`A` or `R`	XY are absolute (A) or relative (R) values. `A` is the default.
`M` or `D`	To perform a move (M) or draw (D) operation to XY. `M` is the default.
`B`	To apply "soft" splines on a line drawn between the coordinate pairs (used only on BLOCK data).
`S`	To plot default symbol at XY.
`S#`	To change default symbol to No # symbol and plot it at XY.
`'TEXT`	To plot `TEXT` at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

BLOCKEND

Use BLOCKEND to terminate the local definition of the graphical operation code defined by the earlier BLOCK command.

CHARSIZE

CHARSIZE redefines the default size of the characters in the plot. The character size has an initial default value, which may vary with the current font setting and the output device (the plot format).



Examples of DATAPLOT Files and Outputs

Syntax	`CHARSIZE $$`
	`$$` must be an unsigned real.

CLIP

CLIP turns clipping on or off. If it is OFF, it allows output outside the ordinary plot area defined by normalized coordinates zero and one.

 Example 2 – Draw Polygons and Symbols and Example 9 - DIGLIB Fonts and Lines

Syntax	`CLIP CLP`
	`clp` is a character string reading ON or OFF.

COLOR

Use COLOR to redefine the current color setting. There are 22 legal color codes (from 0 to 21).



Example 7 – Color Codes

Syntax	`COLOR code`
	`code` is an unsigned integer number (from 0 to 21) identifying the color, or a character string specifying the color.

DIGLIB Color Codes

Code	Color	Equivalent Character
0	Background	Invisible
1	Black	Normal
2	Red	Very_Thick
3	Green	Thin
4	Blue	Thick
5	Yellow	Very_Thin
6	Magenta	Dashed
7	Cyan	Dotted
8	Purple	
9	Gold	
10	Turquoise	
11	Pink	
12	Gray	
13	Orange-red	

Code	Color	Equivalent Character
14	Maroon	
15	Plum	
16	Sea green	
17	Olive	
18	Sienna	
19	Orange	
20	Coral	
21	UserDef	
22 and higher	Any digit larger than 21 has the color effect as 1 (black).	

DATASET

DATASET indicates the beginning of a number of consequent lines comprising a set of user-defined data. The DATASET lines are displayed on the terminal along with the `optional text` when using the `-1` option in the POST-processor as prompted for the DATASET number in the APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT command.

Syntax	`DATASET # optional text`
	`#` is an unsigned integer identifying this set of data.

DATAPOINT

DATAPOINT is not a DATASET command, but the basic DATAPLOT command (see synopsis below) performs an action at the current point determined by the specified X/Y-coordinates. A DATASET may contain various data points, in addition to one or more data BLOCKs. Such data points are separated and independent on each other.

Syntax	`X Y GOC`

	X and Y are unsigned real numbers identifying the X/Y-coordinates for the current data point. GOC stands for Graphical Operation Code (GOC) for the current point. Legal GOC characters.
	Example
	`0.7 0.95 N'Example 6`
	`0.5 0.08 MNA'E^FS18^SQ(^SK^FS10A+5#8*C#^FS10 -!a^FS18)^FS11+B^DIa#b#$`

DRAWLINE

DRAWLINE draws a line starting at (x1,y1) to (xn,yn) through (x2,y2) → (x(n-1), y(n-1)).



Example 1 – Draw Lines and Symbols and Example 2 – Draw Polygons and Symbols

Syntax	`DRAWLINE x1,y1 x2,y2 .... xn,yn`
	`x` and `y` may be reals or integers of any value. This is the same as connecting all points in a table:

```
x1   y1    M
x2   y2    D
...  ...   D
xn   yn    D
```

FONT

FONT redefines the default font setting in the POST-processor.

 Example 9 - DIGLIB Fonts and Lines

Syntax	`FONT #`
	`#` is an unsigned integer.

Font Numbers

Number	Font
1	Bold
2	Normal
3	Italic
5	Bold and Italic
10	Monotype Normal
11	Monotype Italic
12	Monotype Bold
13	Monotype Bold and Italic
14	Narrow Normal
15	Narrow Italic

FUNCTION

FUNCTION defines and plots a user-defined function.



Example 4 – Draw Curves Defined by Functions

Syntax	`FUNCTION Y=f(X); start end number_of_XY_pairs; GOC;` `FUNCTION X=f(Y); start end number_of_XY_pairs; GOC;`
	`f(X)` or `f(Y)` are legal mathematical functions of X or Y, understandable by a FORTRAN program. `start` and `end` are unsigned real numbers, and `number_of_XY_pairs` an unsigned integer. `GOC` is a legal graphical operation code as defined with BLOCK.

GLOBALSIZE

GLOBALSIZE redefines the default global size of the plot. The global size has an initial default value.

Syntax	`GLOBALSIZE $$`
	`$$` must be an unsigned real.

INCLUDE

INCLUDE adds a file into the current input stream.

 Example 5 – Use Included Files for Predefined Symbols.

Syntax	`INCLUDE filename`
	`filename` is a legal filename (with its correct path) for the operation system.

LINETYPE

LINETYPE redefines the current linetype in the plot.



Example 3 – Using Strings and Various Line Types, Example 8 - DIGLIB Symbols and Example 9 - DIGLIB Fonts and Lines

Syntax	`LINETYPE #`
	`#` must be an unsigned integer. Legal linetypes are (for both normal graphical outputs and for PostScript formats): • Solid (default) • Long dashed • Short dashed • Dotted

Line Types

Number	Type
1	Straight line
2	Dashed line
3	Dotted line
4	Dash-Dot line

PAINT

PAINT paints the area enclosed by the current path in the current pattern. The current path starts at the last MOVETO given and includes all subsequent DRAWs. This command only works for the PostScript format (as graphical files or on printed hardcopy).

PCFUNCTION

Syntax	`PAINT <code> <video> <mode>`
	<> denotes optional parameters. To set a new current pattern, supply any or all of the optional parameters. • `<code>` is a single letter 0-9, A-Z or a-t (if `<code>=t`, also supply a space and a number in the range 0.00-1.00). The default is `0`. • `<video>` is a string reading NORMAL (the default) or INVERSE. • `<mode>` is a string reading TRANSPARENT (the default) or OPAQUE.

PCFUNCTION

PCFUNCTION appends a user-defined function to the current path. It is used with PAINT.

Syntax	`PCFUNCTION Y=f(X); start end number_of_XY_pairs; GOC;` `PCFUNCTION X=f(Y); start end number_of_XY_pairs; GOC;`
	`f(X)` or `f(Y)` are legal mathematical functions of X or Y, understandable by a FORTRAN program. `start` and `end` are unsigned real numbers, and `number_of_XY_pairs` an unsigned integer. `GOC` is a legal graphical operation code as defined with BLOCK.

SYMBOLSIZE

SYMBOLSIZE redefines the current symbol size setting. The symbol size has an initial default value.



Example 3 – Using Strings and Various Line Types, Example 7 – Color Codes and Example 8 - DIGLIB Symbols

Syntax	`SYMBOLSIZE $$`
	`$$` must be an unsigned real.

STRING

STRING defines a string containing a text and operation codes (e.g., to change the default font settings).



Example 3 – Using Strings and Various Line Types and Example 5 – Use Included Files for Predefined Symbols

Syntax	`STRING name text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N`
	`name` is a valid alphanumeric name (variable) to represent the text including all text formatting codes. It is highly recommended that all the characters in the name are in CAPITAL CASE (e.g. ACA2SO4); otherwise, the defined STRING can be incorrectly plotted. `text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N` means the text is coded with each of its characters (and/or numeric numbers) that are formatted with various operators (`^S#`, `^G`, `^F#`, `^U#`, `^D#`, `^R#`, `^L#` and/or `^N`). `#'` are unsigned integers. `^` is the caret character and does not mean a control character. Between an `#` (in an operator) and a numeric number (as a part of the text), there must always be a comma sign (`,`) or the number is not plotted in the text, because the `#` with the number is interpreted as another incorrect #. In some of the commands, `#=0` resets the option to previous (or default) value.

String Operation Codes in the DIGLIB Software

For the PostScript hardcopy fonts, these operation codes are not valid; see LaTeX Formatting Codes:

Operator	Operation
`^S#`	Set character size to size #
`^G`	Set font to Greek
`^F#`	Set font to font number #
`^U#`	Move up # units
`^D#`	Move down # units
`^R#`	Move right # units
`^L#`	Move left # units

Operator	Operation
^N	Do not move, remain at current

Examples

```
STRING Alpha1 ^Ga^F0^D0^S8,1^S0^U0
```

is set to α_1

```
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
```

is set to $M_{23}C_6$

```
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0
```

is set to Ca_2CO_3

TEXT

TEXT outputs, at the current position, the text following the keyword TEXT or the text in the string `string_name` that is defined with STRING.

Syntax	`TEXT text` or `~string_name`
	It is possible to mix ^ operators and previously defined string names using the ~ operator.

Examples of DATAPLOT Files and Outputs

Once your Thermo-Calc software is installed you can open the Examples and PDF documentation (*Manuals*) from the main menu:

- To open the Manuals folder select **Help → Manuals Folder**. Note for Linux openSUSE users: This link is not functional. To access the folder, navigate to the default location based on your installation type
- To open the Examples based on whether you are in Console Mode or Graphical Mode, select **File → Examples Files** or **Help → Examples Files**.

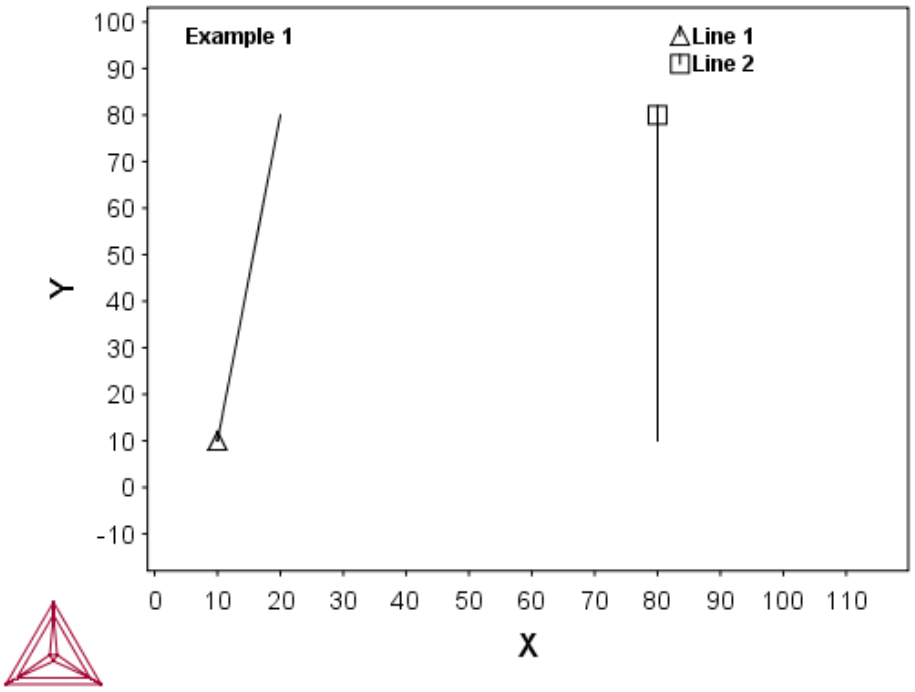
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Example 1 – Draw Lines and Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 1 - Draw Lines and Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

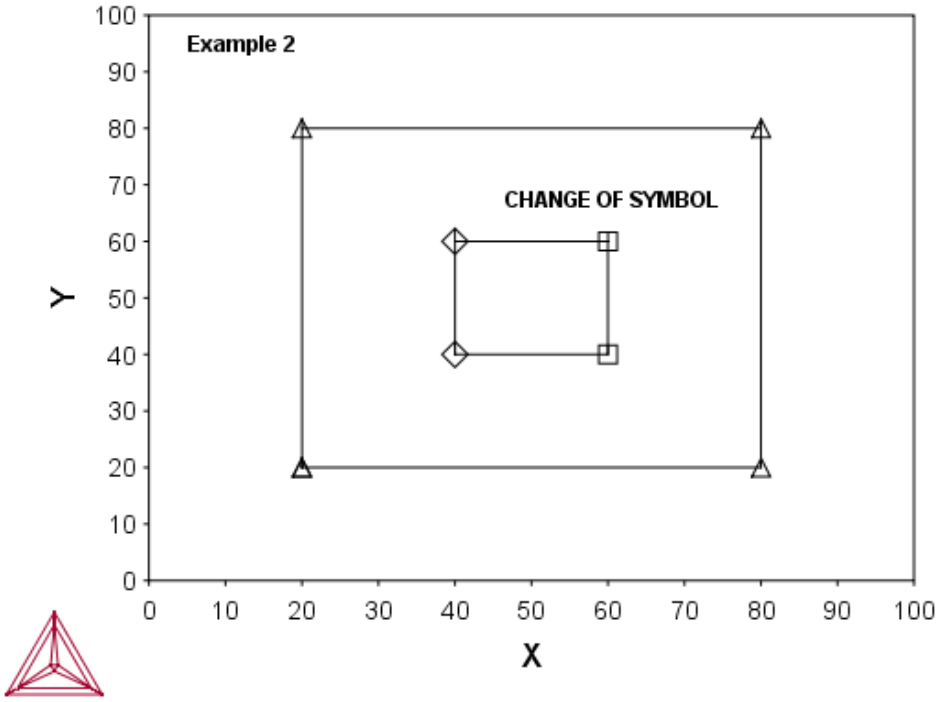
```
DATAPLOT Example 1
PROLOG 1 EXAMPLE 1 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 1
XTEXT X
```

```
YTEXT Y
DATASET 1 Two lines started with two symbols
ATTRIBUTE CENTER
0.05 0.95 N'Example 1
0.7 0.95 NS'Line 1
0.7 0.90 NS2'Line 2
10 10 S1
20 80 D
80 80 S2
80 10 D
50 60
```

Example 2 – Draw Polygons and Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 2 - Draw Polygons and Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

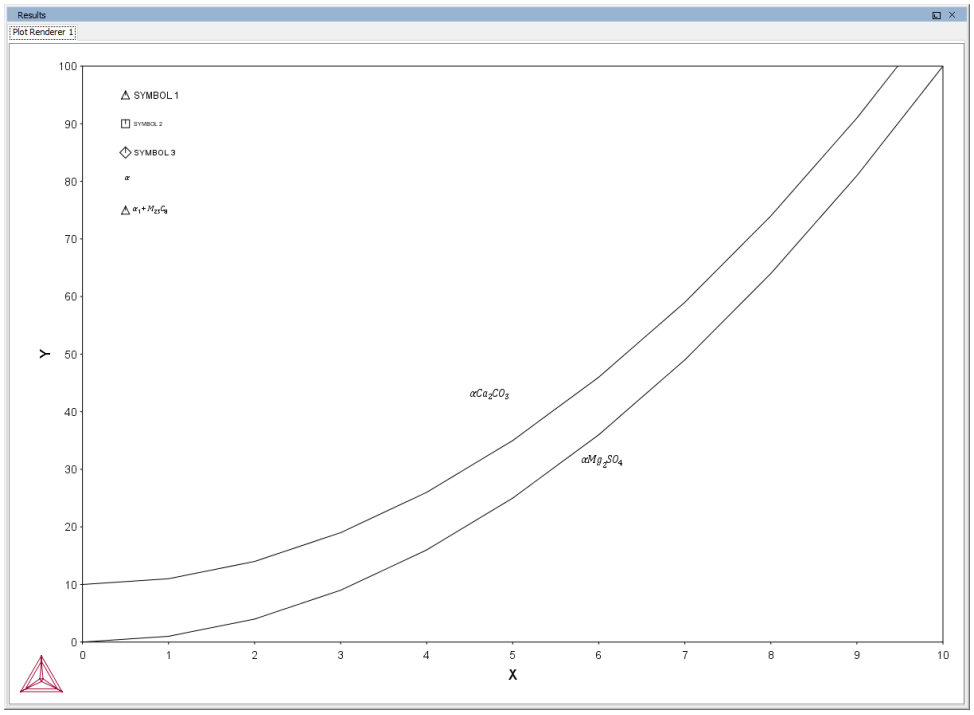
```
$DATAPLOT Example 2
PROLOG 2 EXAMPLE 2 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 2
XTEXT X
```

```
YTEXT Y
DATASET 2 Two ploygons with three types of symbols
ATTRIBUTE CENTER
CLIP OFF
0.05 0.95 N'Example 2
1.1 0.95 NS1'SYMBOL 1
1.1 0.90 NS2'SYMBOL 2
1.1 0.85 NS3'SYMBOL 3
BLOCK X=C1; Y=C2; GOC=C3,DSWA
40 40 M
40 60
60 60 S2'CHANGE OF SYMBOL
60 40
40 40 S0
BLOCKEND
BLOCK X=C1*100; Y=C2*100; GOC=C3,DSWA
0.2 0.2 MS1
0.2 0.8
0.8 0.8
0.8 0.2
0.2 0.2
BLOCKEND
$Draw an additional polygon:
DRAWLINE 20,10 30,15 40,30 50,80
DRAWLINE 50,80 60,60 90,30
```

Example 3 – Using Strings and Various Line Types

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 3 - Using String and Line Types.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 3
PROLOG 3 EXAMPLE 3 0<X<10, 0<Y<100
XSCALE 0.00000 10
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 3
XTEXT X
YTEXT Y
```

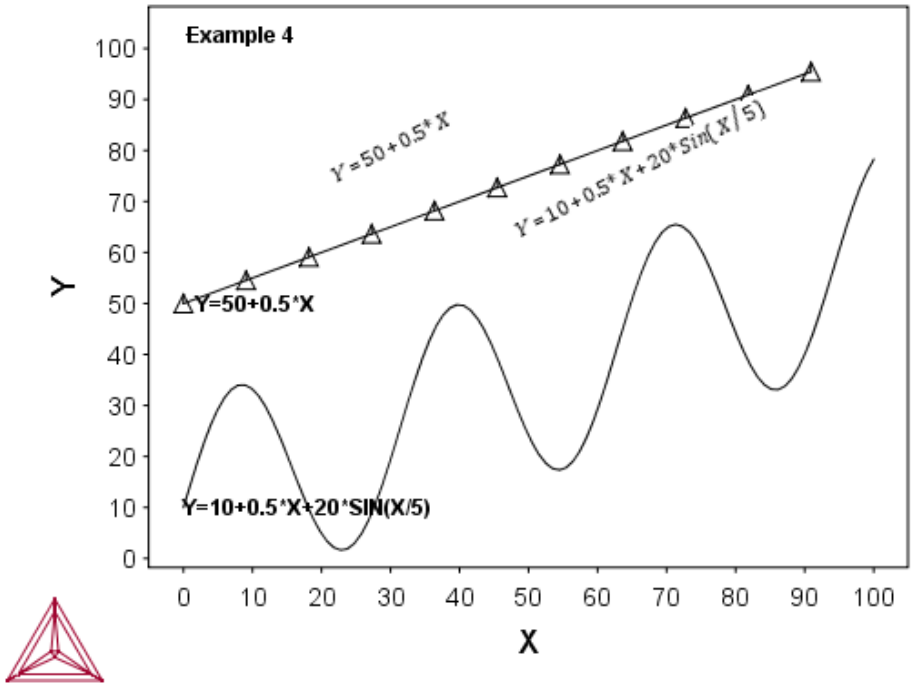
```
DATASET 3 Draw curves; plot formatted texts and symbols
$Define some strings:
STRING BCC \latex \alpha
STRING BCC1 \latex \alpha_1 + M_23C_8
STRING M23C6 M_23C_6
STRING ACA2CO3 \latex \alpha Ca_2CO_3
STRING AMG2SO4 \latex \alpha Mg_2SO_4
ATTRIBUTE CENTER
CLIP OFF
FONT 2
0.05 0.95 NS1'SYMBOL 1
CHARSIZE 0.2
0.05 0.90 NS2' SYMBOL 2
CHARSIZE 0.3
0.05 0.85 NS3'SYMBOL 3
0.05 0.80 N' ~BCC
0.05 0.75 NS1'~BCC1
SYMBOLSIZE 0.4
CHARSIZE 0.4
0.45 0.42 N'~ACA2CO3
0.58 0.30 N'~AMG2SO4
CLIP ON
LINETYPE 1
BLOCK X=C1; Y=C1*C1; GOC=C2, DWA
0 M
1
2
3
4
5
6
7
8
9
10
```

```
BLOCKEND
LINETYPE 2
BLOCK X=C1; Y=C1*C1+10; GOC=C2, DWA
0 M
1
2
3
4
5
6
7
8
9
10
BLOCKEND
```

Example 4 – Draw Curves Defined by Functions

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 4 - Curves and Functions.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 4
PROLOG 4 EXAMPLE 4 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 4
XTEXT X
```

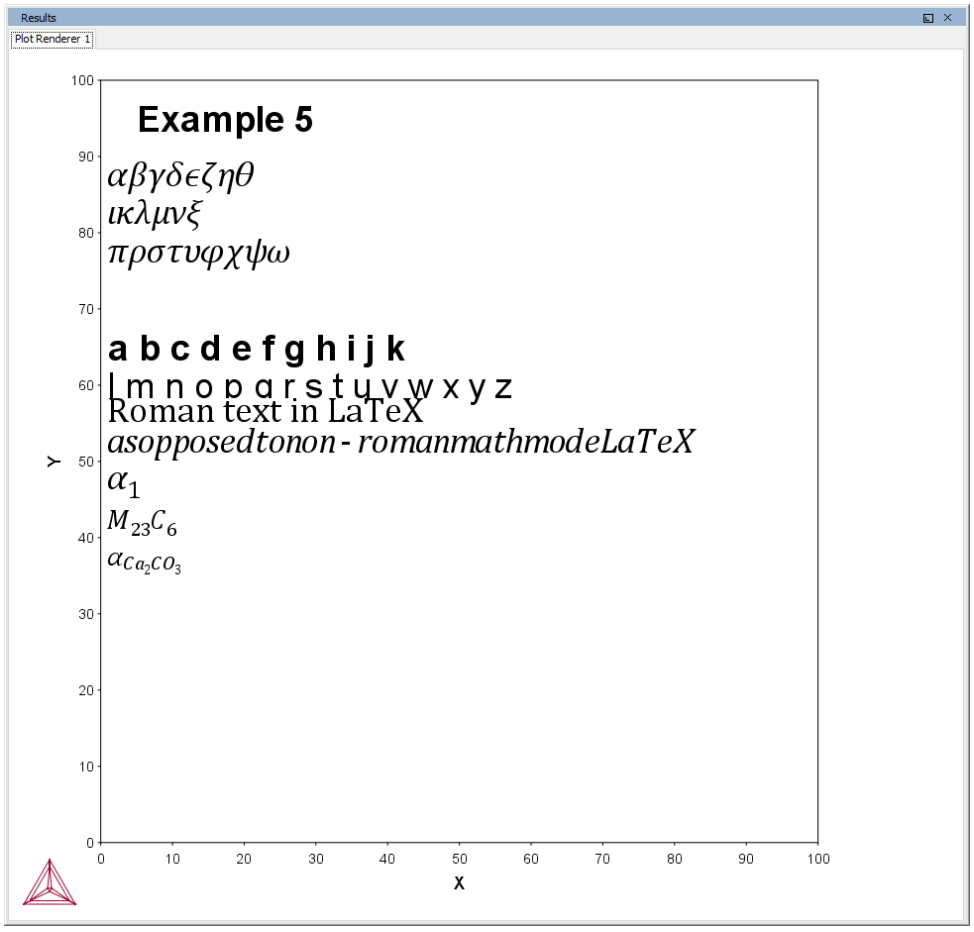
```
YTEXT Y
DATASET 4 Plot two functions as lines:
ATTRIBUTE CENTER
0.05 0.95 N'Example 4
$ Draw two lines defined by FUNCTIONS:
FUNCTION Y=10+0.5*X+20*Sin(X/5); 0 100 100; DWA;
FUNCTION Y=50+0.5*X; 0 100 10; DS1WA;
$ Write functions beside the lines:
$ Note the real rotation angle (27 degree) can be seen
$ only on the PostScript hardcopy
0.25 0.68 N'^RO27Y=50+0.5*X
0.25 0.45 N'^RO27Y=10+0.5*X+20*Sin(X/5)
```

Example 5 – Use Included Files for Predefined Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 5 - Predefined Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example

In the plot result, the hard-to-read LaTeX line is intended to highlight how to type readable text using LaTeX.



Macro Text

```
$DATAPLOT Example 5 Symbols
```

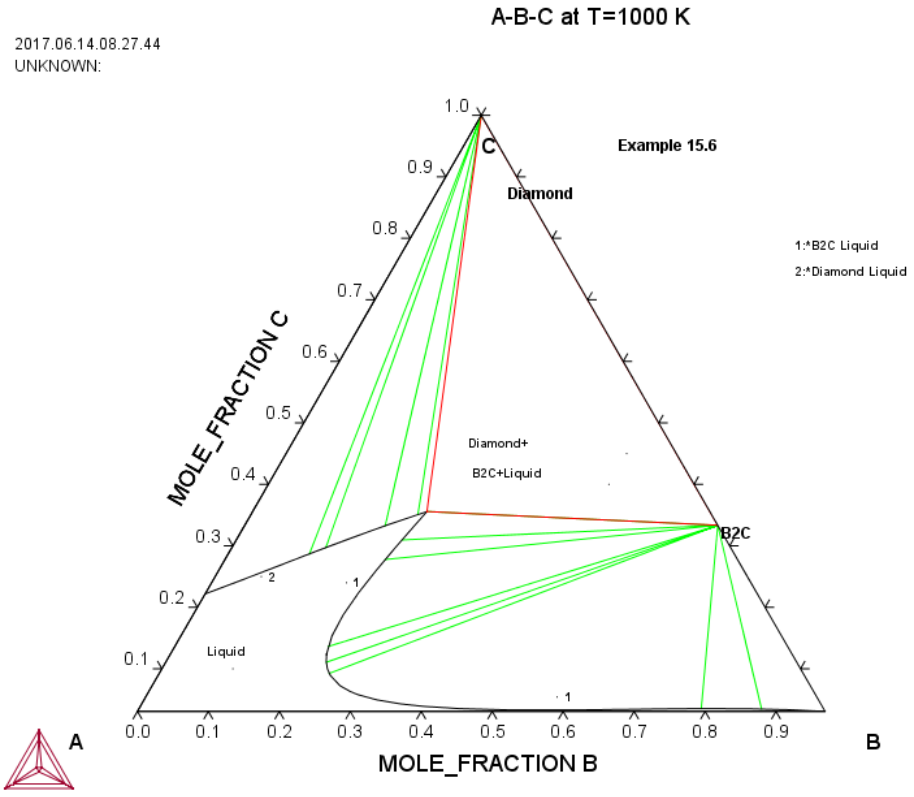
```
PROLOG 5 EXAMPLE 5 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 5
XTEXT X
YTEXT Y
DATASET 5 Write equations and strings with different properties
STRING TEST1A \latex \alpha \beta \gamma \delta \epsilon \zeta \eta \theta
STRING TEST1B \latex \iota \kappa \lambda \mu \nu \xi \omicron
STRING TEST1C \latex \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega
STRING TEST2A a b c d e f g h i j k
STRING TEST2B l m n o p q r s t u v w x y z
STRING BCC1 \latex \alpha_1
STRING ACA2CO3 \latex \alpha_{Ca_2CO_3}
ATTRIBUTE CENTER
CHARSIZE 1
0.05 0.95 N'Example 5
CLIP OFF
0.01 0.85 N'~TEST1A
0.01 0.80 N'~TEST1B
0.01 0.75 N'~TEST1C
FONT 1
0.01 0.65 N'~TEST2A
FONT 2
0.01 0.60 N'~TEST2B
0.01 0.55 N'\latex \textrm{Roman text in LaTeX}
0.01 0.50 N'\latex as opposed to non-roman math mode LaTeX
0.01 0.45 N'~BCC1
CHARSIZE 0.8
0.01 0.40 N'\latex M_{23}C_6
0.01 0.35 N'~ACA2CO3
```

Example 6 – Triangular Diagrams for Ternary Systems

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 6 - Ternary Plots.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example

In the DATAPLOT language, this type of diagram is only available for Console Mode.



Macro Text

$DATAPLOT Example 6 - Ternary Phase Diagram

PROLOG 6 EXAMPLE 6 0<X<0.969224, 0<Y<1.00000

XSCALE 0.00000 0.969224

YSCALE 0.307492E-01 1.00000

```
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE A-B-C at T=1000 K
XTEXT MOLE_FRACTION B
YTEXT MOLE_FRACTION C
DIAGRAM_TYPE TRIANGULAR YES YES
DATASET 6 Plot a ternary phase diagram
CLIP OFF
0.80 0.90 N'Example 6
0.86 0.31 N'B2C
0.52 0.97 N'Diamond
CHARSIZE 0.25
1.4E+01 1.10E+01 MVA'1:*B2C Liquid
1.4E+01 1.05E+01 MVA'2:*Diamond Liquid
0.10 0.10 N'Liquid
0.48 0.45 N'Diamond+
0.48 0.40 N' B2C+Liquid
5.80E-01 5.40E-02 MWA' 1
1.90E-01 2.40E-01 MWA' 1
0.65E-01 2.50E-01 MWA' 2
CHARSIZE 0.45
-0.10 -0.05 N'A
1.06 -0.05 N'B
0.48 1.05 N'C
CHARSIZE 0.35
```

$$ Calculated A-B-C Phase Equilibrium Data:

$ PHASE REGION FOR:

$F0 LIQUID

$E DIAMOND_A4

$F0 B2C

$ INVARIANT EQUILIBRIUM

COLOR 2

BLOCK X=C1; Y=C2; GOC=C3,WAD;

2.4555855989E-01 3.5568857193E-01 M

0.0000000000E+00 9.9999523163E-01

2.4555855989E-01 3.5568857193E-01 M

6.6666668653E-01 3.3333334327E-01

0.0000000000E+00 9.9999523163E-01 M

6.6666668653E-01 3.3333334327E-01

COLOR 1

BLOCKEND

$ PHASE REGION FOR:

$E LIQUID

$F0 B2C

BLOCK X=C1; Y=C2; GOC=C3,WAD;

$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)

2.2030337155E-01 1.2340000272E-01 M

2.2632879019E-01 1.1058768630E-01

2.3371633887E-01 9.9345825613E-02

2.4253317714E-01 8.9345827699E-02

2.6429468393E-01 7.2744041681E-02

2.8429466486E-01 6.2814079225E-02

2.9617273808E-01 5.8319382370E-02

3.2811737061E-01 4.9470417202E-02

3.6353862286E-01 4.3130427599E-02

3.9895987511E-01 3.8979098201E-02

4.5209178329E-01 3.5266116261E-02

5.2293431759E-01 3.3152002841E-02

6.1148744822E-01 3.3077053726E-02

6.4690870047E-01 3.3490389585E-02

6.8232995272E-01 3.4017231315E-02

7.3546189070E-01 3.4814555198E-02

7.5317251682E-01 3.5033416003E-02

8.0630439520E-01 3.5373892635E-02

8.5943627357E-01 3.4983776510E-02

9.1256815195E-01 3.3575300127E-02

9.6747112274E-01 3.0857827514E-02

9.6922445297E-01 3.0749246478E-02

2.2030337155E-01 1.2340000272E-01 M

2.1294665337E-01 1.5308913589E-01

2.1171525121E-01 1.8851040304E-01

2.1532440186E-01 2.2393165529E-01

2.2180187702E-01 2.5935292244E-01

2.2992117703E-01 2.9477417469E-01

2.3888295889E-01 3.3019542694E-01

2.4555855989E-01 3.5568857193E-01

$ PLOTTED COLUMNS ARE : X(B2C,B) and X(B2C,C)

6.6666668653E-01 3.3333334327E-01 M

6.6666668653E-01 3.3333334327E-01

$ TIELINES

COLOR 3

6.6666668653E-01 3.3333334327E-01 M

8.7775242329E-01 3.4625384957E-02

6.6666668653E-01 3.3333334327E-01 M

7.9250496626E-01 3.5342670977E-02

6.6666668653E-01 3.3333334327E-01 M

2.4555824697E-01 3.5568737984E-01

6.6666668653E-01 3.3333334327E-01 M

2.3944084346E-01 9.2542596161E-02

6.6666668653E-01 3.3333334327E-01 M

2.3359020054E-01 3.0954307318E-01

6.6666668653E-01 3.3333334327E-01 M

2.2585247457E-01 2.7766343951E-01

6.6666668653E-01 3.3333334327E-01 M

2.1618695557E-01 1.3621240854E-01

2.2632879019E-01 1.1058768630E-01 M

6.6666668653E-01 3.3333334327E-01

COLOR 1

BLOCKEND

$ PHASE REGION FOR:

$F0 DIAMOND_A4

$E B2C

BLOCK X=C1; Y=C2; GOC=C3,WAD;

$ PLOTTED COLUMNS ARE : X(DIAMOND_A4,B) and X(DIAMOND_A4,C)

0.0000000000E+00 9.9999523163E-01 M

0.0000000000E+00 9.9999976158E-01

BLOCKEND

$ PHASE REGION FOR:

$E LIQUID

$F0 DIAMOND_A4

BLOCK X=C1; Y=C2; GOC=C3,WAD;

$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)

2.4555855989E-01 3.5568857193E-01 M

2.0263540745E-01 3.3483061194E-01

1.6243904829E-01 3.1375369430E-01

1.2243904918E-01 2.9153180122E-01

8.2439050078E-02 2.6854267716E-01

4.2439054698E-02 2.4548016489E-01

2.4390530307E-03 2.2313812375E-01

2.4999999937E-07 2.2181616724E-01

$ TIELINES

COLOR 3

0.0000000000E+00 9.9999511242E-01 M

2.3529186845E-01 3.5085919499E-01

0.0000000000E+00 9.9999469519E-01 M

1.9826586545E-01 3.3260950446E-01

0.0000000000E+00 9.9999409914E-01 M

1.3240024447E-01 2.9716023803E-01

0.0000000000E+00 9.9999397993E-01 M

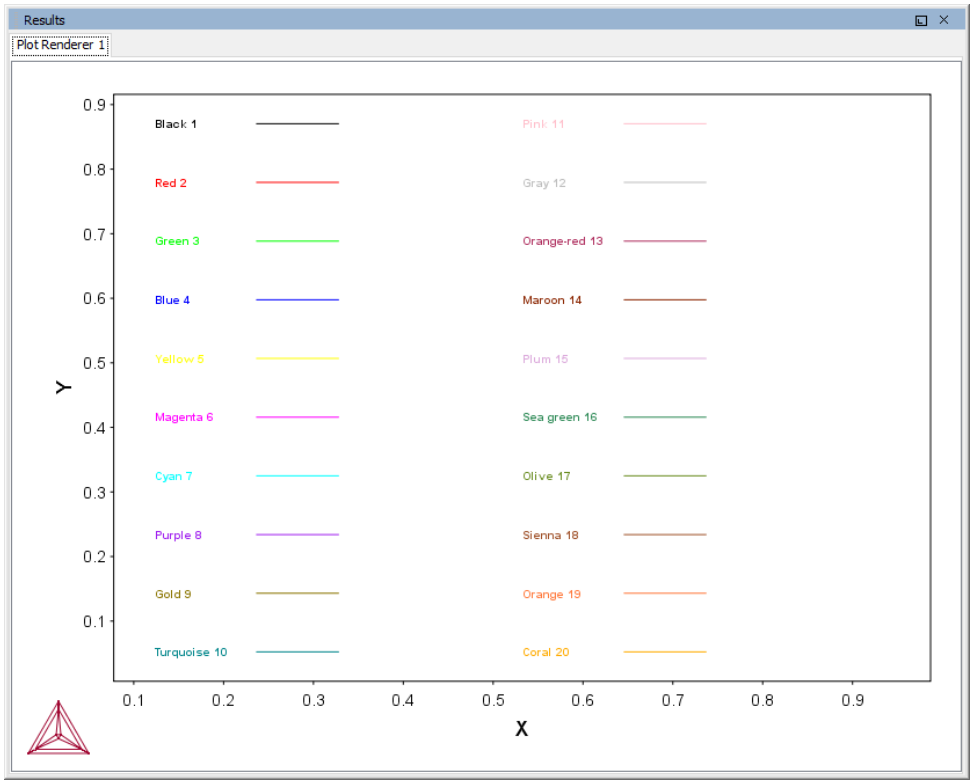
1.1439975351E-01 2.8695335984E-01

BLOCKEND

Example 7 – Color Codes

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 7 - Color Codes.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 7 - DIGLIB Colors
PROLOG 1 DIGLIB Colors
XSCALE 0.0 1.0
YSCALE 0.0 1.0
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 15.5000
YLENGTH 11.5000
TITLE DIGLIB Colors
```

```
XTEXT X
YTEXT Y
DATASET 1 DIGLIB Colors:
$ DIGLIB Colors:
CHARSIZE 0.3
SYMBOLSIZE 0.5
COLOR 1
0.05 0.95 N' Black 1
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.95 M
0.275 0.95 D
BLOCKEND
COLOR 2
0.05 0.85 N' Red 2
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.85 M
0.275 0.85 D
BLOCKEND
COLOR 3
0.05 0.75 N' Green 3
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.75 M
0.275 0.75 D
BLOCKEND
COLOR 4
0.05 0.65 N' Blue 4
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.65 M
0.275 0.65 D
BLOCKEND
COLOR 5
0.05 0.55 N' Yellow 5
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.55 M
0.275 0.55 D
```

```
BLOCKEND
COLOR 6
0.05 0.45 N' Magenta 6
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.45 M
0.275 0.45 D
BLOCKEND
COLOR 7
0.05 0.35 N' Cyan 7
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.35 M
0.275 0.35 D
BLOCKEND
COLOR 8
0.05 0.25 N' Purple 8
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.25 M
0.275 0.25 D
BLOCKEND
COLOR 9
0.05 0.15 N' Gold 9
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.15 M
0.275 0.15 D
BLOCKEND
COLOR 10
0.05 0.05 N' Turquoise 10
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.05 M
0.275 0.05 D
BLOCKEND
COLOR 11
0.5 0.95 N' Pink 11
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.95 M
```

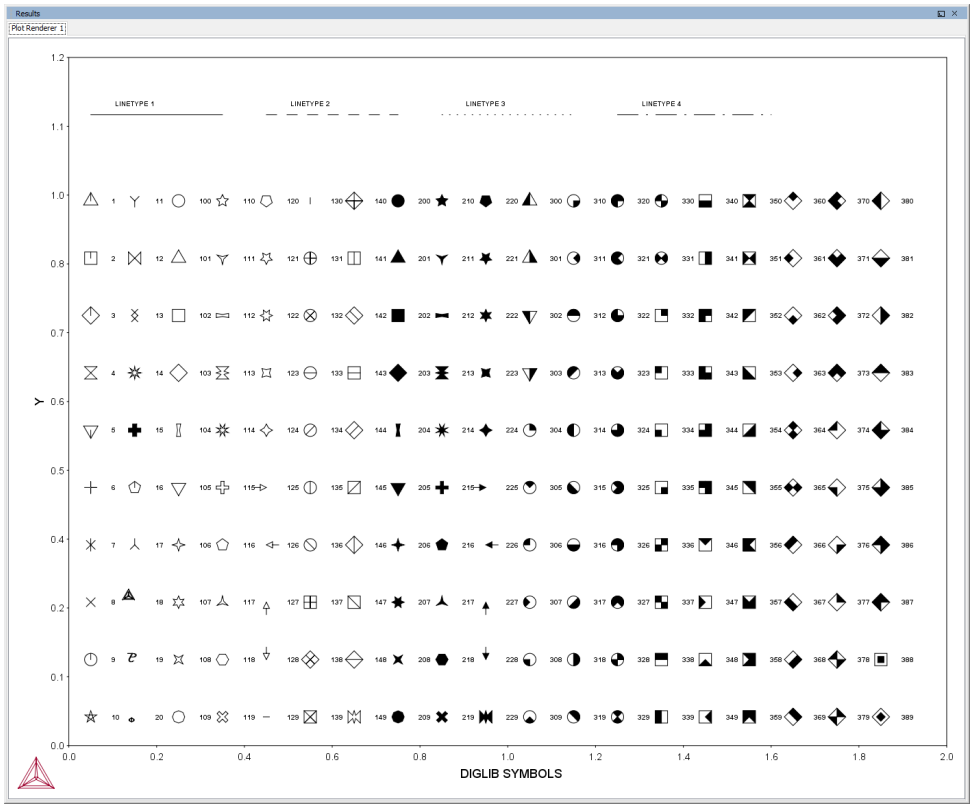
```
0.725 0.95 D
BLOCKEND
COLOR 12
0.5 0.85 N' Gray 12
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.85 M
0.725 0.85 D
BLOCKEND
COLOR 13
0.5 0.75 N' Orange-red 13
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.75 M
0.725 0.75 D
BLOCKEND
COLOR 14
0.5 0.65 N' Maroon 14
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.65 M
0.725 0.65 D
BLOCKEND
COLOR 15
0.5 0.55 N' Plum 15
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.55 M
0.725 0.55 D
BLOCKEND
COLOR 16
0.5 0.45 N' Sea green 16
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.45 M
0.725 0.45 D
BLOCKEND
COLOR 17
0.5 0.35 N' Olive 17
BLOCK X=C1; Y=C2; GOC=C3,N
```

```
0.625 0.35 M
0.725 0.35 D
BLOCKEND
COLOR 18
0.5 0.25 N' Sienna 18
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.25 M
0.725 0.25 D
BLOCKEND
COLOR 19
0.5 0.15 N' Orange 19
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.15 M
0.725 0.15 D
BLOCKEND
COLOR 20
0.5 0.05 N' Coral 20
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.05 M
0.725 0.05 D
BLOCKEND
```

Example 8 - DIGLIB Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 8 - DIGLIB Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



A default symbol is the current symbol in the run of the software (it is usually the No 1 symbol if the POST-processor is switched on for the first time). S (i.e., # is not specified) means that the current symbol is plotted. S0 (i.e., #=0) means that no symbol is plotted.

Macro Text

```
$DATAPLOT DIGLIB Symbols 2
PROLOG 1 DIGLIB Symbols 2 0<X<2.0, 0<Y<1.2
XSCALE 0.0 2.0
YSCALE 0.0 1.2
XTYPE LINEAR
YTYPE LINEAR
```

```
XLENGTH 15.5000
YLENGTH 11.5000
TITLE DIGLIB Symbols
XTEXT DIGLIB SYMBOLS
DATASET 1 Various DIGLIB Symbols:
$ DIGLIB Symbols:
CHARSIZE 0.3
SYMBOLSIZE 0.5
0.05 0.95 WS1' 1
0.05 0.85 WS2' 2
0.05 0.75 WS3' 3
0.05 0.65 WS4' 4
0.05 0.55 WS5' 5
0.05 0.45 WS6' 6
0.05 0.35 WS7' 7
0.05 0.25 WS8' 8
0.05 0.15 WS9' 9
0.05 0.05 WS10' 10
0.15 0.95 WS11' 11
0.15 0.85 WS12' 12
0.15 0.75 WS13' 13
0.15 0.65 WS14' 14
0.15 0.55 WS15' 15
0.15 0.45 WS16' 16
0.15 0.35 WS17' 17
0.15 0.25 WS18' 18
0.15 0.15 WS19' 19
0.15 0.05 WS20' 20
0.25 0.95 WS100' 100
0.25 0.85 WS101' 101
0.25 0.75 WS102' 102
0.25 0.65 WS103' 103
0.25 0.55 WS104' 104
0.25 0.45 WS105' 105
0.25 0.35 WS106' 106
```

```
0.25 0.25 WS107' 107
0.25 0.15 WS108' 108
0.25 0.05 WS109' 109
0.35 0.95 WS110' 110
0.35 0.85 WS111' 111
0.35 0.75 WS112' 112
0.35 0.65 WS113' 113
0.35 0.55 WS114' 114
0.35 0.45 WS115' 115
0.35 0.35 WS116' 116
0.35 0.25 WS117' 117
0.35 0.15 WS118' 118
0.35 0.05 WS119' 119
0.45 0.95 WS120' 120
0.45 0.85 WS121' 121
0.45 0.75 WS122' 122
0.45 0.65 WS123' 123
0.45 0.55 WS124' 124
0.45 0.45 WS125' 125
0.45 0.35 WS126' 126
0.45 0.25 WS127' 127
0.45 0.15 WS128' 128
0.45 0.05 WS129' 129
0.55 0.95 WS130' 130
0.55 0.85 WS131' 131
0.55 0.75 WS132' 132
0.55 0.65 WS133' 133
0.55 0.55 WS134' 134
0.55 0.45 WS135' 135
0.55 0.35 WS136' 136
0.55 0.25 WS137' 137
0.55 0.15 WS138' 138
0.55 0.05 WS139' 139
0.65 0.95 WS140' 140
0.65 0.85 WS141' 141
```

```
0.65 0.75 WS142' 142
0.65 0.65 WS143' 143
0.65 0.55 WS144' 144
0.65 0.45 WS145' 145
0.65 0.35 WS146' 146
0.65 0.25 WS147' 147
0.65 0.15 WS148' 148
0.65 0.05 WS149' 149
0.75 0.95 WS200' 200
0.75 0.85 WS201' 201
0.75 0.75 WS202' 202
0.75 0.65 WS203' 203
0.75 0.55 WS204' 204
0.75 0.45 WS205' 205
0.75 0.35 WS206' 206
0.75 0.25 WS207' 207
0.75 0.15 WS208' 208
0.75 0.05 WS209' 209
0.85 0.95 WS210' 210
0.85 0.85 WS211' 211
0.85 0.75 WS212' 212
0.85 0.65 WS213' 213
0.85 0.55 WS214' 214
0.85 0.45 WS215' 215
0.85 0.35 WS216' 216
0.85 0.25 WS217' 217
0.85 0.15 WS218' 218
0.85 0.05 WS219' 219
0.95 0.95 WS220' 220
0.95 0.85 WS221' 221
0.95 0.75 WS222' 222
0.95 0.65 WS223' 223
0.95 0.55 WS224' 224
0.95 0.45 WS225' 225
0.95 0.35 WS226' 226
```

```
0.95 0.25 WS227' 227
0.95 0.15 WS228' 228
0.95 0.05 WS229' 229
1.05 0.95 WS300' 300
1.05 0.85 WS301' 301
1.05 0.75 WS302' 302
1.05 0.65 WS303' 303
1.05 0.55 WS304' 304
1.05 0.45 WS305' 305
1.05 0.35 WS306' 306
1.05 0.25 WS307' 307
1.05 0.15 WS308' 308
1.05 0.05 WS309' 309
1.15 0.95 WS310' 310
1.15 0.85 WS311' 311
1.15 0.75 WS312' 312
1.15 0.65 WS313' 313
1.15 0.55 WS314' 314
1.15 0.45 WS315' 315
1.15 0.35 WS316' 316
1.15 0.25 WS317' 317
1.15 0.15 WS318' 318
1.15 0.05 WS319' 319
1.25 0.95 WS320' 320
1.25 0.85 WS321' 321
1.25 0.75 WS322' 322
1.25 0.65 WS323' 323
1.25 0.55 WS324' 324
1.25 0.45 WS325' 325
1.25 0.35 WS326' 326
1.25 0.25 WS327' 327
1.25 0.15 WS328' 328
1.25 0.05 WS329' 329
1.35 0.95 WS330' 330
1.35 0.85 WS331' 331
```

```
1.35 0.75 WS332' 332
1.35 0.65 WS333' 333
1.35 0.55 WS334' 334
1.35 0.45 WS335' 335
1.35 0.35 WS336' 336
1.35 0.25 WS337' 337
1.35 0.15 WS338' 338
1.35 0.05 WS339' 339
1.45 0.95 WS340' 340
1.45 0.85 WS341' 341
1.45 0.75 WS342' 342
1.45 0.65 WS343' 343
1.45 0.55 WS344' 344
1.45 0.45 WS345' 345
1.45 0.35 WS346' 346
1.45 0.25 WS347' 347
1.45 0.15 WS348' 348
1.45 0.05 WS349' 349
1.55 0.95 WS350' 350
1.55 0.85 WS351' 351
1.55 0.75 WS352' 352
1.55 0.65 WS353' 353
1.55 0.55 WS354' 354
1.55 0.45 WS355' 355
1.55 0.35 WS356' 356
1.55 0.25 WS357' 357
1.55 0.15 WS358' 358
1.55 0.05 WS359' 359
1.65 0.95 WS360' 360
1.65 0.85 WS361' 361
1.65 0.75 WS362' 362
1.65 0.65 WS363' 363
1.65 0.55 WS364' 364
1.65 0.45 WS365' 365
1.65 0.35 WS366' 366
```

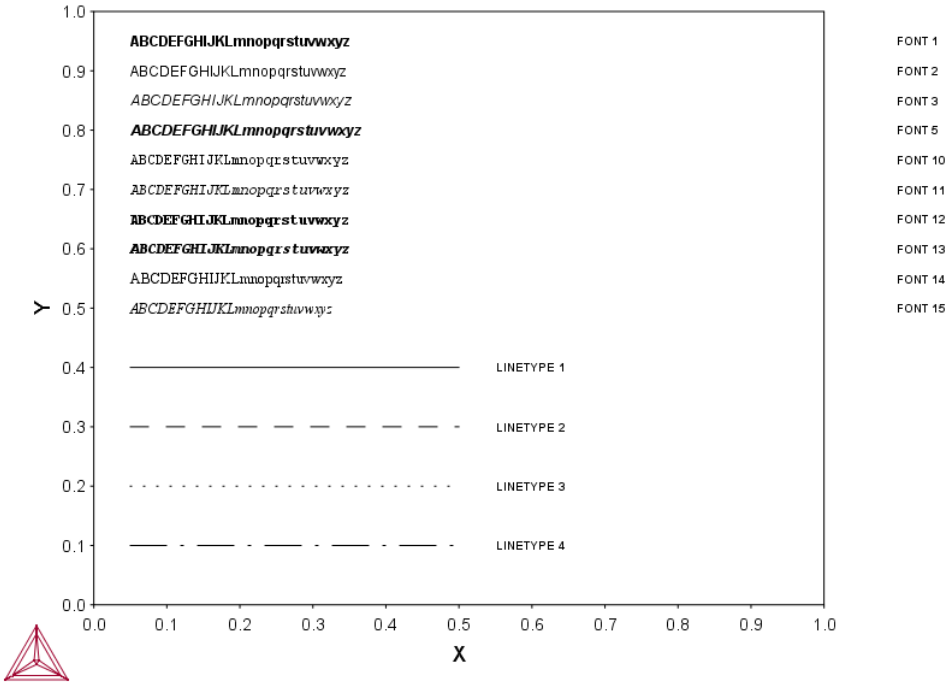
```
1.65 0.25 WS367' 367
1.65 0.15 WS368' 368
1.65 0.05 WS369' 369
1.75 0.95 WS370' 370
1.75 0.85 WS371' 371
1.75 0.75 WS372' 372
1.75 0.65 WS373' 373
1.75 0.55 WS374' 374
1.75 0.45 WS375' 375
1.75 0.35 WS376' 376
1.75 0.25 WS377' 377
1.75 0.15 WS378' 378
1.75 0.05 WS379' 379
1.85 0.95 WS380' 380
1.85 0.85 WS381' 381
1.85 0.75 WS382' 382
1.85 0.65 WS383' 383
1.85 0.55 WS384' 384
1.85 0.45 WS385' 385
1.85 0.35 WS386' 386
1.85 0.25 WS387' 387
1.85 0.15 WS388' 388
1.85 0.05 WS389' 389
$ DIGLIB Line Types:
LINETYPE 1
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 1.10 M
0.35 1.10
BLOCKEND
LINETYPE 2
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.45 1.10 M
0.75 1.10
BLOCKEND
LINETYPE 3
```

```
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.85 1.10 M
1.15 1.10
BLOCKEND
LINETYPE 4
BLOCK X=C1; Y=C2; GOC=C3,DWA
1.25 1.10 M
1.60 1.10
BLOCKEND
0.10 1.12 W' LINETYPE 1
0.50 1.12 W' LINETYPE 2
0.90 1.12 W' LINETYPE 3
1.30 1.12 W' LINETYPE 4
```

Example 9 - DIGLIB Fonts and Lines

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 9 - DIGLIB Fonts.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 9 - DIGLIB Fonts
PROLOG 1 DIGLIB Fonts & Line Types 0<X<1, 0<Y<1
XSCALE 0.0 1.0
YSCALE 0.0 1.0
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE DIGLIB Fonts
XTEXT X
YTEXT Y
```

```
DATASET 1 Various DIGLIB Fonts and Line Types:
$ DIGLIB Fonts:
CHARSIZE .35
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0.55 0.10 N' LINETYPE 4
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Pourbaix Diagrams

Educational Material



Introduction to Pourbaix Diagrams

In this section:

About Pourbaix Diagrams in Thermo-Calc 3
Pourbaix Diagrams 5
Working with Pourbaix Diagrams 7
Key Concepts 9
Basic Settings and Definitions 11

About Pourbaix Diagrams in Thermo-Calc

This guide is for Thermo-Calc software users who know the basics of thermodynamics and want to know more about Pourbaix Diagrams.

You are introduced to the concept of a Pourbaix diagram and shown how to interpret such diagrams through a series of examples.

Materials corrosion occurs almost everywhere. It may lead to serious material damages, unexpected application failures, tremendous economic costs and environmental degradations. Consequently, scientists and engineers must often conduct expensive and time-consuming corrosion experiments as part of failure analyses, risk evaluations, quality improvements and application enhancements.

Under certain conditions, when a metal or alloy is exposed to an aqueous solution with a concentration of inorganic/organic mixture, corrosion phenomena occur at a corresponding degree. During corrosion, some metallic phases dissolve, the metal or alloy surface gets damaged and some secondary solid phases form at the solid-liquid interfaces (such as oxides, hydroxides, silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates, or halides). Such corrosive chemical or electrochemical reactions can be studied by means of the so-called Pourbaix diagrams if the reactions reach their equilibrium states [1973 and 1974, Pourbaix; 2003, Cramer; 2011, Verink; 2011, Thompson].

GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For POURBAIX module users, you need to use GES5. When you try to enter this module, you are instructed to switch to GES5 using the SET_GES_VERSION command.

- About the Gibbs Energy System (GES) Module



To globally set the default from GES6 back to GES5, go to the **Tools → Options → General** tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The SET_GES_VERSION Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

References

[1973, Pourbaix] M. Pourbaix, Lectures on Electrochemical Corrosion (Plenum Press, New York, 1973).

[1974, Pourbaix] M. Pourbaix, Atlas of Electrochemical Equilibria in Aqueous Solutions (National Association of Corrosion Engineers, Houston, TX, ed. 2, 1974).

[2003, Cramer] S. D. Cramer, B. S. Covino Jr., Eds., Corrosion: Fundamentals, Testing, and Protection: ASM Handbook, Volume 13A (ASM International, 2003).

[2011, Verink] E. D. Verink Jr., "Simplified procedure for constructing Pourbaix diagrams", in Uhlig's Corrosion Handbook, R. W. Revie, Ed. (John Wiley & Sons, Inc., Hoboken, NJ, USA, ed. 3, 2011), pp. 93–101.

[2011, Thompson] W. Thompson, M. H. Kaye, C. W. Bale, A. Pelton, "Pourbaix diagrams for multielement systems" in Uhlig's Corrosion Handbook, Revi, Ed. (John Wiley & Sons, Hoboken, NJ, USA, 2011), pp. 103–109.

Pourbaix Diagrams

Marcel Pourbaix applied thermodynamics to predict materials corrosion resistance. He determined the phase stability relations in terms of varied pH and Eh values for an interaction system of metal and pure water or dilute aqueous solution. He presented the stability regions of metal and secondary phases (such as metal-oxides/hydroxides) on a pH-Eh diagram, which is now known as a Pourbaix diagram.

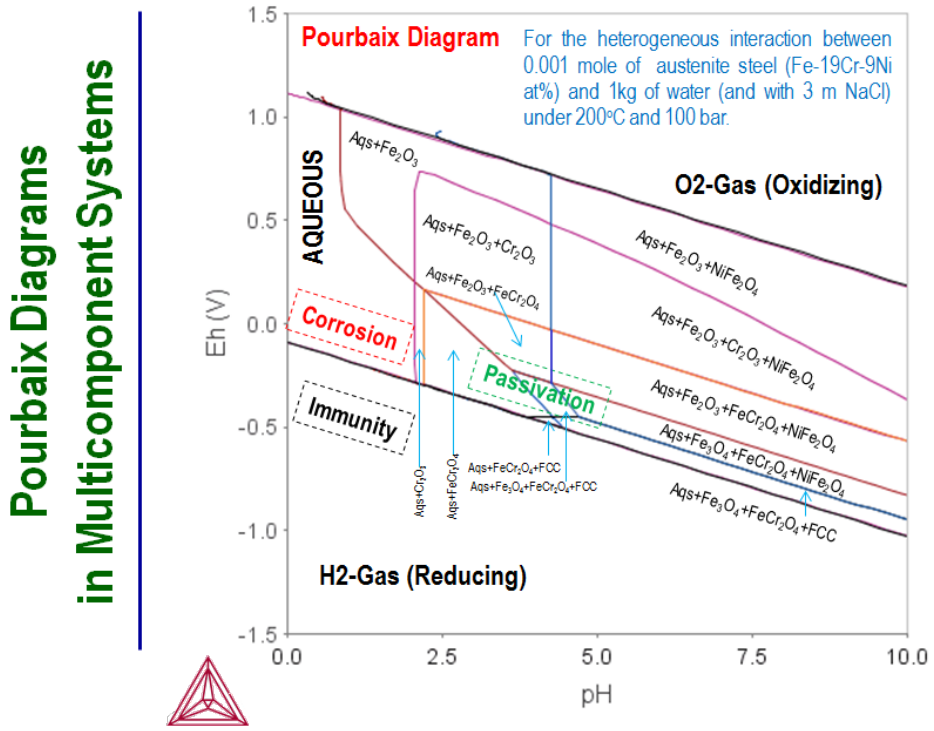
A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

The speciation and partition in the aqueous solution and the interacting phases depend not only on pH and Eh, but also on other factors such as the bulk composition, temperature and pressure in the system. The interacting phases may be gas mixtures, stoichiometric solids or solid solutions.

A Pourbaix diagram is divided in regions of *immunity*, *corrosion* and *passivity*. These regions provides information about the stability of a particular metal or alloy in a specific aqueous electrochemical environment under certain pH, Eh, pressure and temperature conditions.

- The immunity region is the region in which there is no metal dissolution.
- The corrosion region is the region in which there is active metal dissolution.
- The passivation region is the region in which a protective metal-oxide film that prevents metal dissolution is formed.

The following shows these three regions in a Pourbaix diagram for the heterogeneous interaction between 0.001 mole of austenite steel (Fe-19Cr-9Ni [at%]) and 1 kg of water (with 3 m NaCl), at 200° C and 100 bar:



Depending on the system's bulk chemical composition, secondary phases may form during the transformation process. These can not only be oxides, but also be, for example, hydroxides, sulphides, sulphates, carbonates, nitrates, phosphates, borates, silicates, hydrous silicates and halides. Information about these secondary phases may help one understand the passivation behaviours in corrosion processes. For example, it may be important to understand whether any secondary phases are formed in different pH-Eh regions during hydrolysis, oxidation, reduction or other reaction processes.

In a Pourbaix diagram, the predominant ion boundaries are often represented by dashed and straight lines imposed on a traditional Pourbaix diagram for a simple interaction system (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011). Such a predominance boundary is normally an equal molality (or equal activity) line for a pair of two most-concentrated aqueous solute species (charged or neutral) involving a common metal. A line is then simply determined by a reaction constant of its corresponding electrochemical reaction in the homogeneous aqueous solution phase. However, this is not the case in Thermo-Calc.



You cannot get any information about predominant ion boundaries from a Pourbaix diagram in Thermo-Calc.

Working with Pourbaix Diagrams

With the Thermo-Calc software package, Pourbaix diagrams can be calculated over a wide range of pressure, temperature and composition conditions for complex heterogeneous interactions between multicomponent primary alloy solution or compound phases, concentrated aqueous solutions (with dissolved inorganic and organic substances), complicated secondary solids and oxidizing/reducing gaseous mixtures. In the Console Mode, diagrams can be calculated and plotted either using the response-driven POURBAIX module or directly using the DATA, GIBBS, POLY and POST modules.



This command or module is not available with GES6.



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

It is possible in Thermo-Calc to set aqueous properties other than pH and Eh as axis variables. For example, the following properties can also be set as axis variables: `Ah` (electronic affinity), `pe` (electronic activity log10ACRe), `IS` (ionic strength), `TM` (total aqueous concentration, in molality), `OC` (Osmotic coefficient), activity or activity coefficient of solvent H2O, and activities or activity coefficients or concentrations in m (molality) of charged or neutral solute species.

Beside a concentrated aqueous solution phase handled by a proper thermodynamic model named SIT, HKF or PITZ, it is also possible to consider complex alloy solution phases or compound phases, as well as secondary solid phases and gaseous mixtures, which are treated by specific solution models.

Most frequently, a Pourbaix diagram is calculated for a specific alloyed phase with the initial alloying composition, such as the FCC solution phase in an austenite steel. However, it is possible to calculate a Pourbaix diagram for two co-existing phases, such as the FCC+BCC solution phases in a duplex steel for example, or even for more than two co-existing phases in a steel/alloy.



Each point on the line in a pH-Eh diagram in Thermo-Calc represents a certain minimum state of Gibbs energy. When a line is crossed, a phase transformation should occur. This means that a Pourbaix diagram in Thermo-Calc does not provide any information about any predominant ion boundary.

Key Concepts

The following are two key concepts important for understanding how aqueous solutions behave and how an aqueous-bearing heterogeneous interaction system is properly defined and calculated in Thermo-Calc.

Effective Interaction Ratio

A pH-Eh plot is always related to a certain amount of initial alloys or other condensed materials that has effectively reacted with an aqueous solution in the system. This is the amount of condensed material that is fully in equilibrium with the defined aqueous solution phase. The amount is specified relative to an aqueous solution that is normally comprised of 1 kg of water with certain specified solute concentrations at certain temperature and pressure conditions. (This is why a calculated Pourbaix diagram is typically presented for an initial amount of the interacting metal or alloy at a certain level, such as 10-6, 1E-3, 0.1 or 1 mole of metal or alloy.) It is called the *Effective Interaction Ratio* (between the initial alloy or alloyed phases and the initial aqueous solution) and it is expressed in terms of molality (mol/kg).

The Effective Interaction Ratio is important for two reasons. First, the ratio has implications for kinetic or dynamic effects such as chemical reaction mechanism and kinetics, fluid flow dynamics, surface area and interaction time. Secondly, the ratio, being expressed as 10-6 mole of metal (or alloy), is the solubility limit that can be detected for cathodic corrosion protection by immunity.

One should always be careful when setting initial amounts and compositions in the original condensed materials, as well as when setting the initial concentrations of dissolved solutes in the original aqueous solution phase. It is often useful to make a series of calculations for different levels of initial amount of the interacting metal/alloy while the conditions are fixed for other settings (such as initial aqueous concentration, pressure, temperature, pH, and Eh).

Solubility

When a heterogeneous equilibrium has a dissolving solution or mixture phase and a stoichiometric or solution phase, then the concept of solubility becomes important. A solubility of a phase (the solute) is its property of dissolving in the solvent phase. This concept concerns the constitution of a phase and is applied where one or several of the constituents are dominant (which is highly concentrated and dissolving) while there are only small amounts of the other remaining species (which are less concentrated and dissolved). The dissolving solution or mixture phase can be liquid, gas, aqueous or solid, as long as it has dissolving capacity. The stoichiometric or solution phase has some constituents which tend to be dissolved into the dissolving solution or mixture phase.

Key Points about Solubility

- Under certain temperature, pressure and composition conditions, a Fe- or Cr-dominant BCC phase can dissolve certain amounts of Ni and C from a carbide phase such as M23C6, M7C3 or M3C. The Ni and C elements in the carbides have the solubility defined relative to the BCC phase.
- An aqueous solution phase is always dominant in the solvent water, that is, H2O. Under specific temperature, pressure and aqueous composition conditions, any other element (such as Fe and C) or substance (such as a pure SO2 gas, stoichiometric phase Cu2S and solution phase (Fe,Ni)1(O,Va)1) have a certain solubility limit in the defined aqueous solution.
- Under certain temperature and pressure conditions, and under given certain concentrations of other dissolved species in the mixture, an O2-dominant gaseous mixture phase can dissolve certain amounts of Fe+2 or Fe+3 species from magnetite (Fe3O4). The magnetite solid has solubility defined relative to the gaseous mixture under the given conditions.
- Under certain temperature and pressure condition, under specific concentrations of other dissolved species in the liquid phase, a Fe-dominant liquid mixture phase can dissolve certain amounts of, for example, Cr and O. The Cr and O components have the solubility defined in the liquid mixture.

Basic Settings and Definitions

In a homogeneous aqueous solution or an aqueous-bearing heterogeneous interaction system, the most essential definition is for system-components there must be H2O, H+1 and ZE (electron) plus those for elements dissolved in aqueous solution (such as Na, Cl, S) and associated in interacting metals/alloys (such as Fe, Cr, Mn, Mg, Ni, Al, Si, Zn). Three fundamental phases in a system are the AQUEOUS solution, the GAS mixture and the REF_ELECTRODE. The REF_ELECTRODE phase is used for setting the reference state for electrostatic potential in the system and for calculating the Eh condition (defined as MUR(ZE)/RNF). Other phases should be appropriately selected and retrieved from critically-assessed databases that cover not only the target phases (solution or stoichiometric) in interacting metals/alloys but also the secondary phases (solution or stoichiometric). The two public databases PAQ and PAQS are specially designed as single-database choices that cover all kinds of phases necessary for calculations. However, these databases are each limited to a framework of a very small number of elements. When it comes to simulations of complex multicomponent systems with a wide variety of elements and phases, the thermodynamic data must be selected and retrieved from several databases: AQUEOUS solution and REF_ELCTRODE phases must be retrieved from TCAQ or AQS; alloy phases (such as FCC_A1, BCC_A2, HCP_A3, CEMENTITE) from alloy solution databases (such as SSOL for general alloy phases, TCFE for steel/Fe-alloy phases, TCAL for Al-based alloy phases; TCMG for Mg-based alloy phases, and TCNI for Ni-based superalloy phases); gaseous mixture phase and secondary phases from specific substance or solution databases (such as SSUB for GAS phase and various solid compound phases or TCOX for oxide solution phases). Note that the REF_ELECTRODE phase should always be suspended in equilibrium calculations, while GAS phase could be set as ENTERED, SUSPENDED or DORMANT, depending on the purpose of the calculation.

When defining an interaction system, the initial condition for the H2O component is always set as 1 kg of water. The initial composition conditions for dissolving and interacting elements are normally defined in moles (such as n(Fe)=0.009, n(Cr)=5E-4, n(Ni)=3E-4, n(Mn)=5E-5, n(S)=5E-5, n(Na)=3, n(Cl)=3). This makes it straightforward and convenient to count various related aqueous solution properties based on molality. The initial conditions for the H+1 and ZE components can be given as molar compositions (such as n(H+1)=0, n(ZE)=0) or their activities or potentials (such as lnACR(H+1)=-9.21, MUR(ZE)=8400).

The pH and Eh properties of the aqueous solution in the interacting system are always defined in the following way:

```
pH = -log10[ACR(H+1,AQUEOUS)*AH2O]]Eh = MUR(ZE)/RNF
```

The symbol AH2O is the molecular weight of solvent H2O (equals 55.508435) and RNF is the Faraday constant (equals 96485.309).

The activity of the solvent water (ACRH2O, Aw), the osmatic coefficient of aqueous solution (OSMC, Os), electronic affinity (Ah), electronic activity log10ACRe (pe), ionic strength (IS), total aqueous concentration, in molality (TM) and total alkaline concentrations under two definitions (At1/AT2) are calculated and listed for each equilibrium state.

POLY3 calculations for mass balances in Thermo-Calc are always based on site-fractions. Consequently, when functions for describing various properties of aqueous solutes are defined, such as molality (MLi), activity coefficient (RCi) and activity (AIi), they should be converted to molality-based quantities:

```
MLi = Y(AQUEOUS,i)*AH2O/YH2O
RCi = ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i)
AIi = ACR(i,AQUEOUS)*AH2O
```

Here, YH2O is the site-fraction of solvent H2O and AH2O equals 55.508435.

Many more variables, functions and tables can be entered for various purposes. For instance, an equilibrium constant for a homogeneous reaction or a solubility product for a solid dissolution reaction can be entered.

Thermodynamic Data Requirements

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Required Thermodynamic Data

To calculate a Pourbaix diagram, thermodynamic data for at least the following four types of phases must be available:

- The aqueous solution phase which applies a certain aqueous solution model. In Thermo-Calc, information about this phase could be retrieved from, for instance, the TCAQ or AQS database (these also include data for the `REF_ELECTRODE` phase that is used for setting the reference state of the standard hydrogen electrode).
- The alloy solution and/or compound phases for the primary matrix phases (and possibly also for the precipitated phases in the alloy. Examples of such phases include FCC_A1, BCC_A2, HCP_A3, SIGMA and CEMENTITE. In Thermo-Calc, information about such phases could be retrieved from, for example, the TCFE database for steels/Fe-alloys, the TCNI database for Ni-based superalloys, the TCAL database for Al-based alloys, the TCMG database for Mg-based alloys, the TCSLD for Sn-/Au-/Bi-/Zn-based solder alloys or the SSOL for general alloys.
- The secondary solid phases that would form as a result of the heterogeneous chemical or electrochemical reactions. These phases could be, for example, oxides, hydroxides, silicates, hydrous silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates or halides. In Thermo-Calc, information about such phases could be retrieved from, for example, the SSUB database for pure solid compounds or the TCOX database for complex oxide solids.
- The gaseous mixture phase. Information about this phase could be retrieved from, for example, the SSUB database. However, note that is also possible to perform Pourbaix diagram calculations that ignore the gaseous mixture phase.

All this thermodynamic data about the various phases must be critically assessed and internally consistent. Furthermore, when the data is retrieved from several databases, the data taken from each database must be consistent with the data taken from the other databases. When Pourbaix diagrams and other diagrams of steel corrosion processes are calculated, it is typically recommended that the TCAQ, TCFE, SSUB and TCOX databases or the AQS, TCFE, SSUB and TCOX are used in combination.

The public PAQ database contains thermodynamic data for all four phase types and can be used for calculating Pourbaix diagrams. They have been designed specifically for the purpose of demonstrating the POURBAIX module functionality in Thermo-Calc. However, these databases only allow you to perform test calculations for simple cases with major phases in which only a few elements can be considered.

Including or Excluding the Gas Phase

Under defined pressure and temperature conditions, the solvent water's thermodynamic stability limits are determined by the following two electrochemical reactions:

```
H2O(water) + 2e- = H2(gas) + 2OH-1
2H2O(water) = O2(gas) + 4H+1 + 4e-
```

The first reaction describes the formation of H2-dominated gaseous mixture, under reducing conditions. The second reaction describes the formation of O2-dominated gaseous mixture, under oxidising conditions.

If the system reaches global equilibrium, then the water component is electrolyzed to H+ and O-2 at all pH conditions. The degree of electrolysis depends on the pH value in the aqueous solution phase. If Eh gets high enough, then the O-2 anion is oxidized to O2 (aqs). On the other hand, if Eh gets low enough, then the H+ cation is reduced to H2 (aqs). The major electrolysis and redox reactions are the following:

```
H2O (water) = H+ + OH- → Electrolysis of water at all pH.
H2O (water) = 2H+ + O-2 → Electrolysis of water at all pH.
O-2 - 2e- = 0.5O2 (aqs) → Oxidation or de-electronization of O-2 at high
Eh.
2H+ + 2e- = H2 (aqs) → Reduction or electronization of H+ at low Eh.
```

At a critically high Eh value under a given pH condition, an aqueous solution phase with a high enough O2 activity becomes less stable than an O2-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system. The replacement process can be characterised by the following phase-transformation on the aqueous-gas phase boundary and oxidation of remaining water:

```
O2 (aqs)  = O2 (gas)
H2O (water) - 2e- = 2H+(gas) + 0.5O2 (gas)
```

Similarly, at a critically low Eh value under a given pH condition, an aqueous solution phase with a high enough H2 activity becomes less stable than a H2-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system, through the following phase-transformation on the aqueous-gas phase boundary and reduction of remaining water:

```
H2 (aqs)  = H2 (gas)
H2O (water) + 2e- = O-2 (gas) + H2 (gas)
```

The phase transformation from an aqueous solution phase to an O2- or H2-dominated gaseous mixture phase also depends on the total molar Gibbs energies of the phases (which

are complex functions of the phase constituents, the temperature and the pressure). The Gibbs energy minimization technique used in Thermo-Calc ensures that the phase transformation is accurately simulated.

The following Pourbaix diagrams show the result of a calculation where the gaseous mixture phase was included. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase has been oxidized and reduced, respectively, to an O2- or H2-dominated gaseous mixture phase.

The two example diagrams show that the upper and lower boundaries between the aqueous phase (water) and the gas phase (dominated by either O2 or H2) can shift when solutes dissolve or when the temperature and pressure change.

Accordingly, if one does not take a gaseous mixture phase into account when performing a calculation of Pourbaix diagram (as above), then the aqueous solution phase may end up with an extremely high O2 (aqs) concentration at high Eh condition, or an extremely high H2 (aqs) concentration at low Eh condition. Under either of these two extreme circumstances, the concept of “aqueous solution phase” is no longer valid and consequently no proper aqueous solution model can actually be applied. Therefore, from a restrictive thermodynamic equilibrium point of view, one shall normally include a gaseous mixture phase in an aqueous-bearing heterogeneous interaction system. This is true for all types of equilibrium calculations for an aqueous-bearing heterogeneous interaction system, not only of Pourbaix diagram calculations.

Hence, to perform a completely accurate Pourbaix diagram calculation, the gaseous mixture phase must be taken into account. However, since these electrochemical reactions normally have much higher kinetic barriers and are slower than other electrochemical and chemical reactions in the interaction system, one can sometimes ignore the gaseous mixture phase in the calculation. Note that if the gaseous mixture phase is ignored in this way, then the Pourbaix diagram does not show the H2O-stability limiting lines.

Examples

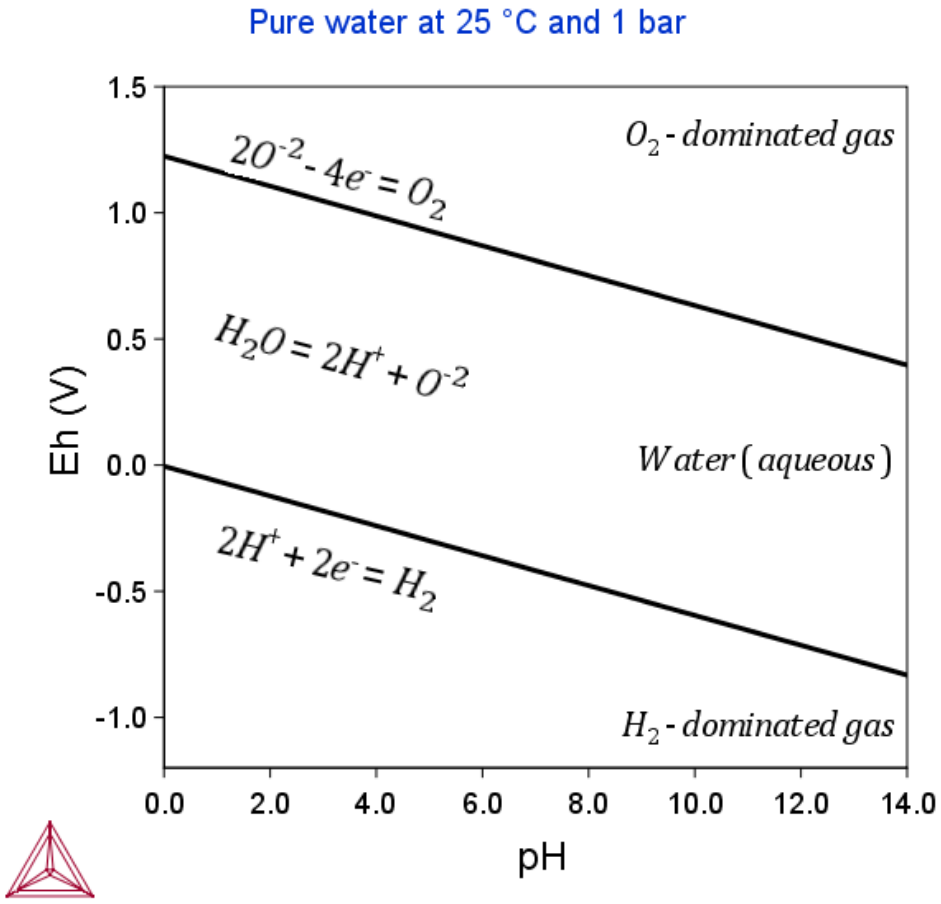


Figure 114: A pH-Eh diagram for pure water at 25° C and 1 bar.

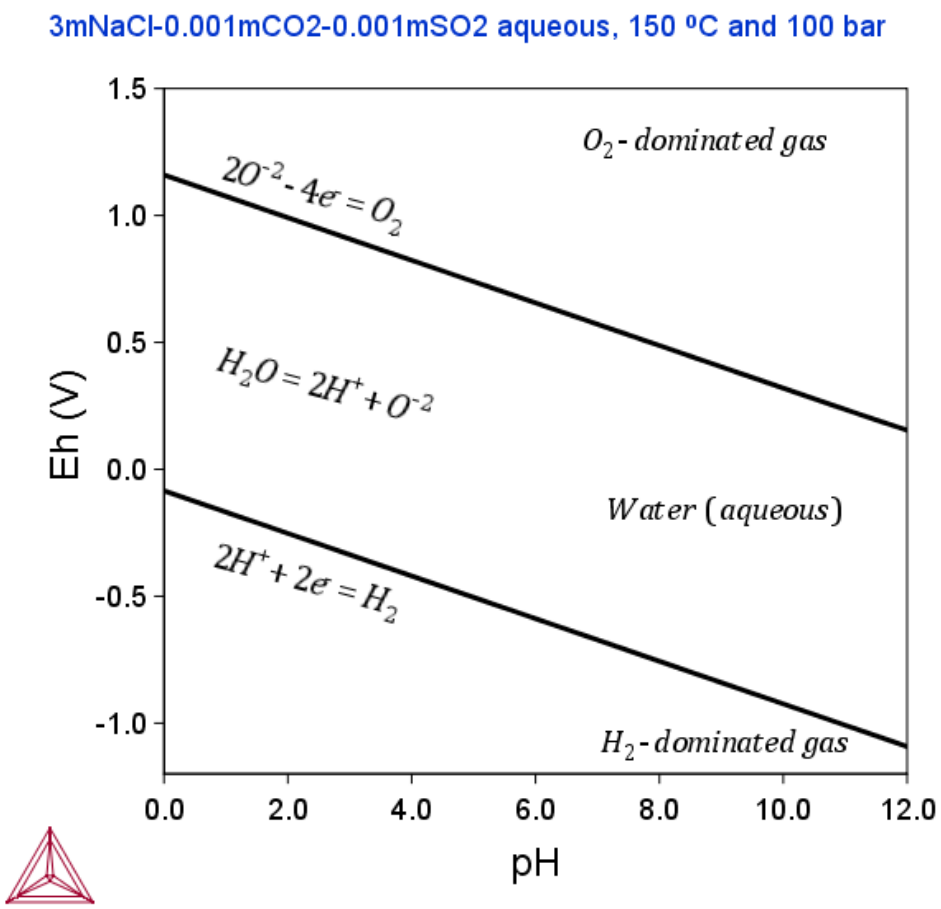


Figure 115: A pH-Eh diagram for 3mNaCl-0.001mCO2-0.001mSO2 aqueous solution at 150° C and 100 bar.

Examples of Pourbaix Diagrams for Fe

The following two topics are examples of Pourbaix diagrams for Fe. For the first example, the calculations on which the diagrams are based have not taken the gas phase into account. The diagrams in the second example are based on calculations that have taken the gas phase into account.

In this section:

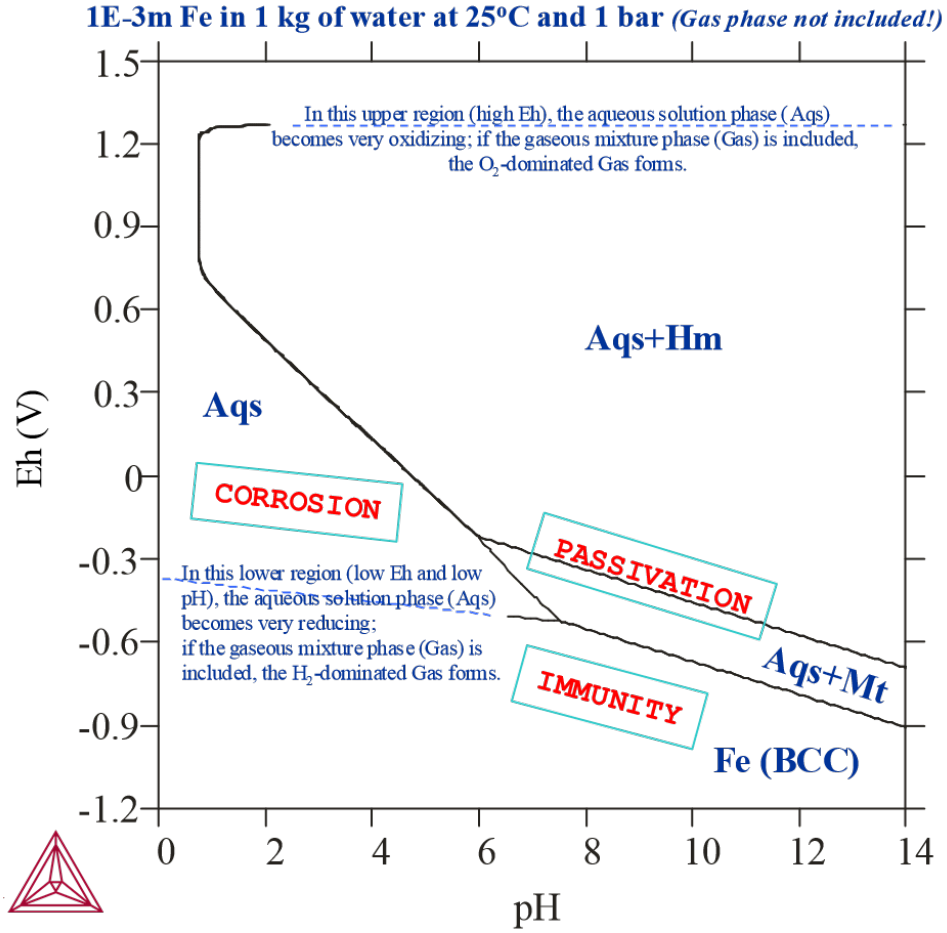
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Pourbaix Diagrams with Gas Phase Included 21

Pourbaix Diagrams with Gas Phase Excluded

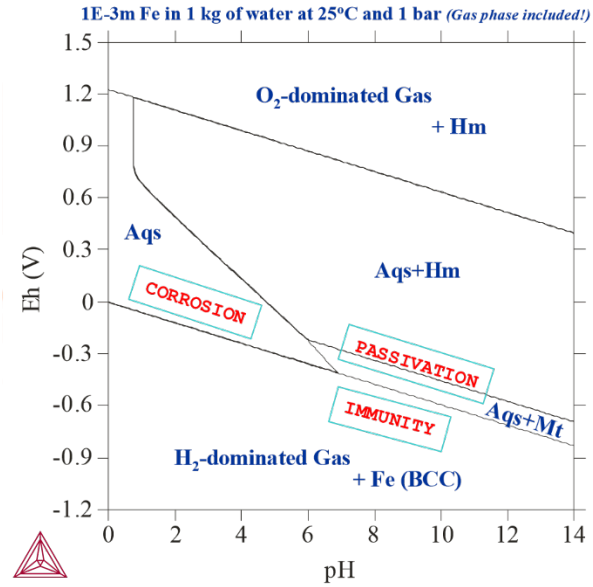
This is an example of a Pourbaix diagram of Fe, in which the gas phase has not been considered in the calculation. The system has 0.001 mole of Fe in 1 kg of pure water at a temperature of 25oC and a pressure of 1 bar. Magnetite (Mt, Fe3O4) and hematite (Hm, Fe2O3) co-exist with the Fe-containing dilute aqueous solution. The formation of magnetite and hematite represent the passivation of iron in the upper right pH-Eh field.

If pH is low and Eh is relatively high, then Fe eventually completely dissolves into the aqueous solution phase. Under conditions of low Eh, Fe remains in its stable solid state, the BCC phase, and neither dissolves into water nor into alternates to Fe (the immunity of Fe).



Pourbaix Diagrams with Gas Phase Included

With all the possible redox reactions involving the aqueous solution phase and gaseous mixture phase being considered in the equilibrium system, that is, the gaseous mixture phase is included in the calculation, the Pourbaix diagram of Fe in a system with 0.001 mole of Fe in 1 kg of pure water at 25oC and 1 bar.



Comparing this Pourbaix diagram with that from Basic Settings and Definitions, you can see that both diagrams are for the same interaction system under the same temperature-pressure condition, but the present diagram shows the results of calculations where the gaseous mixture phase has been included. It presents the complete Pourbaix diagram for the defined interaction system, in a full thermodynamic equilibrium. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase is oxidised and reduced to the O2- or H2-dominated gas phase. Hematite coexists with the O2-dominated gas, while Fe-BCC is stable with the H2-dominated gas. The stability field of magnetite may extend slightly into the H2-dominated gas region, where it coexists with the gaseous mixture instead of the aqueous solution. Its boundary with Fe (BCC) cannot be drawn due to the absence of aqueous solution phase.

It is not possible to calculate the pH value in both the O2- and H2-dominated gaseous mixture phase stability regions where the aqueous solution phase is absent. Hence, in a normal Pourbaix diagram, no line is drawn that indicates a phase boundary between the gas phase and the metallic phases or secondary phases (that is, metal-oxides).

Other Examples of Pourbaix Diagrams

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Variations of Pourbaix Diagrams 23

Pourbaix Diagrams for Complex Alloys 26

Variations of Pourbaix Diagrams

The shape of a Pourbaix diagram of an alloy or condensed material and the stability relations of various secondary phases depend upon the following system factors:

- Initial amount of the alloy or other condensed materials
- Initial composition of the alloy or other condensed materials
- Initial amount of the interacting aqueous solution phase
- Initial composition of the interacting aqueous solution phase
- Temperature and pressure conditions

In the interaction system that the diagrams in Pourbaix Diagrams with Gas Phase Excluded and Pourbaix Diagrams with Gas Phase Included are based on, the initial amount of pure Fe that was taken to have effectively reacted with 1 kg of pure water at 25° C and 1 bar was 0.001 m. The following diagrams are Pourbaix diagrams of Fe where other initial amounts of pure Fe have been used, or where the interacting aqueous solution compositions have been alternated, or the temperature and/or pressure have been changed. Gaseous mixture phases have been included in all the calculations that these diagrams are based on.

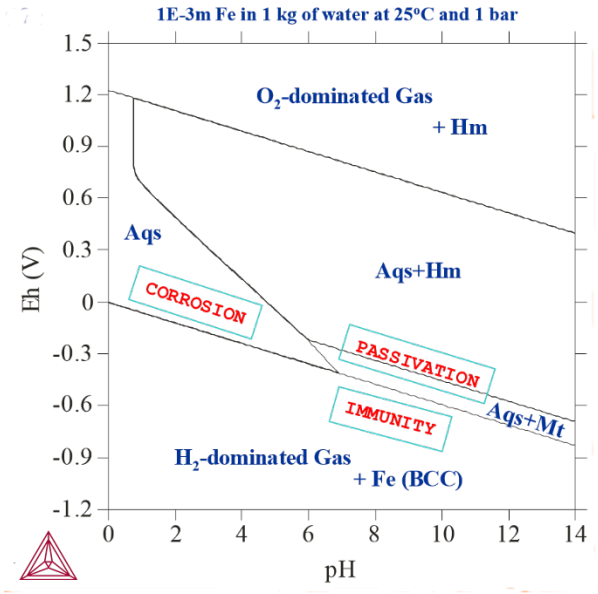


Figure 116: 1E-3 m Fe actively reacted with 1 kg of pure water at 25° C and 1 bar (as in the calculation in Pourbaix Diagrams with Gas Phase Included).

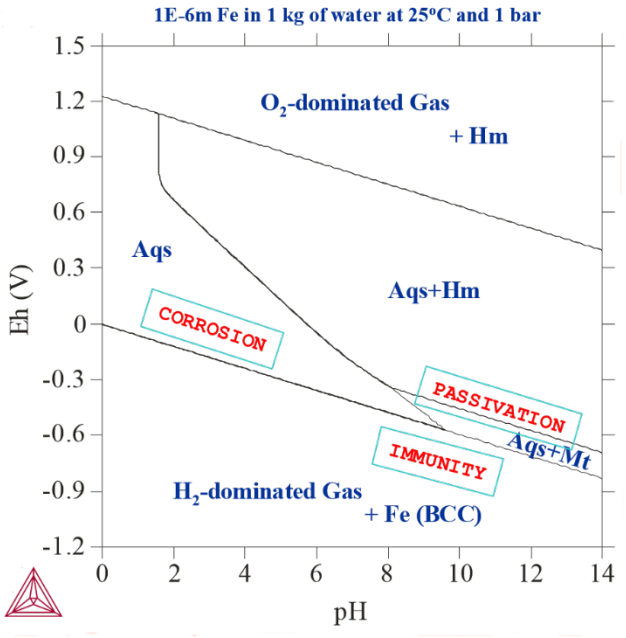


Figure 117: 1E-6 m Fe actively reacted with 1 kg of pure water at 25° C and 1 bar. Note that the active metal corrosion region gets enlarged as the initial Fe amount decreases from 1E-3m to 1E-6m.

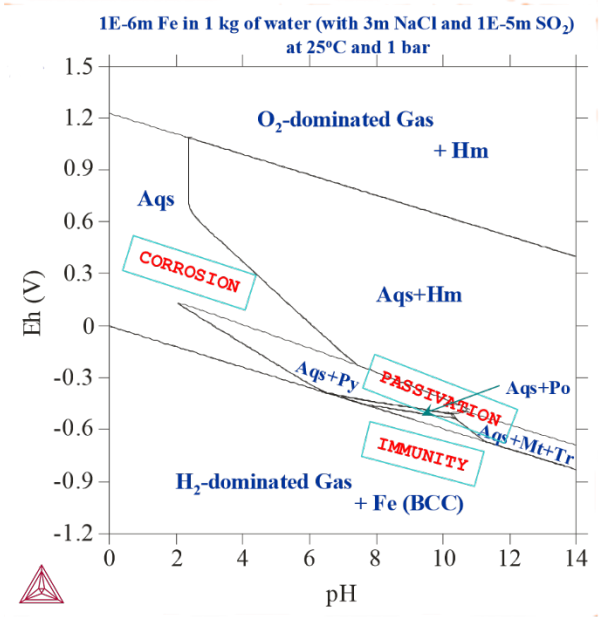


Figure 118: 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO2 at 25° C and 1 bar. Introducing SO2 into the system leads to the formation of various metal-sulphides (Py-pyrite, Popyrrhotite, Tr-troilite). In addition, the passivation region becomes larger.

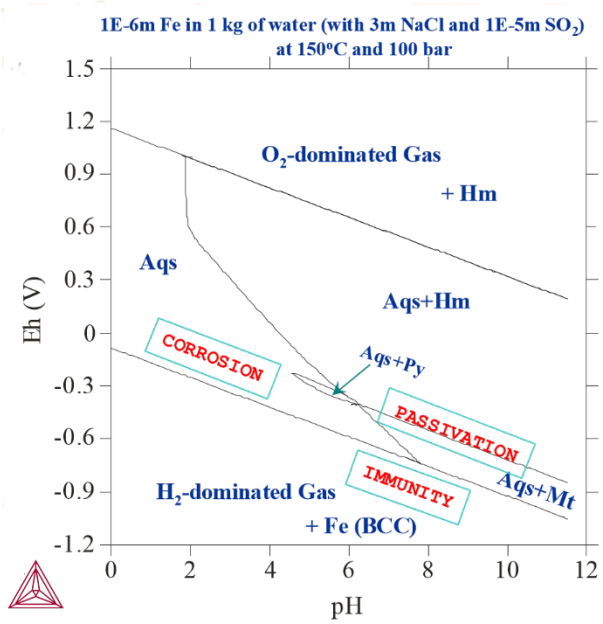


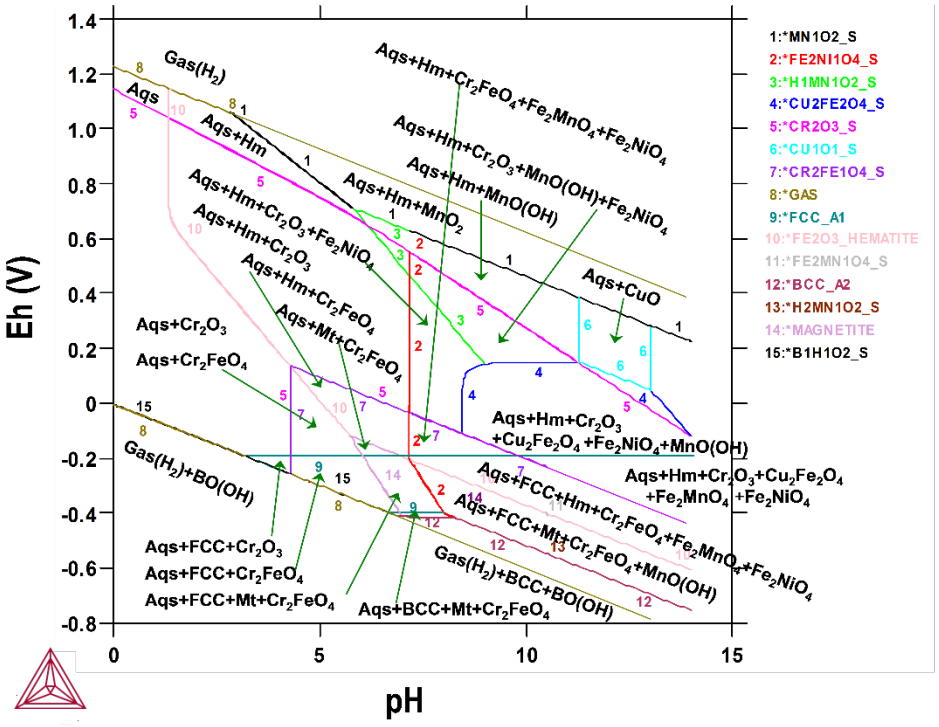
Figure 119: 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO2 at 150° C and 100 bar. Here, changing the temperature and pressure affects the stability fields of various Fe-oxides/sulphides.

As you can see from the figures, the aqueous-gas phase boundaries shift as the initial bulk compositions, pressure and temperature conditions in the interaction system change.

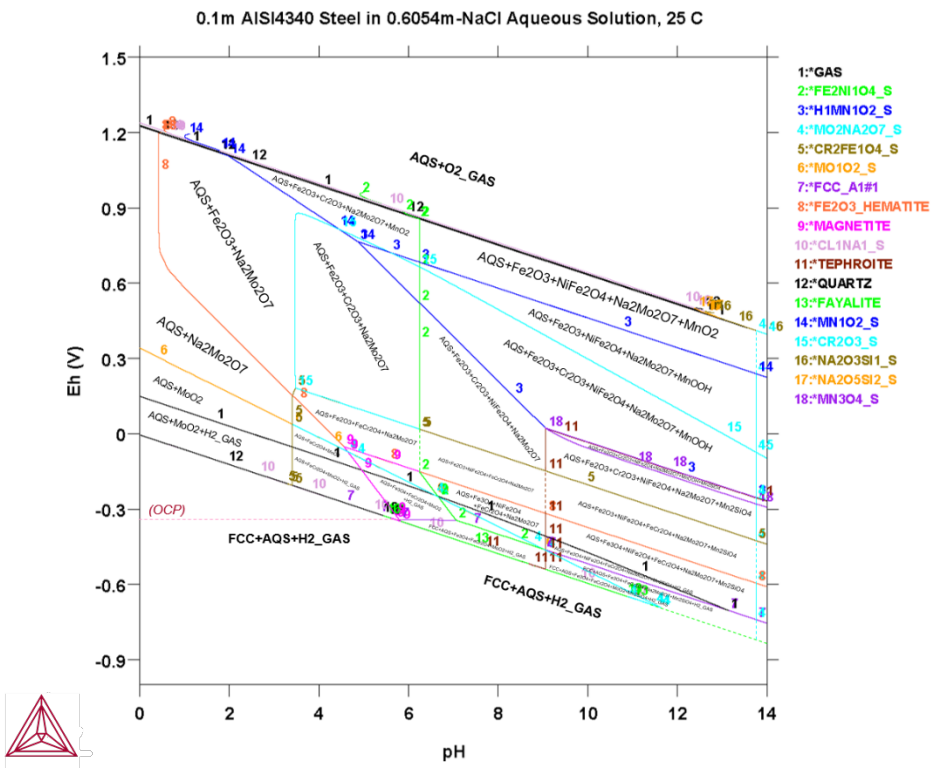
Pourbaix Diagrams for Complex Alloys

Thermo-Calc can not only be used to simulate how pure metals interact with pure water or simple aqueous solutions under normal pressure and temperature conditions. It can also be used to calculate how complex alloys and concentrated aqueous solutions interact over a very wide pressure, temperature and composition ranges. This is illustrated with the two examples.

The first example is a Pourbaix diagram calculated for the heterogeneous interaction between 0.001 mole of steel (Fe-7.676Cr-5.0Ni-2.1887Mn-1.0Cu [at%]) and 1 kg of water (and with 1.2 m H3BO3, 0.022 m Li and 0.001 m NH3), at 25° C and 1 bar. This application is particularly useful for safety assessments of nuclear reactors and nuclear waste repositories.



The next example is a Pourbaix diagram calculated for the heterogeneous interaction systems between 0.1 mole of AISI4340 stainless steel (Fe-0.80Cr-1.85Ni-0.70Mn-0.25Mo-0.25Si-0.40C [wt%]) and 1 kg of seawater (with the equivalent of 0.6054 m NaCl), at 25° C and 1 bar. This application is particularly useful for failure analysis of petroleum exploitation industry.



Pourbaix Diagram References

1. Andersson J-O., Helander T., Höglund L., Shi P., and Sundman B. (2002). Thermo-Calc and DICTRA, Computational tools for materials science. *Calphad*, 26: 273-312.
2. Ciavatta, L. (1990). The specific interaction theory in equilibrium analysis. Some empirical rules for estimating interaction coefficients of metal ion complexes. *Ann Chim. (Rome)*, 80, 255-263.
3. Cramer, S.D. and Covino, B.S. Jr. (2003). *Corrosion: Fundamentals, Testing, and Protection*. ASM Handbook, Volume 13A.
4. Helgeson, H.C., Kirkham, D.H., and Flowers, G.C. (1981). Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600° C and 5 kb. *Am. J. Sci.*, 281, 1249- 1516.
5. Johnson, J.M. and Norton, D. (1991). Critical phenomena in hydrothermal system: State, thermodynamic, electrostatic, and transport properties of H_2O in the critical region. *Am. J. Sci.*, 291, 541-648.

6. Kaufman, L. (2002). Calculation of Pourbaix diagrams for C22 in various well water chemistries. In: *Proceedings for the 5th Nickel Development Institute Workshop on Fabrication of Welding of Nickel Alloys* (R. Moeller, ed.), Nickel Development Institute, Las Vegas, Nevada, 16-17 Oct., 2002.
7. Kaufman, L., Perepezko, J.H., Hildal, K., Farmer, J., Day, D., Yang, N., and Branagan, D. (2009). Transformation, stability and Pourbaix diagrams of high performance corrosion resistant (HPCRM) alloys. *Calphad,* 33: 89-99.
8. Pourbaix, M. (1973). *Lectures on Electrochemical Corrosion*. Plenum Press, New York.
9. Pourbaix, M. (1974). *Atlas of Electrochemical Equilibria in Aqueous Solutions, 2nd Ed*, Houston, Tex., National Association of Corrosion Engineers.
10. Shi, P. (2013a). *Thermo-Calc 3.0 (Console Mode) Manual* (including *TC3-CM User's Guide*, and *Thermo-Calc Software System*), Thermo-Calc Software, Stockholm, Sweden.
11. Shi, P. (2013b). *Materials Corrosion Applications with Thermo-Calc Software.* Thermo-Calc Software, Stockholm, Sweden.
12. Shi Pingfang, Engström A, and Sundman B (2011a). Thermodynamic investigations on materials corrosion in some industrial and environmental processes. *Journal of Environmental Sciences*, 23 (Supplement): S1-S7.
13. Shi, P., Engström, A., Sundman, B., and Ågren, J. (2011b). Thermodynamic calculations and kinetic simulations of some advanced materials. *Materials Science Forum*, 675-677: 961-974.
14. Thompson, W.T., Kaye, M.H., Bale, C.W., and Pelton, A.D. (2011). Pourbaix diagrams for multielement systems. In: *Uhlig's Corrosion Handbook, 3rd Edition (Revie RW, Ed.)*, The Electrochemical Society and Jon Wiley & Sons, New Jersey.
15. Verink, E.D. (2011). Simplified procedure for constructing Pourbaix diagrams. In: *Uhlig's Corrosion Handbook, 3rd Edition (Revie RW, Ed.)*, The Electrochemical Society and Jon Wiley & Sons, New Jersey.

Thermo-Calc: General Reference

Miscellaneous Information

Generally applicable to multiple applications within Thermo-Calc, i.e. in both Console Mode and Graphical Mode, or needed for a specific database calculation in Thermo-Calc (i.e. thermophysical properties), etc.



Parameters, Functions, and Variables

This section is applicable to both Console Mode and Graphical Mode with respect to understanding the format these are to be written in for Thermo-Calc to use the parameter, function, or variable. However, many of the sections are specific to Console Mode where the explicit use of these terms is more often used.

To learn about using variables and functions, in Graphical Mode, see T_07: User-Defined Functions and in Console Mode, see example 44 .

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Specifying Parameters



This section or topic is specific to Console Mode.

Running a command typically requires that several parameter values are specified, which can be done directly in the command line after the command name. For example, to set an axis variable for a stepping or mapping operation, enter:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

You can also use SET_AXIS_VARIABLE and press <Enter>. At the command line prompt, you then specify the parameters one at a time.

On all command lines, you can enter a question mark (`?`) for help. For some parameters, enter two question marks (`??`) for more detailed information.

Default Parameters Values

When you are requested to specify a parameter, Thermo-Calc usually suggests an appropriate default value, which is displayed at the prompt between two slash signs (//). For example, this prompt means the default answer is `TERMINAL`:

```
OUTPUT FILE /TERMINAL/:
```

Press <Enter> to accept the default.

If you specify some parameters directly after the command name, then you can still choose to accept default values for some parameters.

To accept the default value for a parameter, type a comma (,) instead of a value for that parameter. For the comma to be interpreted correctly, type a blank space on each side of the comma. However, if you accept the default values for several parameters that follow each other, then the commas can be typed in without blank spaces separating them: (, , ,) is interpreted in the same way as (, , ,).

For some commands and parameters, Thermo-Calc treats the values previously assigned as default values if the command is used again. For example, if the first stepping or mapping axis variable is specified as:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

Then if you want to change a parameter value for this axis variable, type:

```
SET_AXIS_VARIABLE 1 , 0.1 ,,,
```

This changes the minimum value from 0 to 0.1 at which a stepping or mapping operation halts. The other parameter values remain the same. Consequently, what is typed is equivalent to:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0.1 0.89 0.025
```

About Operators and Functions

Sometimes you need to specify functions when setting up a system. For example, to make global conditions vary as a function of time.

The following operators can be used in writing functions. Use a semi-colon (;) to mark the end of a function.

Available Operators for Writing Functions

Operator	Description
+, -, *, /	Addition, subtraction, multiplication, division
**	Exponentiation, raising one quantity to the power of another, e.g. x^2.
ABS()	Absolute value
ERF(X)	Error function
EXP(X)	Exponential
LOG(X)	Natural logarithm
LOG10(X)	Base 10 logarithm
SIGN(X)	Sign function SIGN(X) is -1 when X<0, is 0 when X=0 and is 1 when X>0.
SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)	• Trigonometric functions: sine, cosine, tangent • Inverse trigonometric functions: arcsine, arccosine, arctangent
SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH (X)	• Hyperbolic trigonometric functions • Inverse hyperbolic functions
SQRT(X)	Square root

Thermodynamic Variables

There are different thermodynamic variables in Thermo-Calc. Some are *state variables*, for example temperature, pressure and mole fraction. These characterize the equilibrium state of a system. You set them when you define your system in the POLY module before performing a calculation. They are also used in other modules such as DATA, GIBBS and PARROT. State variables that involve components can be used for the defined components, but not for any species. (To define new components in a defined system, use DEFINE_COMPONENTS).

Other useful thermodynamic variables are derive from state variables with a mathematical function. Some derived variables are pre-defined by Thermo-Calc, such as normalized energetic and compositional extensive state variables for example. You use these by appending various normalizing suffixes to abbreviations that are associated with the state variables.

Thermodynamic variables can also be divided into extensive variables and intensive variables. An extensive variable is a variable whose value depends on the size of the system, whereas an intensive variable is a variable whose value is independent of system size.

More information about thermodynamic variables is available in the online help in Thermo-Calc Console Mode. Use the command INFORMATION, with a subject keyword such as one of the following as argument: STATE VARIABLES, INTENSIVE VARIABLES, EXTENSIVE VARIABLES, DERIVED VARIABLES, CONDITIONS (for condition settings), AXIS-VARIABLES (for stepping/mapping variable settings).

Common Thermodynamic Variables

The tables below list common thermodynamic variables. Most of these can be used to define equilibrium conditions in the POLY module unless otherwise indicated.

The variables are divided into the following tables:

- Intensive variables
- Energy-related extensive variables for whole system or for a phase
- Compositional extensive variables (overall amount of components in the whole system, or amount of a component in system or in a phase)
- Constitutional composition-related extensive variables (amount of a constituent/species on a sublattice site in a phase)
- Special quantities

How to Read the Tables

- The *Abbrev*. column shows the abbreviation that you use in the POLY module for referring to the variable. If the variable must be given any arguments, then these are given in parenthesis directly after the abbreviation. For most variables, this is also the abbreviation that you use to refer to the variable in other modules. However, some variables are referred to with a different abbreviation in the POST module. If this is the case, then this is noted at the bottom of the table.
- Variables that are specific to a species, in which case the species is specified as an argument (*sp* in the table below). If there are two or more sublattices in a given phase, then this argument is given as `constituent#sublattice`. This indicates a constituent on a specific sublattice or site in the phase (referred to by the # sign and a digit). For example, `y(BCC,C#2)` stands for the site fraction of the C species on the second sublattice site of the BCC_A2 solution phase.
- The *Unit* column show which unit that you can use to express the variable in the POLY module. This unit is always the SI unit. In other modules, state variables may be expressed in other units.
- The *Suffix* column shows the suffixes you can append to the variables. The `R` suffix can be used with all compositional extensive state variables, but the suffix does not always change the value of the variable. This is indicated by putting the `R` in parenthesis.

These types of variables are listed in the following topics:

- Intensive Variables
- Extensive Variables
- Special Quantities
- The u-Fraction Variable
- Suffixes

Intensive Variables

V	Abbrev.	Unit	Descript.	Domain	Suffix
T	T[1]	K	Temperature	System	
P	P	Pa	Pressure	System	
μ	MU(comp)	J/mol	Chemical potential	Component	R
	MU(sp,ph)[2]			Species relative to a solution phase	R
a	AC(comp)	N/A	Activity	Component	R
	AC(sp,ph)[2]			Species relative to a solution phase	R
	LNAC (comp)[3]		ln(Activity)	Component	R
	LNAC (sp,ph) [2]			Species relative to a solution phase	R

[1] When plotting in POST, besides T (Kelvin), you can also use T_C or T_F to plot temperature in °C or °F.

[2] Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASeous mixture phases and for interacting species on the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).

[3] In natural logarithm (lnAC=MU/RT)

Extensive Variables

Energy-Related Extensive Variables for Whole System or for a Phase

V	Abbrev.	Unit	Descript.	Domain	Suffix
V	V	m^3	Volume	System	M, W, V, R
	V(ph)[1]			Phase	M, W, F, R
	VP(ph) [2]			Phase	M, W, V, R
G	G	J	Gibbs energy	System	M, W, V, R
	G(ph) [1]			Phase	M, W, V, F, R
A	A	J	Helmholtz energy	System	M, W, V, R
	A(ph) [1]			Phase	M, W, V, F, R
U	U	J	Internal energy	System	M, W, V, R
	U(ph) [1]			Phase	M, W, V, F, R
H	H	J	Enthalpy[6]	System	M, W, V, R
	H(ph)			Phase	M, W, V, F
S	S	J/K	Entropy[6]	System	M, W, V, R
	S(ph) [1]			Phase	M, W, V, F, R
Cp	HM.T^3	J/mol/K	Heat capacity at constant pressure	System	R
	HM(ph).T^3			Phase	R
Cv	HM.T^4	J/mol/K	Heat capacity at constant volume	System	R
	HM(ph).T^4			Phase	R

V	Abbrev.	Unit	Descript.	Domain	Suffix
D	DG(ph) [5]	N/A	Driving force (thermodynamic factor)	Phase	Always use with M, W, V or F. R can also be used.

[1] For this variable, if the phase is unstable, then the variable gets a value of zero.

[2] Do not use VP(ph) as a condition in POLY. Instead, use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to VPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then VP(ph) and its normalized quantities get zero value.

[3] Use only if pressure has been set as a condition.

[4] Use only if volume has been set as a condition.

[5] Already divided by RT.

[6] When working in the POST module you can also enter the abbreviation for this variable into the Console, for example, `enth` or `enthalpy`, which corresponds to `HM`, and `entr` and `entropy`, which corresponds to `SM`.

Compositional Extensive Variables

These are for the overall amount of components in whole system, or amount of a component in system or in a phase.

Do not use NP(ph) or BP(ph) as conditions in the POLY module. Instead use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to NPF(ph) or BPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then NP(ph) or BP(ph) (and its normalized quantities) get zero value.

When plotting the following quantities in POST, refer to each as indicated:

- X(comp) -> `Mole-Fraction <comp>` (or `M_F`)
- W(comp) -> `Weight-Fraction <comp>` (or `W_F`)
- X%(comp) -> `Mole-Percent <comp>` (or `M_P`)
- W%(comp) -> `Weight-Percent <comp>` (or `W_P`).
- u-f(ph,comp) -> `U-F`

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
n	N	mole	Moles	All	M, W, V,	

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
				components	(R)	
	N(comp)			Component	M, W, V, (R)	
	N(ph,comp)			Component in a phase	M, W, V, (R)	
	NP(ph)[1]			Phase	M, W, V, (R)	See above
b	B	gram	Mass	All components	M, W, V, (R)	
	B(comp)			Component	M, W, V, (R)	
	B(ph,comp)			Component in a phase	M, W, V, (R)	
	BP(ph) [1]			Phase	M, W, V, (R)	See above
x	X(comp)	N/A	Mole fraction	Component	(R)	See above
	X(ph,comp)			Component in a phase	(R)	
w	W(comp)	N/A	Mass (weight) fraction	Component	(R)	See above
	W(ph,comp)			Component in a phase	(R)	
x%	X%(comp)[2]	N/A	Mole percent	Component	(R)	See above
w%	W%(comp)[2]	N/A	Mass (weight) percent	Component	(R)	See above
u	u-f (ph,comp)[1]	N/A	u-fraction	Component in a stable phase	(R)	See above
in	IN(sp)[2]	mole	Input mole number	Phase species in the system	(R)	See above

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
im	IM(sp)[2]	gram	Input mass unit	Phase species in the system	(R)	See above

[1] Do not use as a condition in the POLY module.

[2] Only available in TQ-Interface and TC-API.

Constitutional Composition-Related Extensive Variable

This is the amount of a constituent/species on a sublattice site in a phase.

V	Abbrev.	Unit	Descript.	Domain
y	Y(ph,cons#sub)	N/A	Site fraction	Constituent on a sublattice site (denoted by # and a digit) in a phase

Special Quantities

Variable	Abbrev.	Unit	Description or Example	Domain	Suffix
Q	QF(ph)[1]	n/a	Phase stability function	Phase	R Under a condition and system definition, QFR(ph) = QF (ph)
Tc	TC(ph) [2]	K	Curie temperature	Phase	R Under a condition and system definition, TCR(ph) = TC (ph)
Mb	BMAG(ph)[3]	n/a	Bohr magneton number	Phase	R Under a condition and system definition, BMAGR (ph) = BMAG (ph)
D1G	D1G(phase, site-fraction)	n/a	For example, D1G(FCC_A1#1, Cr#1) for first derivative of G for first composition set of FCC_A1 phase with respect to Cr site fraction on first sublattice. ▶ Search for TQGMDY in the *TQ-Interface Guide*	Phase	n/a
D2G	D2G(phase, site-fraction, site-fracton)	n/a	For example, D2G(FCC_A1#2, Cr#1, Cr#1) for second derivative of G for second composition	Phase	n/a

Variable	Abbrev.	Unit	Description or Example	Domain	Suffix
			set of FCC_A1 phase with respect to Cr site fraction on first sublattice. ▶ Search for TQDGYY in the *TQ-Interface Guide*		

[1] Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.

[2] Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST or evaluated in POLY using SHOW_VALUE.

[3] Calculated for phases with magnetic contributions in an equilibrium state.

n/a = not applicable

The u-Fraction Variable

The u-fraction is an important quantity in some single-point or stepping paraequilibrium calculations in the POLY module and in the DICTRA module. You can apply the variable in a paraequilibrium calculation to the substitutional matrix component, the substitutional alloying components or the interstitial component. The u-fraction is denoted as ui for the i-th system component *n* of a whole system or of a specific phase in various equilibrium states (such as full-equilibria, partial-equilibria, para-equilibria, local-equilibria).

Generally, the u-fraction is defined as:

$$\frac{x_i}{\sum_{j \in S} x_j}$$

The sum of x_j in the denominator is calculated for all substitutional alloying elements in the whole system or in a specific phase. The variable x_i in the numerator stands for the mole-fraction of the *i*-th component in the whole system or in the specific phase.

Suffixes

Suffixes may be appended to all extensive variables and to some intensive variables. Some suffixes can be used to enter the value of variables in normalized form. These are referred to as normalizing suffixes. If the variable that you create with a normalizing suffix is based on a state variable that can be set as a condition in POLY, then the normalized variable can also be set as a condition in POLY.

The normalizing suffixes are M (per mole), W (per mass in gram), V (per volume in m^3) and F (per mole formula unit). There is also a reference state suffix R, which you can use if you want the value of a thermodynamic variable to be calculated with respect to a reference state that have previously set.

Normalizing Suffixes

When variables that express system and phase quantities are normalized, the following general rules are used:

- System quantities are normalized by the total system size (in terms of N, B or V).
- Phase quantities are normalized by the phase amount [in terms of NP(ph), BP(ph) or VP(ph)].

The normalized quantities of G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) are calculated according to the thermodynamic model used for the phase (e.g. GM(ph), AM(ph), UM(ph), HM(ph), SM(ph) and VM(ph)). These quantities are calculated using the first derivatives of the Gibbs energy expressed for the phase with respect to the current composition of the system.

The tables describe the normalizing suffixes for the different state variables.

G, A, U, H, S and V of a Whole System

Suffix	Description	Example
M (per mole)	Total system size in terms of N.	GM is the Gibbs energy per mole of the system (J/mol). $\mathrm{GM} = \mathrm{G}/\mathrm{N}$
W (per mass in gram)	The total system size in terms of B.	GW is the Gibbs energy per mass of the system (J/g).

Suffix	Description	Example
		$GW = G/B$
V (per volume in m^3)	The total system size in terms of V. VV does not have to be evaluated.	GV is the Gibbs energy per volume of the system (J/m^3). $GV = G/V$

G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) of a Phase

Suffix	Example
M (per mole)	For example, GM(ph) is Gibbs energy of the phase per mole of the phase (J/mol). $GM(ph) = G(ph)/NP(ph)$
W (per mass in gram)	For example, GW(ph) is Gibbs energy of the phase per mass of the phase (J/mol). $GW(ph) = G(ph)/BP(ph)$
V (per volume in m^3)	For example, GV(ph) is Gibbs energy of the phase per volume of the phase (J/mol). $GV(ph) = G(ph)/V(ph)$
F (per mole formula unit)	For example, GF(ph) is the Gibbs energy of the phase per formula unit of the phase (J/mol). $GF(ph) = G(ph)/NP(ph)^*NA$

DG(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGM(ph) is driving force for precipitation of the phase per mole of components. $DGM(ph) = \delta DG(ph)/\delta NP(ph)$

Suffix	Description	Example(s)
W (per mass in gram)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of BP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGW(ph) is driving force for precipitation of the phase per mass of components. DGW(ph) = ∂DG(ph)/∂BP(ph)
V (per volume in m^3)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of VP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGV(ph) is driving force for precipitation of the phase per volume of components. DGV(ph) = ∂DG(ph)/∂VP(ph)
F (per mole formula unit)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGF(ph) is driving force for precipitation of the phase per formula unit of components. DGF(ph) = ∂DG(ph)/∂NP(ph)*∂NA

N and B of a System

Suffix	Description	Example(s)
M (per mole)	The total system size in terms of N. NM does not have to be evaluated. BM cannot be set as a condition.	BM is mass (gram) of components per mole of the system (g/mol). $\mathrm{BM} = \mathrm{B}/\mathrm{N}$
W (per mass in gram)	The total system size in terms of B. BW does not have to be evaluated. NW cannot be set as a	NW is mole number of components per mass of the system (mol/g). $\mathrm{NW} = \mathrm{N}/\mathrm{B}$

Suffix	Description	Example(s)
	condition.	
V (per volume in m^3)	The total system size in terms of V. BV is the density of the entire system.	NV is mole number of components per volume of the system (mol/m^3). $\mathrm{NV} = \mathrm{N}/\mathrm{V}$ BV is the density of the entire system (g/m^3). $\mathrm{BV} = \mathrm{B}/\mathrm{V}$

N (comp) and B(comp) of a Component in the System

Suffix	Description	Example(s)
M (per mole)	The total system size in terms of N. BM(comp) cannot be set as a condition.	NM(comp) is the mole of a component per mole of the system (i.e. mole fraction, which also is expressed as X(comp)). $\mathrm{NM(comp)} = \mathrm{N(comp)}/\mathrm{N}$
W (per mass in gram)	The total system size in terms of B. NW(comp) cannot be set as a condition.	BW(comp) is mass (gram) of a component per mass of the system (i.e. mass fraction, which also is expressed as W(comp)). $\mathrm{BW(comp)} = \mathrm{B(comp)}/\mathrm{B}$
V (per volume in m^3)	The total system size in terms of V.	NV(comp) is mole number of a component per volume of the system (mol/m^3). $\mathrm{NV(comp)} = \mathrm{N(comp)}/\mathrm{V}$

NP(ph), BP(ph) and VP(ph) of a Phase in the System

Suffix	Description	Example(s)
M (per mole)	BPM(ph) and VPM(ph): The phase amount in terms of NP(ph). NPM(ph): The total system size in terms of N.	BPM(ph) is mass (gram) of a phase per moles of the system (g/mol). $\mathrm{BPM(ph)} = \mathrm{BP(ph)}/\mathrm{N}$ NPM(ph) is number of moles of a phase per moles of the system (mole fraction).

Suffix	Description	Example(s)
		$$\mathrm{NPM(ph) = NP(ph)/N}$$
W (per mass in gram)	NPW(ph) and VPW(ph): The phase amount in terms of BP(ph). BPW(ph):The total system size in terms of B.	VPW(ph) is volume (m^3) of a phase per mass of the system (m^3/g) $$\mathrm{VPW(ph) = VP(ph)/B}$$ BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction) $$\mathrm{BPW(ph) = BP(ph)/B}$$
V (per volume in m^3)	NPV(ph) and BPV(ph): The phase amount in terms of VP(ph). VPV(ph): The total system size in terms of V.	NPV(ph) is number of moles of a phase per volume of the system (mol/m^3). $$\mathrm{NPV(ph) = NP(ph)/V}$$ VPV(ph) is volume (m^3) of a phase per volume of the system (volume fraction). $$\mathrm{VPV(ph) = VP(ph)/V}$$

N(ph,comp) and B(ph,comp) of a Component in a Phase

Suffix	Description	Example(s)
M (per mole)	The phase amount in terms of NP(ph) of the phase.	NM(ph,comp) is number of moles of a component per mole of a phase (i.e. mole fraction of a component in a phase, which is equivalent to X(ph, comp)). $$\mathrm{NM(ph,comp)} = \mathrm{N(ph,comp)/NP(ph)}$$
W (per mass in gram)	The phase amount in terms of BP(ph) of the phase.	BW(ph,comp) is mass (gram) of a component per mass of a phase (i.e. mass fraction of a component in a phase, which is equivalent to W(ph,comp)). $$\mathrm{BW(ph,comp)} = \mathrm{B(ph,comp)/BP(ph)}$$
V (per volume in m^3)	The phase amount in terms of VP(ph) of the phase.	NV(ph,comp) is mole number of a component per volume of a phase (mol/m^3). $$\mathrm{NV(ph,comp)} = \mathrm{N(ph,comp)/VP(ph)}$$

The Reference State Suffix R

- SET_REFERENCE_STATE

You can use the reference state suffix `R` for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the SET_REFERENCE_STATE command in POLY (or in response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the `R` suffix depends on the reference states of all the components in the defined system.



It is possible to use an `R` suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then MUR(comp)= MU (comp), ACR(comp)= AC(comp) and LNACR(comp)= LNAC(comp).

In the case of some thermodynamic variables, you can also use the R suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

Derived Variables and Partial Derivatives

Many derived variables can be obtained easily by using partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others.

Derivatives of state variables can be defined or evaluated by putting a dot (.) between two state variables. The variable after the dot must be a condition that you have set when you defined your system. For example, the heat capacity (at constant pressure or volume) of a system is the partial derivative of the state variable enthalpy with respect to temperature. To evaluate this derivative, use the designation HM.T, where temperature is a state variable that you have set already.

Any partial derivative of a state variable with respect to another can be defined or evaluated as a derived variable by using the dot (.) notation.

Derived Variables Dot Notation Examples

The following table shows some examples:

Derived variable	Description
$\mathrm{HM.T} = \partial \mathrm{HM}/\partial \mathrm{T}$	Heat capacity for the system at either constant P if pressure is a condition or constant V if volume is a condition.
$\mathrm{HM(ph).T} = \partial \mathrm{HM(ph)}/\partial \mathrm{T}$	Heat capacity for a phase at either constant P if pressure is a condition or constant V if volume is a condition.
$\mathrm{H.T} = \partial \mathrm{H}/\partial \mathrm{T}$	Heat capacity for the system multiplied by total mole number of components, i.e., $\partial \mathrm{H}/\partial \mathrm{T} = \mathrm{C_p}{*}\mathrm{N}$ if pressure is a condition in a closed system or $\partial \mathrm{H}/\partial \mathrm{T} = \mathrm{C_v}{*}\mathrm{N}$ if volume is a condition in a closed system.
$\mathrm{H(ph).T} = \partial \mathrm{H(ph)}/\partial \mathrm{T}$	Heat capacity for a phase multiplied by the sum of $\mathrm{NP(ph)}$ and $\mathrm{HM(ph)}{*}\partial \mathrm{NP(ph)}/\partial \mathrm{T}$, i.e., $\mathrm{C_p(ph)}{*}\mathrm{NP(ph)}+\mathrm{HM(ph)}{*}\partial \mathrm{NP(ph)}/\partial \mathrm{T}$ if pressure is a condition or $\mathrm{C_{v(ph)}}{*}\mathrm{NP(ph)}+\mathrm{HM(ph)}{*}\partial \mathrm{NP(ph)}/\partial \mathrm{T}$ if volume is a condition.
$\mathrm{VM.T} = \partial \mathrm{VM}/\partial \mathrm{T}$	Thermal expansivity of the system (already multiplied by the total molar volume), i.e., $\partial \mathrm{VM}/\partial \mathrm{T} = \alpha{*}\mathrm{VM}$.
$\mathrm{VM(ph).T} = \partial \mathrm{VM(ph)}/\partial \mathrm{T}$	Thermal expansivity of a phase (already multiplied by its molar volume), i.e., $\partial \mathrm{VM(ph)}/\partial \mathrm{T} = \alpha\mathrm{(ph)}{*}\mathrm{VM(ph)}$.

Derived variable	Description
$V.T = \partial V/\partial T$	Thermal expansivity of the system (already multiplied by the total volume), i.e., $\partial V/\partial T = \alpha^* V$.
$V(ph).T = \partial V(ph)/\partial T$	Thermal expansivity of a phase (already multiplied by the phase volume) plus the $VM(ph)^*\partial NP(ph)/\partial T$ term, i.e., $\partial V(ph)/\partial T = \alpha(ph)^* V(ph) = \alpha(ph)^* VM(ph)^* NP(ph) + VM(ph)^*\partial NP(ph)/\partial T$.
$VM.P = -\partial VM/\partial P$	Isothermal compressibility of the system (already multiplied by the total molar volume), i.e., $\partial VM/\partial P - \kappa^* VM$.
$VM(ph).P = -\partial VM(ph)/\partial P$	Isothermal compressibility of a phase (already multiplied by its molar volume), i.e., $\partial VM(ph)/\partial P = -\kappa(ph)^* VM(ph)$.
$V.P = -\partial V/\partial P$	Isothermal compressibility of the system (already multiplied by the total volume), i.e., $\partial V/\partial P = -\kappa^* V$
$V(ph).P = -\partial V(ph)/\partial P$	Isothermal compressibility of a phase (already multiplied by the phase volume) plus the $VM(ph)^*\partial NP(ph)/\partial P$ term, i.e., $\partial V(ph)/\partial P = -\kappa(ph)^* V(ph) = -\kappa(ph)^* VM(ph)^* NP(ph) + VM(ph)^*\partial NP(ph)/\partial P$.
$T.X(comp) = \partial T/\partial X(comp)$	Slope of a phase boundary on a T-X(comp) phase diagram with respect to mole fraction of the component in the system.
$T.W(comp) = \partial T/\partial W(comp)$	Slope of a phase boundary on a T-W(comp) phase diagram with respect to mass of the component in the system.
$T.X(ph,comp) = \partial T/\partial X(ph,comp)$	Slope of a phase boundary on a T-X(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$T.W(ph,comp) = \partial T/\partial W(ph,comp)$	Slope of a phase boundary on a T-W(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$P.T = \partial P/\partial T$	Slope of a phase boundary on a P-T phase diagram (Note that the equilibrium with phase assemblage must be calculated first).

Defining New Derived Variables and Functions

You can define additional derived variables or functions based on a state variable by using ENTER_SYMBOL. Any derived variable or function must have a unique name that starts with a

letter and has a maximum number of eight characters. These characters can include both uppercase and lowercase letters, numerical digits and the underscore (_). No other characters are allowed.

The difference between new derived variables introduced with the ENTER_SYMBOL command and new functions introduced with the same command is as follows. Whenever Thermo-Calc calculates the value of a function (as part of an equilibrium calculation for example), all functions related to the defined system is evaluated. An entered derived variable, on the other hand, is only evaluated when it is defined and when it is re-evaluated with EVALUATE_FUNCTIONS.

Derived Variables for Aqueous Solutions

Standard state variables used for other phases can be directly applied to the aqueous solution phase. In addition, there are pre-defined derived variables for the aqueous solution phase in particular.

Examples of predefined derived variables for the aqueous solution phase are listed and briefly described in the following tables. Some derived variables for a gaseous mixture phase are also shown. This is because EOS (Equation of State) expressions, standard thermodynamic properties and transport properties of the pure solvent H2O are also expressions and properties of the pure gaseous species H2O.

For Aqueous Solution Phase

Name	Abbrev.	Units	Description	Comments
pH	PH	N/A	Acidity	of the aqueous solution phase pH = -log10(AC(H+)) = -log10 (ACR(H+,AQ))
Eh	EH	V, mV	Hypothetical electric potential	of the aqueous solution phase Eh = u(ZE)/96485.309
Pe	PE	N/A	Logarithm of the hypothetical electron activity	of the aqueous solution phase pe = u(ZE)/(2.3025851*RT)
Ah	AH	kJ, kcal	Thermodynamic affinity per electron	of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase Ah = u(ZE)

Name	Abbrev.	Units	Description	Comments
yw	YH2O	N/A	Mole fraction	of the solvent H2O in the aqueous solution phase YH2O = Y(AQ,H2O)
Nw	AH2O	mole	Mole number	of 1.0 kg of solvent H2O AH2O = 55.508435
Nsp	NSH2O	mole	Mole number, NS(AQ,H2O)	of the solvent (H2O) in the aqueous solution phase NS(AQ,H2O) = YH2O*NP(AQ)
	NS#		Mole number, NS(AQ,sp)	of a solute species in the aqueous solution phase NS(AQ,sp) = Y(AQ,sp)*NP(AQ)
M	ML#	mol/kg_H2O	Molality, ML(AQ,sp)	of a solute species in the aqueous phase ML(AQ,sp) = Y (AQ,sp)*AH2O/YH2O
m*	TIM	equivalent molality	Total molality	of all solute species in the aqueous solution phase TIM = sum[ML(AQ,sp)]ions + sum[ML(AQ,sp)]complexes
mt	TIC#	equivalent molality	Total ionic concentration, TIC (AQ,sp)	of a cation I in the aqueous phase TIC(AQ,spI) = sum[ML (AQ,spJ)*V(spI-in-spJ)]
I	ISTR	N/A	Ionic strength	of the aqueous solution phase ISTR=1/2*sum[ML(AQ,sp)*Z (AQ,sp)**2]
γ	RCH2O	N/A	Activity coefficient, RC(H2O,AQ)	of the solvent (H2O) RC(H2O,AQ) = ACR (H2O,AQ)/YH2O
	RC#		Activity coefficient, RC(sp,AQ)	of a solute species RC(sp,AQ) = ACR(sp,AQ)/Y

Name	Abbrev.	Units	Description	Comments
				(AQ,sp)*YH2O
αi	AIH2O	N/A	Activity, AI(H2O,AQ)	of the solvent (H2O), AI(H2O,AQ) = ACR(H2O,AQ)
	AI#		Activity, AI(sp,AQ)	of a solute species related to the aqueous solution phase, AI(sp,AQ) = ACR (sp,AQ)*AH2O
	LogAI#		Log10 Activity, LogAI(H2O,AQ), LogAI(sp,AQ)	of the solvent or a solute species related to the aqueous solution phase in common logarithm, LogAI(H2O,AQ) = log10[AI (H2O,AQ)] LogAI(sp,AQ) = log10[AI (sp,AQ)]
αw	AW	N/A	Activity	of H2O in the aqueous solution phase AW = ACR(H2O,AQ)
ϕ	OS	N/A	Osmotic coefficient	of aqueous solution phase OS = -55.508435*lnAW/TIM
At1	AT1	equil_mol/kg_ H2O	Titration alkalinity (definition 1)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate at the methyl orange endpoint (pH=4.5).
At2	AT2	equil_mol/kg_ H2O	Titration alkalinity (definition 2)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate, plus sulfide, at the methyl orange endpoint (pH=4.5).

For Gaseous Mixture Phase

Name	Abbrev.	Units	Description	Comments
γ	RA#	N/A	Activity coefficient, RA(sp,GAS)	of a gaseous species in the gaseous mixture RA(sp,GAS) = function(Y,T,P)
γ*	RF#	N/A	Fugacity coefficient, RF(sp,GAS)	of a pure gaseous species under TP RF(sp,GAS) = function(T,P/V)
F	FUG#	pa, bar, psi	Fugacity, FUG(sp,GAS)	of a gaseous species in the gaseous mixture FUG(sp,GAS) = RA(sp,GAS)*RF (sp,GAS)*Y(GAS,sp)*P
ft	TFUG	pa, bar, psi	Total gas fugacity	of the gaseous mixture phase TFUG = sum[FUG(sp,GAS)]

Defining New Derived Variables for Aqueous Solutions

You can define many different additional derived variables and functions. For instance, the partition coefficient of a component between two phases is defined as follows:

```
Pc<name> = X(phase1,component)/X(phase2,component)
```

Another example is the activity coefficient of a component in the system. It is defined as follows:

```
Rc<name> = ACR(component)/X(component)
```

The activity coefficient of a species in a solution phase depends on which model definitions on the reference states that are used and it depends on the standard states for the species. If the standard state of a species is defined to be the same as the pure species in a substitutional phase, then the activity coefficient of the species can be calculated as:

```
RC<name> = ACR(species,phase)/Y(phase,species)
```

In some cases, there are more than one sublattice in the phase and the reference states for the phase species cannot be presented by the pure species, as in the case of C in FCC [(Fe)1 (C,N,VA)1], where the model may end at fifty percent C and fifty percent Fe. In those cases, the chemical potential and activity of all phase constituents is not well defined and you cannot properly define the activity coefficients of the species in the phase.

For an aqueous solution phase, no matter what model is used, the reference state and standard state for both the solvent and solutes are defined in a special way in the Thermo-Calc software. The reference state for the solvent is set as pure water, the same as its standard state (according to Raoults's Law). The standard state for a solute species is set the hypothetical solute species, whilst its reference state is defined as the hypothetical state at unit molality (one mole dissolved into 1.0 kg of solvent) but in which the environment of each molecular is the same as at infinite dilution (according to Henry's Law). Under these definitions, the activity coefficients for solvent species can be calculated as follows:

```
RC<H2O> = ACR(H2O,aqueous)/ Y(aqueous,H2O)
```

The coefficients for the solute species can be calculated as follows:

```
RC<spec> = AI(species,aqueous)/ML(aqueous,species)
= ACR(species,aqueous)/ Y(aqueous,species)*Y(aqueous,H2O)
```

AI is here the activity of solute species calculated from the model, and ML is the molality of the species.

Thermodynamic Variables and Wildcard Characters

The ACR (species,phase) and the MUR (species,phase) quantities can only be appropriately and meaningfully applied to substitutional solution phases (such as GAS, AQUEOUS, LIQUID) and to solution phases without an interstitial sublattice set. This means that the wild card characters `*` and `$` normally don’t work properly for the activity and/or chemical potential properties.

For example, do not use ACR(*,*) or MUR(*,*) for all the species relative to all phases, nor ACR(*,phase) or MUR(*,phase) for all the species relative to a specific phase, nor ACR (species,*) or MUR(species,*) for a specific species relative to all phases.

Instead, use specific names for species and (applicable) phase, as in the following examples:

```
SHOW_VALUE acr(fe+2,aqueous)Lists activity of the Fe+2 species referred to
AQUEOUS solution phase
```

```
SHOW_VALUE mur(c2,gas)Lists chemical potential of the C2 species referred to GAS
mixture phase
```

```
SET_AXIS_VAR y ac(o2,gas)Sets activity of the O2 species referred to GAS mixture
phase as Y-axis
```

Units of State Variables and Derived Variables

The units for the state variables in the Units column in the table in User-Specified Units are the SI units that are used in the POLY module. However, in the POST module, you can both use pre-defined symbols and define your own symbols which are based on state variables and derived variables. By doing this, you can express the value of the thermodynamic variables in non-default units. The following topic briefly describes how you can create your own symbols and suggests expressions that you can use to convert default units into other standard units which are not default units in Thermo-Calc.

The topic Examples of User-Defined Units describes some variables of specific species in a phase and the units in which they are expressed. These variables are not used in POLY or POST, but in the GIBBS, DATA, PARROT and ED_EXP modules.

User-Specified Units

You do not always need to use the default units for variables. Using ENTER_SYMBOL, you can convert the value of variable from the default unit to your preferred unit. (Some response-driven modules also allow you to set conditions in non-default units.) User-defined symbols in the form of functions can be used for plotting in the POST module, but they cannot be used as conditions in POLY. User defined symbols in the form of variables can be used as conditions.

For example, if you want pressure to be plotted in bar rather than Pa, then you define the following function `PB`:

```
Enter_symbol function PB = P/1E5 ;
```

If you wanted heat capacity of a system to be shown as in terms of J/mol/K, then you can define the following function Cp:

```
Enter_symbol function Cp = Hm.T ;
```

If the variable you want to convert is a function of one or more derivatives, then you must enter the symbol as a variable rather as a function. For instance, a symbol expressing heat capacity of a system in a unit of cal/mol/K can be defined as the following variable `Cp2`:

```
Enter_symbol variable Cp2 = Hm.T/4.1858 ;
```

- Examples of User-Defined Units for information about entering conventional functions and the associated units.

Examples of User-Defined Units

The following tables give examples of expressions you can use to enter symbols. This enables you to show the values of thermodynamic variables in a variety of units.

Units of State Variables and Derived Variables and User-Specified Units

You can also use thermodynamic variables with normalizing suffixes in the expression when you enter a symbol. However, the tables do not have examples of these expressions.

In the expressions these are defined as follows:

- `i` is for an auxiliary index or letter that corresponds to the component `c`
- `j` is for an auxiliary index or letter that corresponds to the phase `ph`, and
- `ij` stands for an auxiliary index or letter that corresponds to the component `c` in the phase `ph`.

Intensive and Extensive Variables of a Defined System

Quantity	Suggested name and expression	Unit
For intensive variables of a defined system		
Temperature	TempC = T-273.15	Celsius (C)
	TempF = 1.8*T-459.67	Fahrenheit (F)
	TempF = 1.8*TempC+32	

Quantity	Suggested name and expression	Unit
Pressure	PB = P/1E5	bars (bar)
	PKb = P/1E8	kilobars (kbar)
	PAtm = P/101325	atmosphere (atm)
	PSI = P/6894.76	pounds/sq. inch (psi)
	PIHg = P/3342.11	inches of Hg
	PTor = P/133.322	Tors (millimeters of Hg)
For extensive variables of a defined system		
Amount	BKg = 1E-3*B	kilograms (kg)
	BTon = 1E-6*B	tons
Volume	VDM = 1E-3*V	cubic decimeters (dm^3, l)
	VCM = 1E-6*V	cubic centimeters (cm^3)
	VMM = 1E-9*V	cubic millimeters (mm^3)
	VCI = 1.6387064E-5*V	cubic inches (in^3)
	VLi = 1E-3*V	liters (l)
Energy	GCal = G/4.1858	cal
	ACal = A/4.1858	cal
	UCal = U/4.1858	cal
	HCal = H/4.1858	cal
	SCal = S/4.1858	Cal/K

Quantity	Suggested name and expression	Unit
Heat Capacity	Cp2 = HM.T/4.1858	cal/mol/K
	Cp3 = HW.T/4.1858	cal/g/K
	Cp4 = HV.T/4.1858	cal/m^3/K
Thermal Expansion	A2 = VM.T*1E-6/VM	1/K
	A3 = VW.T*1E-6/VW	1/K
Isothermal Compressibility	B2 = -VM.P*1E-9/VM	1/Pa
	B3 = -VW.P*1E-9/VW	1/Pa

Intensive and Extensive Variables of a System Component

Quantity	Suggested name and expression	Unit
For intensive variables of a system component		
Chemical Potential	MUi = MU(c)/4.1858	cal/mol
	MURi = MUR(c)/4.1858	cal/mol
Special quantity for aqueous solution	pH = -LOG10(ACR(H+1))	dimensionless
	Eh = MUR(ZE)/RNF where RNF=96485.309	volts (V)
For extensive variables of a system component		

Quantity	Suggested name and expression	Unit
Amount	MFi = N(c)/N = X(c)	dimensionless
	MPi = N(c)/N*100	dimensionless
	WFi = B(c)/B = W(c)	dimensionless
	WPi = B(c)/B*100	dimensionless
	BKgi = 1E-3*B(c)	kilograms (kg)
	BToni = 1E-6*B(c)	tons

Extensive Variables of a Phase

Quantity	Suggested name and expression	Unit
Amount	MFj = NP(ph)/N	dimensionless
	MPj = NP(ph)/N*100	dimensionless
	WFj = BP(ph)/B	dimensionless
	WPj = BP(ph)/B*100	dimensionless
	BKgj = 1E-3*BP(ph)	kilograms (kg)
	BTonj = 1E-6*BP(ph)	tons
Volume	VCMj = 1E-3*V(ph)	cubic decimeters (dm^3, l)
	VCMj = 1E-6*V(ph)	cubic centimeters (cm^3)
	VMMj = 1E-9*V(ph)	cubic millimeters (mm^3)

Quantity	Suggested name and expression	Unit
Energy	GCalj = G(ph)/4.1858	cal
	ACalj = A(ph)/4.1858	cal
	UCalj = U(ph)/4.1858	cal
	HCalj = H(ph)/4.1858	cal
	SCalj = S(ph)/4.1858	Cal/K
Driving Force	DG2j = DGM(ph)/4.1858	cal/mol
	DG3j = DGW(ph)/4.1858	cal/g
	DG4j = DGV(ph)/4.1858	Cal/m^3
	DG5j = DGF(ph)/4.1858	cal/mole_formula_unit
Heat Capacity	Cp2j = HM(ph).T/4.1858	cal/mol/K
	Cp3j = HW(ph).T/4.1858	cal/g/K
	Cp4j = HV(ph)/.T/4.1858	$cal/m^3/K$
	Cp5j = HF(ph)/.T/4.1858	cal/mole_formula_unit/K
Thermal Expansion	A2j= VM(ph).T/VM(ph)	1/K
Isothermal Compressibility	B2j = -VM(ph).P/VM(ph)	1/Pa

Extensive Variables of a Component in a Phase

Quantity	Suggested name and expression	Unit
Amount	MFij = N(ph,c)/NP(ph) = X(ph,c)	dimensionless
	MPij = N(ph,c)/NP(ph)*100	dimensionless
	WFi = B(ph,c)/BP(ph) = W(ph,c)	dimensionless
	WPij = B(ph,c)/BP(ph)*100	dimensionless
	BKgij = 1E-3*B(ph,c)	kilograms (kg)
	BTonij = 1E-6*B(ph,c)	tons

Intensive and Extensive Variables of a Species in a Phase

Quantity	Suggested name and expression	Unit
For intensive variables of a species in a phase		
Chemical Potential	MUCalij = MU(sp,ph)/4.1858	cal/mol
	MUErgij = MU(sp,ph)*1E7	cal/mol
Fugacity	FAij = AC(sp,ph)*PATM	atmosphere (atm)
	FBij = AC(sp,ph)*PB	bars (bar)
	FCij = AC(sp,ph)*PKB	kilobars (kbar)
	FTij = AC(sp,ph)*PTOR	Tors (millimeters of Hg)

Quantity	Suggested name and expression	Unit
ln(Fugacity)	LnFAij = LNAC(sp,ph)+LN(PATM)	atmosphere (atm)
	LnFBij = LNAC(sp,ph)+LN(PB)	bars (bar)
	LnFCij = LNAC(sp,ph)+LN(PKB)	kilobars (kbar)
	LnFTij = LNAC(sp,ph)+LN(PTOR)	Tors (millimeters of Hg)
Special quantity for aqueous solution	AIij=ACR(FE+3,AQ)*AH2O	dimensionless
	RCij=ACR(FE+3,AQ)*YH2O/Y(AQ,FE+3) where AH2O=55.508435 and YH2O=Y(AQ,H2O)	dimensionless
	WRCalij = WR(AQ,sp)/4.1858 (WR(AQ,sp) is only valid for aqueous species in a system in which the AQUEOUS solution phase is considered)	cal/mol
For extensive variables of a species in a phase		
Special quantity for aqueous solution	MLij=Y(AQ,FE+3)*AH2O/YH2O	molality (m)
	ISTR=1*IS1+1*IS2+1*IS3 where AH2O=55.508435, YH2O=Y(AQ,H2O) and ISn=.5*MLi*Zi**2+.5*MLj*Zj**2+.5*MLk*Zk**2	molality (m)

Units for Variables of Specific Species in a Phase

In the GIBBS, DATA, PARROT and ED_EXP modules, there are quantities that describe various thermodynamic, physical, chemical and transport properties for a compound phase, and for a certain species or a given species combination in a specific solution phase. The following table describes the units for those variables.

These variables cannot be directly used in the POLY or POST modules.

Variables	Description and unit
G(ph,sp) G(ph,sp;0) G(ph,sp1;sp2;...;0)	Gibbs energy (J/mol) of a pure substance or end-member.
G(ph,sp1,sp2,...) L(ph,sp1,sp2,...) G(ph,sp1,sp2,...;0) L(ph,sp1,sp2,...;0) G(ph,sp1,sp2,...;...;0) L(ph,sp1,sp2,...;...;0)	Zero-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
G(ph,sp1,sp2,...;i) L(ph,sp1,sp2,...;i) G(ph,sp1,sp2,...;...;i) L(ph,sp1,sp2,...;...;i)	The ith -order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp) TC(ph,sp;0) TC(ph,sp1;sp2;...;0)	Curie temperature (K) of a pure substance or end-member.
TC(ph,sp1,sp2,...) TC(ph,sp1,sp2,...;0) TC(ph,sp1,sp2,...;...;0)	Zero-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp1,sp2,...;i) TC(ph,sp1,sp2,...;...;i)	The ith -order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
BMAGN(ph,sp) BMAGN(ph,sp;0) BMAGN (ph,sp1;sp2;...;0)	Bohr magneton number (dimensionless) of a pure substance or end-member.
BMAGN(ph,sp1,sp2,...) BMAGN (ph,sp1,sp2,...;0)	Zero-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

Variables	Description and unit
BMAGN (ph,...;sp1,sp2,...;0)	
BMAGN (ph,sp1,sp2,...;i) BMAGN (ph,sp1,sp2,...;...;i)	The ith -order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp) V0(ph,sp;0) V0(ph,sp1;sp2;...;0)	Molar volume (m^3) at 1 bar and reference T0 of a pure substance or end-member.
V0(ph,sp1,sp2,...) V0(ph,sp1,sp2,...;0) V0(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent molar volume (m^3) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp1,sp2,...;i) V0(ph,sp1,sp2,...;...;i)	The ith-order composition-dependent molar volume (m^3) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp) VA(ph,sp;0) VA(ph,sp1;sp2;...;0)	Integrated thermal expansivity (m^3/mol/K) of a pure substance or end-member.
VA(ph,sp1,sp2,...) VA(ph,sp1,sp2,...;0) VA(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent thermal expansivity (m^3/mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp1,sp2,...;i) VA(ph,sp1,sp2,...;...;i)	The ith -order composition-dependent thermal expansivity (m^3/mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp)	High pressure fitting parameter (m^3/mol) of a pure substance or endmember.
VC(ph,sp1,sp2,...)	Zero-order composition-dependent high pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp1,sp2,...i)	The ith -order composition-dependent high pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site

Variables	Description and unit
	in a solution phase.
VK(ph,sp)	Isothermal compressibility (m^3/mol/Pa) of a pure substance or endmember.
VK(ph,sp1,sp2,...)	Zero-order composition-dependent isothermal compressibility (m^3/mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp1,sp2,...i)	The ith -order composition-dependent isothermal compressibility (m^3/mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
WR(ph,sp) WR(ph,sp;0)	Standard Born function (J/mol) of a specific aqueous species in the AQUEOUS solution phase (always with a single sublattice) under the reference-state temperature and pressure.

State Variables for Scheil

Post processing is done the same way as POLY-3: specific variables for plotting in the Scheil module are listed.

POLY Module Commands

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

Abbreviation	State variable
T	Temperature in Celsius
NL/BL	Mole/mass fraction of liquid
NS/BS	Mole/mass fraction of all solid phases
NS(ph)/BS(ph)	Mole/mass fraction of a solid phase
W(ph,el)	Weight fraction of an element in a phase
X(ph,el)	Mole fraction of an element in a phase
Y(ph,el)	Site fraction of an element in a phase
NN(ph,el)	Distribution of an element in a phases
NH/BH	Heat release and Latent heat per mole/gram
CP/BCP	Apparent heat capacity per mole/gram
NV/NV(ph)	Molar volume of the system or a phase
DS/DS(ph)	Average density of the system or a phase
BT	Apparent volumetric CTE of the system

State Variables in Console Mode DICTRA

State variables in the DICTRA POST module are similar to those defined in Thermo-Calc POLY-3 module. Examples of state variables are temperature, mole fraction, enthalpy, etc. In POLY-3 a general notation method based on character mnemonics is designed for a predefined set of state variables.

The numerical values of some state variables, e.g. activity, chemical potential, and the energetic extensive properties, are given relative to some reference state which has been defined in the thermodynamic database file. Sometimes you may have specified a reference state using SET_REFERENCE_STATE. To get numerical values relative to the user-defined reference state, append an R to the mnemonic names as defined.

Intensive Properties

Mnemonic	Description
T	temperature
P	pressure
AC(component)	activity
MU(component)	chemical potential

Extensive Properties

NORMALIZATION of extensive properties: For all extensive properties a suffix can be added to the mnemonic name to indicate a normalized extensive property. The following tables describe each mnemonic .

Extensive Property `Z at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z at each grid point.
ZM	Extensive property `Z per moles of atoms.
ZW	Extensive property `Z per mass (gram).

Mnemonic	Description
ZV	Extensive property `Z per volume (m^3).

Extensive Property `Z for a Phase at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z for the current amount of the phase.
ZM	Extensive property `Z per mole of atoms of the phase.
ZW	Extensive property `Z per mass (gram) of the phase.
ZV	Extensive property `Z per volume (m^3) of the phase.
ZF	Extensive property `Z per mole formula unit of the phase.

Energetic Extensive Properties



Suffixes M, W, V and F can be applied.

Mnemonic	Description
S	entropy
S(phase)	entropy of a phase
V	volume
V(phase)	volume of a phase
G	Gibbs energy
G(phase)	Gibbs energy of a phase
H	enthalpy

Mnemonic	Description
H(phase)	enthalpy of a phase
A	Helmholtz energy
A(phase)	Helmholtz energy of a phase

Amount of Components

Suffixes M, W and V can be applied.

Mnemonic	Description
N(component)	Number of moles of a component.
N(phase,component)	Number of moles of a component in a phase.
B(component)	Mass of a component.
B(phase,component)	Mass of a component in a phase.

Total Amount

Suffixes M, W and V can be applied.

Mnemonic	Description
N	Number of moles
B	Mass The legal combination BW is not very interesting as it will always be unity. BV is the density

Amount of a Phase

Suffixes M, W and V can be applied.

The normalizing properties are calculated at each grid point.

Mnemonic	Description
NP(phase)	Number of moles of a phase.
BP(phase)	Mass of a phase.
VP(phase)	Volume of a phase.
Y(phase,species#sublattice)	site fraction  This quantity is dependent upon the model chosen for the phase.

Constitution

 This quantity is dependent upon the model chosen for the phase.

Mnemonic	Description
Y(phase,species#sublattice)	site fraction

Thermophysical Properties Data and Variables

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About Thermophysical Properties Data Parameters

You can find information on our website about the thermophysical properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

- Parameters, Functions, and Variables
- Thermophysical Properties Variables

The so-called classic syntax is used in the examples below. It can be used in Console Mode or when using the APIs, e.g. TC-Python. Graphical Mode in Thermo-Calc has readable names for all of these.

All Available Properties Data Parameters and Variables

Below is a summary of the available parameters and variables for this database when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	Model Parameters	Variables to Show or Plot in Console Mode and TC-Python
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI*	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)` **

Property	Model Parameters	Variables to Show or Plot in Console Mode and TC-Python
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)` **
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI
* XI is not used in the TCS Metal Oxide Solutions Database (TCOX) ** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)		

Viscosity Model

- Viscosity of the Metallic Liquids Model
- Viscosity of the Ionic Liquids Model

To use this model, the database parameter VISC is needed. It can be used for liquids.

- Dynamic viscosity (DVIS)
- Kinematic viscosity (KVIS)

Examples in Console Mode:

- In POLY module: SHOW DVIS(LIQUID)
- Set as plot variable: SET-DIAGRAM-AXIS Y KVIS(LIQUID)

Thermal Conductivity Model

- Thermal Conductivity Model

To use the thermal conduction parameters, the database parameter THCD is needed. The other two related properties are derived from THCD. These properties can be obtained for a phase or for the whole system.

- Thermal conductivity (THCD)
- Thermal diffusivity (THDF)
- Thermal resistivity (THRS)

Examples in Console Mode:

- In POLY module: SHOW THCD
- Set as plot variable: SET-DIAGRAM-AXIS Y THDF(FCC_A1)

Electrical Resistivity Model

Electrical Resistivity Model

To use the electric properties parameters, the database parameter ELRS is needed. ELCD is derived from that. These properties can be obtained for a phase or for the whole system.

- Electrical conductivity (ELCD)
- Electrical resistivity (ELRS)

Examples in Console Mode:

- In POLY module: SHOW ELCD
- Set as plot variable: SET-DIAGRAM-AXIS Y ELRS(FCC_A1)

Surface Tension Model

Surface Tension of Metallic Liquid Alloys Model

Surface Tension Model for Oxide Slag

Surface tension for liquids can be calculated if the database contains the two database parameters SIGM and XI. From these, the surface energy is calculated:

- Surface energy (SURF)



XI is not used in the TCS Metal Oxide Solutions Database (TCOX)

Examples in Console Mode:

- In POLY module: SHOW SURF(LIQUID)
- Set as plot variable: SET-DIAGRAM-AXIS Y SURF(LIQUID)

Thermophysical Properties Variables

The Thermo-Calc databases have a variety of properties data included such as molar volume, thermal conductivity, dynamic and kinematic viscosity, thermal resistivity, and surface tension. These properties data are being integrated into databases as each new version of a database is released.

Availability of properties data is dependent on both the database and its version. Some information is specific to use in Console Mode. There is more information also available for Graphical Mode and TC-Python for each of the databases where the properties data is included. More advanced information is also contained in the *Database Manager User Guide* PARAMETER section included with this documentation set.

To determine if the database you are using has this properties data, search the help (press F1) to review the technical information. The availability of properties data is also included with the Database Overview document available on the Thermo-Calc website.

Variables	Abbrev.	Unit	Descript.	Domain
DVIS	DVIS(ph)	Pa·s	Dynamic viscosity	Liquid phase
KVIS	KVIS(ph)	m^2/s	Kinematic viscosity	Liquid phase
ELRS	ELRS	Ωm	Electric resistivity	System
ELRS	ELRS(ph)	Ωm	Electric resistivity	Phase
ELCD	ELCD	S/m	Electric conductivity	System
ELCD	ELCD(ph)	S/m	Electric conductivity	Phase
THCD	THCD	W/(mK)	Thermal conductivity	System
THCD	THCD(ph)	W/(mK)	Thermal conductivity	Phase
THRS	THRS	mK/W	Thermal resistivity	System

Variables	Abbrev.	Unit	Descript.	Domain
THRS	THRS(ph)	mK/W	Thermal resistivity	Phase
THDF	THDF	m^2/s	Thermal diffusivity	System
THDF	THDF(ph)	m^2/s	Thermal diffusivity	Phase
SURF	SURF(ph)	J/m^2	Surface tension	Liquid phase

Electrical Resistivity Model

The modeling starts with unaries in their stable and metastable structures. The temperature dependence of electrical resistivity is described with polynomials for each unary and each end-member of compounds. In order to guarantee the reliability of the extrapolation, experimental data were first fitted to a semi-empirical model, which was established based on relevant theories. The experimental data, together with the extrapolated values, are then used for deriving the polynomials that are saved in the database. The magnetic contribution to electrical resistivity can be separately treated with a model implemented in Thermo-Calc.

The composition dependence of electrical resistivity is described with the Redlich-Kister expression. All binary systems are modeled by using experimental data or theoretical estimations. Ternary and higher-order parameters can be used if necessary.

Electrical resistivity is modeled and its descriptions are stored in the databases. Electrical conductivity is derived from electrical resistivity and can be retrieved from calculated results as well.

Model Description

The semi-empirical model for electrical resistivity is built based on the Matthiessen's rule [1997DeB]. In general, the electrical resistivity of a metallic alloy consists of residual resistivity (ρ_0) and electron-phonon resistivity (ρ_{e-p}), as well as magnetic resistivity (ρ_m). The residual resistivity is due to the scatterings of impurities and defects that exist in well-annealed and high purity alloys, and the value of ρ_0 is generally considered independent of temperature.

[*Eq. 1*] $$\rho = \rho_0 + \rho_{e-p} + \rho_m$$

ρ_{e-p} is described with the modified Bloch-Grüneisen equation [1928Blo; 1933Gru] and corrections can be made in cases where other types of scatterings play considerable roles.

[*Eq. 2*] $$\rho_{e-p} = A \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right)$$

[*Eq. 3*] $$A = \frac{\frac{3}{2} h q_D^6 (G')^2}{4e^2 (m^*)^2 n_c k_B \theta_D k_F^2 \nu_F^2}$$

[*Eq. 4*] $$J_n\left(\frac{\theta_D}{T}\right) = \int_0^{\frac{\theta_D}{T}} \frac{x^n e^x}{(e^x - 1)^2} dx$$

The characteristic temperature θ_R plays a similar role and is also approximated as the Debye temperature (θ_D), which can be readily obtained from low-temperature heat capacity and elastic constants data as well as theoretical computations. The approximation of θ_R as θ_D indicates that transverse phonons play a role in electron scattering. k_F is the electron wave number at the Fermi surface. q_D is the phonon Debye wave number. h is the Planck constant. G' is a constant representing the strength of the e-p interaction and cannot be easily estimated. m^* is the electron effective mass. n_c is the number of unit cells per unit volume. v_F is the electron velocity at the Fermi surface.

To describe the drastic change of the magnetic resistivity (ρ_m) around the Curie (or Neel) temperature, T_C, of a magnetic alloy, an empirical model is proposed using the dimensionless temperature T/T_C and a parameter ρ_{spd} that stands for the resistivity due to spin disordering. According to this model, Eq. 5, ρ_m approaches ρ_{spd}, when the temperature is well above T_C, and is 0 when the temperature is far below T_C. ρ_{spd} depends only on composition and is described with the Redlich-Kister (R-K) expression. Apparently, ρ_{spd} has a positive value for magnetic elements, and compounds as well as endmembers, and is 0 for non-magnetic ones.

In a typical binary system made of a magnetic element A and a non-magnetic element B, ρ_{spd} decreases usually from ρ_{spd}^{A} to 0 at a certain composition (x_*). Such a behavior is also seen in magnetic moment and Curie temperature. ρ_{spd} is expected to be zero in the composition range from x_* to element B, and will be forced to zero when the R-K expansion leads inevitably to negative values over this composition range. T_C is available from the thermodynamic description in the database.

[*Eq. 5*]
$$\rho_m = \rho_{spd} \cdot \left(1 - e^{\left(-\frac{3}{2}\left(\frac{T}{T_c}\right)^3\right)}\right)$$

The semi-empirical model (as given in Eq. 1 to Eq. 5) is first fitted to experimental data. The description is then extrapolated to a wider temperature range if necessary, either to extreme temperatures where the structure is no longer stable or to where experimental data are missing. Polynomials are then derived with the experimental data, together with the extrapolated values, and stored in the database. The model as given in Eq. 5 is implemented in Thermo-Calc, so the magnetic contribution can be excluded from the polynomials and separately modeled, and it will be automatically included during the calculations.

Model Parameters

The extended TDB format accepts parameters describing electrical resistivity and thermal conductivity, together with spin disordering resistivity. Examples for unary and binary systems are given below:

```
ELRS(FCC_A1,AL:VA;0)
ELRS(FCC_A1,AL,CO:VA;0)
ESPD(FCC_A1,CO:VA;0)
ESPD(FCC_A1,AL,CO:VA;0)
```

Calculation and Plot Variables

- `ELRS` – Electrical resistivity
- `ELCD` – Electrical conductivity

All the above quantities can be calculated, retrieved, shown and plot in Thermo-Calc via the variables in the Console Mode or via the quantity names in the Graphic Mode (see sections below).

Console Mode

The quantities corresponding to the variables of `ELRS` and `ELCD` can be calculated in Console Mode for a phase, e.g. `ELRS(FCC_A1)`, or for a system, i.e. `ELRS`. The results can be shown in the POLY module with the command SHOW_VALUE or illustrated as a plot in the POST module with the command PLOT_DIAGRAM.

Graphical Mode

On the **Plot Renderer** in Graphical Mode, electrical resistivity, electrical conductivity, thermal conductivity, thermal resistivity, and thermal diffusivity can be selected from the axes lists, tabulated and plotted using the quantity names, with options for a specific phase, all phases or for a system.

TC-Python

The quantities of `ELRS` and `ELCD` can be retrieved, for a phase, e.g. `ELRS(FCC_A1)`, or for a system, i.e. `ELRS`, via `get_value_of()` or `get_values_of()`, from most phase equilibrium calculations in TC-Python, for instance,

- `with_single_equilibrium_calculation()`,
- `with_property_digram_calculation()` or
- `with_batch_equilibrium_calculation()`.

References

[1928Blo] F. Bloch, Über die Quantenmechanik der Elektronen in Kristallgittern (About the quantum mechanics of electrons in crystal lattices). Zeitschrift fur Phys. 52, 555–600 (1928).

[1933Gru] E. Grüneisen, The dependence of the electrical resistance of pure metals on the temperature. Ann. Phys. 16, 530–540 (1933).

[1997DeB] R. De-Bruyn-Ouboter, Heike Kamerlingh Onnes's discovery of superconductivity. Sci. Am., 98–103 (1997).

Thermal Conductivity Model

The modeling starts with unaries in their stable and metastable structures. The temperature dependence of thermal conductivity is described with polynomials for each unary and each end-member of compounds. Thermal resistivity and thermal diffusivity can be derived from thermal conductivity and retrieved from calculated results. The composition dependence is described with the Redlich-Kister expression in the CALPHAD spirit, but the relation is applied to thermal resistivity (or the inverse of thermal conductivity).

Model Description

Experimental data of thermal conductivity are used to derive descriptions in polynomials, which are stored in the database, despite that it consists of two components, electronic thermal conductivity (κ_e) and lattice thermal conductivity κ_g. In other words, they are not separately treated.

In cases where experimental data are absent or sparse, however, κ_e and κ_g can be separately predicted and summed up to give the total thermal conductivity. κ_e can be predicted from ρ or vice versa, by employing the Wiedemann-Franz Law [1853Fra; 1985Jon], respectively, to the residual resistivity, magnetic resistivity and intrinsic resistivity.

[*Eq. 1*]
$$\frac{1}{\kappa_e} = W_e = \frac{\rho_0 + \rho_m + \rho_i}{L_0 T}$$

L_0 is known as the Sommerfeld value of the Lorenz number: $2.4453 \times 10^{-8} W\Omega/K^2$.

[*Eq. 2*]
$$\rho_i = \frac{A}{L_0 T} \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right) \cdot f$$

[*Eq. 3*]
$$f = 1 + \frac{3}{\pi^2} \cdot \left(\frac{k_F}{q_D}\right)^2 \cdot \left(\frac{\theta_R}{T}\right)^2 - \frac{1}{2\pi^2} \cdot \frac{J_7\left(\frac{\theta_R}{T}\right)}{J_5\left(\frac{\theta_R}{T}\right)}$$

The intrinsic resistivity (ρ_i) is based on Eq. 4

[*Eq. 4*]
$$\rho_{e-p} = A \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right)$$

for the e-p processes, but corrections are provided, as given in Eq. 3: the first term corresponds to large-angle scattering that satisfies the original Wiedemann-Franz Law; the second one is due to inelastic small-angle (vertical processes) and has no counterpart in the

electrical resistivity; the third term is a correction that accounts for situations where large-angle scattering can reverse the electron direction without actually assisting to restore the distribution back to equilibrium.

κ_g can be predicted with the Slack model in a temperature range where only anharmonic Umklapp phonon-phonon interactions are important. In other words, normal processes are neglected as a first approximation [1979Sla; 2002Mor]. The most reasonable version among several ones is given below [1965Jul].

[*Eq. 5*]
$$\kappa_p^U = A' \cdot \frac{M_a \cdot \theta_D^3 \cdot \delta}{\gamma^2 \cdot n_c^{\frac{2}{3}}} \cdot \frac{1}{T}$$

[*Eq. 6*]
$$A' = \frac{2.43 \cdot 10^{-5}}{1 - \frac{0.514}{\gamma} + \frac{0.228}{\gamma^2}}$$

The Debye temperature, θ_D can be obtained from low-temperature heat capacity or elastic constant data. M_a is the average atomic mass, δ^3 the volume per atom, n_c the number of atoms in a unit cell, and γ the Grüneisen coefficient. A typical value for A' is evaluated to be 3×10^{-5} using $\gamma = 2$ as the Grüneisen coefficient, and can be used in the absence of experimental information. It can also be obtained from e.g. DFT calculations of elastic properties.

Model Parameters

The extended TDB format accepts parameters describing electrical resistivity and thermal conductivity, together with spin disordering resistivity. Examples for unary and binary systems are given below:

```
THCD(FCC_A1,AL:VA;0)
THCD(FCC_A1,AL,CO:VA;0)
```

Calculation and Plot Variables

- `THCD` – Thermal conductivity
- `THRS` – Thermal resistivity
- `THDF` – Thermal diffusivity

All the above quantities can be calculated, retrieved, shown and plot in Thermo-Calc via the variables in the Console Mode or via the quantity names in the Graphic Mode (see sections below).

Console Mode

The quantities corresponding to the variables of THCD, THRS, and THDF can be calculated in Console Mode for a phase, e.g. THCD(FCC_A1), or for a system, i.e. THCD. The results can be shown in the POLY module with the command SHOW_VALUE or illustrated as a plot in the POST module with the command PLOT_DIAGRAM.

Graphical Mode

On the **Plot Renderer** in Graphical Mode, electrical resistivity, electrical conductivity, thermal conductivity, thermal resistivity, and thermal diffusivity can be selected from the axes lists, tabulated and plotted using the quantity names, with options for a specific phase, all phases or for a system.

TC-Python

The quantities of THCD, THRS, and THDF can be retrieved, for a phase, e.g. THCD(FCC_A1), or for a system, i.e. THCD, via get_value_of() or get_values_of(), from most phase equilibrium calculations in TC-Python, for instance,

- with_single_equilibrium_calculation(),
- with_property_digram_calculation() or
- with_batch_equilibrium_calculation().

References

[1852Fra] R. Franz, G. Wiedemann, Ueber die Wärme-Leitungsfähigkeit der Metalle. Ann. der Phys. und Chemie. 165, 497–531 (1853).

[1965Jul] C. L. Julian, Theory of Heat Conduction in Rare-Gas Crystals. Phys. Rev. 137, A128–A137 (1965).

1979[Sla] G. A. Slack, The Thermal Conductivity of Nonmetallic Crystals, in Solid State Physics Volume 34, 1–71 (1979).

[1985Jon] W. Jones, N. H. March, Theoretical Solid State Physics (Courier Dover Publications, 1985).

[2002Mor] D. T. Morelli, J. P. Heremans, G. A. Slack, Estimation of the isotope effect on the lattice thermal conductivity of group IV and group III-V semiconductors. Phys. Rev. B. 66, 195304 (2002).

Surface Tension of Metallic Liquid Alloys Model

For each database where the properties data are included, the assessments for particular binary and elements is based on the specific database. In general, all the surface tension for all elements and binary systems are assessed.



Search the help (press F1) to review the technical information for the database you are using.

Model Description

The chosen model for the surface tension of metallic liquid alloys is the modified Guggenheim model [2019, Vermot des Roche]:

$$\sigma(x_i^B,T) = -\frac{RT}{S(x_i^B,T)}\ln\left[x_1^B \exp\left(-(1+\Xi_1 \cdot x_2^S(x_i^B,T))\frac{\sigma_1(T)S_1(T)}{RT}\right) + x_2^B \exp\left(-(1+\Xi_2 \cdot x_1^S(x_i^B,T))\frac{\sigma_2(T)S_2(T)}{RT}\right)\right]$$

where

- x_i^B is the bulk composition
- σ_i is the surface tension
- S and S_i are the total and the partial molar surface of species i defined as

$$S_{(i)} = 1.901 \cdot N_A^{1/3} \cdot V_{m,(i)}^{2/3}$$

- N_A being the Avogadro number and $V_{m,(i)}$ the molar volume of the system or the species i.
- x_i^S is the composition of i in surface, which is a function of bulk composition and T and defined as follows:

$$x_i^{S,id}(x_i^B,T) = \frac{x_i^B}{x_i^B + x_j^B \exp\left(\frac{S(x_i^B,T)[\sigma_i(T)-\sigma_j(T)]}{RT}\right)}$$

- Ξ_1 and Ξ_2 are called damping factors and these parameters are fitted for species 1 and 2 of binary systems.

The extrapolation to higher-order systems is straightforward. The ideal surface composition for a multicomponent system is:

$$x_i^{S,id}(T, x_i^B, x_j^B, \dots) = \frac{x_i^B}{x_i^B + \sum_{j \neq i} x_j^B \exp\left(\frac{S_{ij}(x_i^B, T) \cdot [\sigma_i(T) - \sigma_j(T)]}{RT}\right)}$$

and the surface tension of a multicomponent alloy is obtained from:

$$\sigma(T, x_i^B, x_j^B, \dots) = -\frac{RT}{S(T, x_i^B, x_j^B, \dots)} \cdot \ln\left[\sum_{i=1}^{n} \sum_{j \neq i} x_i^B \exp\left(-(1 + x_j^S(T, x_i^{B,ij}) \cdot \Xi_i^{ij}) \frac{\sigma_i(T) S_i(T)}{RT}\right)\right]$$

Reference

[2019, Vermot des Roche] M. Vermot des Roches, A. E. Gheribi, P. Chartrand, "A versatile multicomponent database for the surface tension of liquid metals," Calphad. 65, 326–339 (2019).

Corresponding Variables

The corresponding variable for surface energy of pure elements is SIGM. For instance, the surface tension of pure A is written as SIGM(LIQUID,A;0). The corresponding X_1 and X_2 parameters for A-B binary system are respectively written as following:

```
PARAMETER XI(LIQUID,A,B:0)
PARAMETER XI(LIQUID,A,B:1)
```

The surface energy of the liquid is accessed via SURF(LIQUID).

Plot Variables

Console Mode

The surface energy can be calculated through step calculations in Console Mode. The plot variable is `SURF(LIQUID)`.

Graphical Mode

The surface energy is calculated using the **One-axis calculation** type in Graphical Mode. The corresponding plot variable is *Surface tension*.

TC-Python

In TC-Python, it can be plotted using `property-diagram_calculation()` or `with_batch_equilibrium_calculation()`. The plot variable is `SURF(LIQUID)`.

Graphical Mode and Console Mode Examples

There are two basic examples included with your software installation and that use demonstration (DEMO) databases.

Search the help (press F1 when in Thermo-Calc) for brief descriptions of these examples, or browse to the examples located in your installation. From the main menu, **Help→ Examples Files**:

- Graphical Mode **T_11_Surface_tension_in_Cu-Zr.tcu**
- Console Mode `tcex56`

Surface Tension Model for Oxide Slag

The model for TCS Metal Oxide Solutions Database (TCOX) surface tension of oxide slag:

$$\sigma = \sum y_i \sigma_i + \sigma^E$$

$$\sigma^E = \sum_i y_A \cdot y_B (y_A - y_B)^i \cdot SIGM^i$$

where y_i and σ_i indicate the site fraction and surface tension for pure component i. For pure component, the surface tension is described with $a + b * T$. The excess term is expressed using Redlich-Kister polynomial, as one can find the example of a binary A-B.

SIGM is the parameter used for optimization, for example,

```
PARAMETER SIGM (IONIC_LIQ, A;0)
PARAMETER SIGM (IONIC_LIQ, B;0)
PARAMETER SIGM (IONIC_LIQ, A:B,0)
```

The user can calculate the surface tension of liquid oxide by calling the variable `SURF (IONIC)`.

Viscosity of the Metallic Liquids Model

Model Description

The viscosity of metallic liquid alloys is modeled as follows:

$$RT\ln\eta = RT\ln\eta_0 + E$$

where

- η is the dynamic (or shear) viscosity of the liquid,
- η_0 is the viscosity at finite temperatures,
- E is the activation energy in J/mole,
- R is the gas constant, and
- T is the absolute temperature.

The SI unit of viscosity is pascal.second (Pa.s). The viscosity parameters are expanded via Redlich-Kister polynomials.

For example, viscosity of a liquid A-B alloy is:

$$\begin{aligned} RT\ln\eta_{alloy} = x_A(E_A + RT\ln\eta_0^A) \\ +x_B(E_B + RT\ln\eta_0^B) \\ +x_Ax_B(L_0 + (x_A - x_B)\cdot L_1) \end{aligned}$$

The two first terms are the contributions for the end-members, A and B elements and the last term accounts for the excess viscosity. Basically, the activation energies are optimized. L_0 and L_1 etc. are the parameters that are optimized to fit the viscosity data.

The kinematic viscosity, ν, is the ratio of the dynamic viscosity, η, to the density, ρ, of the alloy:

$$\nu = \eta/\rho$$

The SI unit of kinematic viscosity is square meter per second (m^2/s).

Corresponding Variables

In Console Mode, the viscosity can be plotted via a step calculation vs. temperature or composition. The calculated property in Thermo-Calc is VISC of the liquid phase. The calculated VISC property is not the viscosity (η) but is related to η via $RT\ln(\eta)$, thus in order to plot the viscosity or η you define a function for η as follows:

$$\eta = \exp(VISC(LIQUID)/RT)$$

The default unit is Pa.s.

However, it is also possible to directly get the values for dynamic and kinematic viscosity in Console Mode and using TC-Python. The relevant properties are DVIS (dynamic viscosity) and KVIS (kinematic viscosity). For example, once the equilibrium is calculated in Console Mode, one can get the viscosity value by:

`show DVIS(liq)` or `show KVIS(liquid).`

In Graphical Mode, the viscosity (η) is directly plotted when using the One-axis calculations available with various calculators.

Graphical Mode and Console Mode Examples

There are two basic examples included with your software installation and that use demonstration (DEMO) databases.

Search the help (press F1 when in Thermo-Calc) for brief descriptions of these examples, or browse to the examples located in your installation. From the main menu, **Help→ Examples Files**:

- Graphical Mode **T_12_Viscosty_in_Cr-Ni.tcu**
- Console Mode `tcex55`

Viscosity of the Ionic Liquids Model

The model for TCS Metal Oxide Solutions Database (TCOX) viscosity of slag:

$$RTln\eta = RTln\eta_0 + E$$

where η is viscosity, $\eta_0 = \frac{hN_A}{V_m}$ and E is activation energy.

The excess parameters are expanded via R-K. An example of viscosity of A-B liquid oxide:

$$RTln\eta_{A-B} = y_A(RTln\eta_0^A + E_A) + y_B(RTln\eta_0^B + E_B) + \sum_i y_A \cdot y_B(y_A - y_B)^i \cdot VISC^i$$

The parameter of *VISC* stands for *R· T· ln(viscosity)*. In Thermo-Calc software, VISC is implemented as *VISC(ionic)*. In order to quickly acquire the actual viscosity, the parameter of *DVIS(ionic)* should be used. By coupling to the database, it makes use of the site fractions of each species, which reflects the structural change in the oxide melt.

Units for the viscosity of oxide slag:

- Pa·s (pascal-second) is the SI unit, mostly used for oxide slag
- CGS unit is poise (P), 1 poise=0.1 Pa·s
- Centipoise is also common (cP) because it is equivalent to mPa·s.

Molar Volume Model

Molar volume can be used to establish a connection with some significant physical properties, for example, viscosity, electrical conductivity and surface tension. It is the reciprocal of density multiplied by molar mass.

Model Description

The model used to describe the molar volume at ambient pressures is:

$$V_m(T) = V_0 exp(\int_{T_0}^{T} 3\alpha dT)$$

A simple polynomial is used to model non-magnetic volumetric expansivity above 298 K:

$$3\alpha = a + bT + cT^2 + dT^3 + eT^{-2}$$

The model described above is implemented in Thermo-Calc software with two parameters, V0 and VA, and α is the linear thermal expansivity at 1 bar and 3α is the volumetric thermal expansivity.

Molar Volume Descriptions

Parameter	Unit	Description
V0 (phase, constituent array)	m^3/mol	Volume at 1 bar and reference temperature T0
VA (phase, constituent array)	None	$\int_{T_0}^{T} 3\alpha dT$

Database Files

In this section:

About the Database Files 71
Database Installation Folder 73
About Cached Database Files 74
Editing the Database Initialization File or Unencrypted Database File 75
Database Checker 76

About the Database Files

- Database Manager User Guide

Encrypted vs Unencrypted Database Files

Any licensed databases purchased from Thermo-Calc Software are encrypted in files with the extension `.TDC`; these files cannot be edited. These are referred to as *encrypted databases*.

Unencrypted databases have the file extension `.TDB` and can be edited. For example, PURE5 or PG35 (the free databases), or a user-defined database file.

- Editing the Database Initialization File or Unencrypted Database File
- If you develop your own databases on a regular basis, also see About the TDB Editor.

Database Initialization File

The *database initialization file* is called `tc_initd.tdb`. Individual licenses are still required to use each database.

The file is used differently by the program depending on whether you are working with databases in Console Mode or Graphical Mode. For this reason, editing the file can be problematic if you do not understand the differences.

- About Cached Database Files and Editing the Database Initialization File or Unencrypted Database File

User Database Files

A user-defined database is considered to be an unencrypted database because you can make changes to it.

In Graphical Mode you can add user databases via the **Options → Graphical Mode → System Definer** window. Once you have added the user database it is available from the database list in the System Definer Configuration window.

- Global Settings: System Definer to add a user database.

In Console Mode, users can decide to add their own user-defined database to the database initiation file, which then makes it available in the Console window.

- Editing the Database Initialization File or Unencrypted Database File

Custom Databases: GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For custom database users, you may sometimes see messages in the log indicating that additional preparation is being done by Thermo-Calc prior to a calculation. The preparation is carried out automatically; it is usually fast and only needed the first time a custom database is used after a modification. While databases with warnings are tolerated, databases that contain errors can only be loaded by GES6 after the errors are corrected.

The Database Checker tool uses the same parser as GES6 and can be used to verify the consistency and correctness of databases during development, before the databases are actually used.

- Database Checker



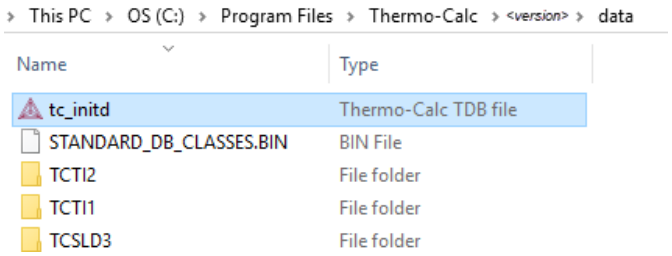
To globally set the default from GES6 back to GES5, go to the **Tools → Options → General** tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The SET_GES_VERSION Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Database Installation Folder

The standard Thermo-Calc databases and the database initialization file `tc_initd.tdb` are located in a subfolder to the Thermo-Calc installation. For example, in a Windows Standalone installation, you can find these in a folder called **data** where the file path is *C:\Program Files\Thermo-Calc\<version>\data*.



About Cached Database Files

This is applicable to Graphical Mode.

Also see Global Settings General where you can set the default database directory path. There is also an option to clear the database cache, which may be helpful if you are having issues.

The first time you open a database in Graphical Mode it can take a little while for it to load, especially if it is one of the large databases such as TCFE or TCNI. However, the next time the database opens quickly because the databases are now cached, or stored, in Graphical Mode.

Think of a cache as an intermediate storage area. Once a database cache is established the file is made easily accessible, even if you close the software program. It is the same concept as when you load a web page for the first time. The next time the page opens faster. This is also how it works for the databases in Thermo-Calc Graphical Mode.

Thermo-Calc caches the database files, both encrypted and unencrypted types, at two points—when you first open a database, sometimes called an *in-memory cache*, and then as a *disk-based cache*. The disk-based cache is what speeds up database loading and it is at this point that Thermo-Calc refers to the database initialization file for information. The disk-based cache uses a lookup key to find the abbreviated database name (e.g. TCFE or TCNI) contained in this initialization file.

It is important to understand the way databases are cached in Graphical Mode to ensure best practices for those who also use Console Mode, especially if the database initialization file is edited. If you plan to edit this file, see Editing the Database Initialization File or Unencrypted Database File.

Editing the Database Initialization File or Unencrypted Database File

Some advanced users may decide to edit the database initialization file, for example to reorder the list of encrypted databases displaying in the Console window or to add a user-defined database for use in Console Mode. It is important to understand that changes to this file impact the database caching process used in Graphical Mode.

- About the Database Files
- About Cached Database Files

The following recommendations are also applicable if you edit an unencrypted database file, which includes user databases and free databases such as PURE5 or PG35.

Best Practice Recommendations

- Database Installation Folder

If you edit the database initialization file (`tc.initd.tdb` in Windows or `initd.tdb` in Mac and Linux), then:

- If a user database is added to the file, it is subject to the same caching as the encrypted databases. This means that further changes (to the user database) are not detected when you are working with databases in the System Definer in Graphical Mode.

If you have a user database, which is subject to regular updates, then:

- If you make changes to a user database, you then need to clear the cache.
- It is recommended that you create a separate directory to store unencrypted database files.

If you edit an unencrypted database file included with the installation (such as the PURE5 and PG35 files):

- Do not edit the file in the installation folder. Instead make a local copy and load it into the application as a user database.

Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.



Thermo-Calc accepts some deviations from these syntax rules. Although warnings can be ignored, errors must be corrected.

For example, a warning is reported if an abbreviated phase name is found and phase name abbreviations are accepted by Thermo-Calc and its Add-on Modules. However, reported errors must be corrected in the TDB file before the database can be loaded by the application.

With respect to using this tool, the executable `DatabaseChecker` file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu in Thermo-Calc.

- Database Manager User Guide

Global Settings

In the **Options** window (select **Tools → Options**) you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

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Global Settings: Equilibrium Calculator 87

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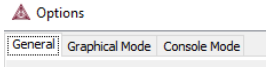
Global Settings: Process Metallurgy 91

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General



These settings are for both Graphical Mode and Console Mode. To open this window, from the main menu select **Tools → Options**.

Tooltips enabled

Select whether to turn on tooltips information. By default the **Tooltips enabled** check box is selected. This displays a small text box when you hover the cursor above some buttons or other items.

Localization

To change the GUI language from the **Localization** list choose **English** (the default), **Swedish**, **Spanish**, **German**, **Russian**, **Chinese**, **Japanese** or **French**.

Look and feel

To change the **Look and feel** of the GUI layout, choose **FlatLAF Light** (the default), **Metal**, **Nimbus**, **CDE/Motif**, **Windows**, or **Windows Classic**.

Log level

Select the level and type of information to display in the **Event Log** window using the **Log level** slide bar. Choose from a **Debug**, **Info**, **Warning** or **Error** level of detail.

Database directory

In the **Database directory** field, specify the path to the directory that contains the **data** directory. This is where the Thermo-Calc database directory called **data** is located. Do not specify the path to where the database files are found (that is, in the **data** directory).

Modifying the Database Directory Path (Graphical Mode Only)



Important Note: Database Directory Path (Graphical Mode only)

When you open a database for the first time, it is stored in a cache (an intermediate storage area), that is maintained even if you close the program. This improves the speed of loading the next time you open that database. The cache is used for all databases that are listed in the database initialization file, typically all the standard databases that are included with Thermo-Calc.

If you modify your own user-defined database, or if you choose to edit an unencrypted database, it is recommended that you create a separate directory to store these database files. This way the most recent version of the user-defined or edited databases are loaded into the program when the System Definer is performed.

- About the Database Files

Model directory

This is where the predefined and custom Property Models (used with the Property Model Calculator or TC-Python) are saved and stored by default. Click **Modify** to open the default folder or to create a custom folder for your own models.



All Property Models (whether these are predefined or custom models) must be located in a subdirectory of the Property Model directory. For that reason it is recommended that you do not change the directory location.



See Property Model Calculator for information about using the predefined models. Also see the TC-Python help on the website for details about creating custom models.

Property model Python interpreter

This is the path to the executable Python file that is needed to work with custom property models. See the **Property Model Framework → Best Practices** section in the TC-Python help on the website.

Check update interval

From the **Check update interval** list, choose not to check (**Do not check**, the default) or **On startup**. You can also manually check for updates – choose **Help→Check for Updates**.

Preferred Gibbs Energy System

- About the Gibbs Energy System (GES) Module.

Use this setting to globally set the default GES version to be either GES6 (the default) or GES5.

This setting is useful if you are using the POURBAIX module (aqueous solutions) or if you have a custom database that is not compatible with GES6. The SET_GES_VERSION Console Mode command can also be used to change GES versions for a single Thermo-Calc session.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

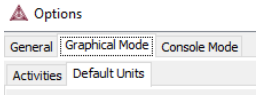
Reset all settings and the database cache to defaults

Click **Factory reset** to reset all the settings to the original defaults, including clearing the database cache. The changes are applied when Thermo-Calc is restarted. This may be useful when there are several versions of Thermo-Calc installed and there are conflicts between settings or loading databases becomes problematic. See About Cached Database Files.

Reset to original settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Graphical Mode - Default Units



To open this window, from the main menu select **Tools → Options** and click the **Default Units** tab.

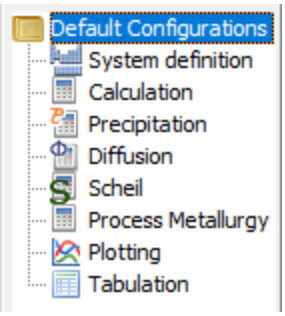
Reset to original settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Setting	Options
Temperature	**Kelvin** (the default), **Celsius**, or **Fahrenheit**
Pressure	**Pascal** (the default), **Atmospheres**, or **Bar**
Amount	**Mole** (the default), **Gram**, **Kilogram**, **Tonne**, or **Pound**
Mass	**Tonne** (the default), **Kilogram**, **Gram**, or **Pound**
Composition	**Mass percent** (the default), **Mole percent**, **Mass fraction**, or **Mole fraction**
Mass composition	**Mass percent** (the default) or **Mass fraction**
Energy	**Joule** (the default), **Calorie** , **Electron volt**, **Gigajoule**, **Watt hour**, or **Kilowatt hour**
Power	**Watt** (the default), **Kilowatt**, or **Megawatt**
Volume	**Cubic meter** (the default), **Cubic decimeter**, **Cubic centimeter**, or **Normal cubic meter**
Density	**Kilogram per cubic meter** (the default) or **Gram per cubic meter**
Entropy	**Joule per Kelvin** (the default), **Calorie per Kelvin**, or **Electron volt per Kelvin**
Dynamic viscosity	**Pascal-second** (the default), **milliPascal-second**, **Poise**, or **centiPoise**
Kinematic viscosity	**Square meter per second** (the default), **Stokes**, or **Centistokes**

Setting	Options
Length	**Meter** (the default), **Micrometer**, or **Nanometer**
Time	**Seconds** (the default), **Minutes**, **Hours**, or **Days**
Velocity	**m/s** (the default), **µm/s**, or **nm/s**
Surface tension	**Joule per m^2** (the default) or **Millijoule per m^2**
Surface energy	**Joule per m^2** (the default) or **Millijoule per m^2**

Graphical Mode: Activities



To open this window, from the main menu select **Tools → Options** and click the **Activities** tab.

There are **System definition**, **Calculation**, **Precipitation**, **Diffusion**, **Scheil**, **Process Metallurgy**, **Plotting** and **Tabulation** settings windows.

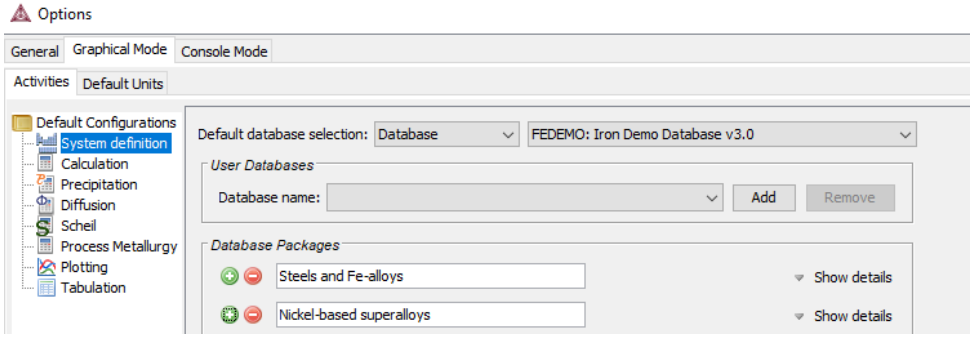
For Plotting, the default settings are shared with the Graphical and Console Modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa).

Global Settings: Graphical and Console Mode Plotting

Global Settings: System Definer

When you create a new System Definer, the default databases are taken from these defaults. The database selections for each System Definer can then be configured individually. Once created, the specific (local) settings for a System Definer are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **System definition**.



- System Definer
- Creating a Database Package and Clearing a Database Package Message

> **Reset to original settings**: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Default database selection

The **Default database selection** can be either for a **Database** or a **Database Package**.

- If you choose **Database**, then select the default installed database to use globally for all System Definer nodes. For example, choose the latest version of the TCS Steel and Fe-alloys Database (TCFE) from the list if you have a license.
- If you choose **Database Package**, select an option from the list. These Database Packages are defined in the *Database Packages* section described below.

User Databases

Under *User Databases*, define the **Database name** after adding a custom database.

Click **Add** to navigate to a custom database on your computer. After you have added the user database it is available from the list to choose as the default.

Once a user database is added to the **Database name** list, you can also click the **Remove** button to delete it from your project.

Database Packages

Based on the installed databases, there are also default *Database Packages* available. Use this section to organize your own sets of databases that you use together often.

Create and remove *Database Packages* by clicking the **Add a database package** button or **Remove this database package** button.



The addition or removal of a database package does not take effect until a new System Definer node is defined.

Click **Show details** to display the list of databases included with the package. Click **Hide details** to only display the name of the package.

- Creating a Database Package

Global Settings: Equilibrium Calculator

When you create a new Equilibrium Calculator, its initial settings are taken from these defaults. The settings of each Equilibrium Calculator can then be configured individually. Once created, the specific (local) settings for an Equilibrium Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Calculation**.

- Options Tab Settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Global Settings: Diffusion Calculator

When you create a new Diffusion Calculator, its initial settings are taken from these defaults. The settings for each Diffusion Calculator can then be configured individually. Once created, the specific (local) settings are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Diffusion**.

- Options Tab Settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Global Settings: Precipitation Calculator

When you create a new Precipitation Calculator, some of its initial settings are taken from these defaults. The settings for each Precipitation Calculator can then be configured individually. Once created, the specific (local) settings for a Precipitation Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Precipitation**.

- Conditions Tab Settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Global Settings: Scheil Calculator

When you create a new Scheil Calculator, its initial settings are taken from these defaults. The settings of each Scheil Calculator can then be configured individually. Once created, the specific (local) settings for a Scheil Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Scheil**.

- Configuration Window Settings



Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Global Settings: Process Metallurgy

When you create a new **Process Metallurgy Calculator**, its initial settings are taken from these defaults. The settings for each Process Metallurgy Calculator can then be configured individually. Once created, the specific (local) settings are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options → Graphical Mode** and click the **Activities** tab. Then click **Process Metallurgy**.



Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Global Settings: Tables

When you create a new Table Renderer, its initial settings are taken from these default settings. The settings of each Table Renderer can then be configured individually. Once created, the settings of a Table Renderer are not affected by changes in the default settings.

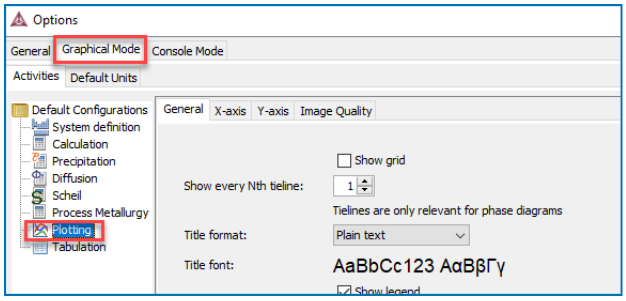
To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

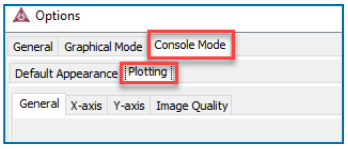
- Configuration Settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Global Settings: Graphical and Console Mode Plotting

The default settings are shared with both modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa).





Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Local Plot Property Settings

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. In the **Plot Properties** window a variety of settings can be made. These are the same settings as in the **Options** window.

You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included). In the **Results** window, hover the mouse over a plot line. The crosshair cursor turns into a cursor resembling a pointing hand when it is over a line that can clicked. Alternatively, hold down the <Ctrl> key while you move the cursor around the plot to only display it as a crosshair and prevent unintended edits.

Global Configuration (Options)

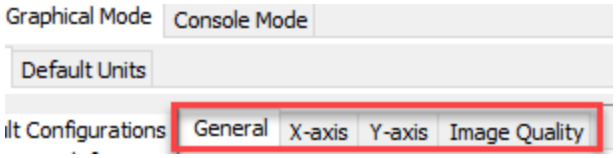
To globally configure the default settings for plotting, from the main menu select **Tools → Options**. You access the same settings either from the **Graphical Mode** or **Console Mode** tabs.

- Click the **Graphical Mode → Activities** tabs and then click the **Plotting** node in the tree, or
- Click the **Console Mode → Plotting** tabs.

> When you create a new Plot Renderer, its initial settings are taken from these default settings. The settings can then be configured individually. Once created, the settings of a Plot Renderer are not affected by changes to the default global settings.

To configure the settings of an individual Plot Renderer rather than the default settings, right-click a plot in the **Results** window and select **Properties** from the menu.

The following global settings are available for both Console Mode and Graphical Mode. Most of the settings are found on the **General** tab. Additional settings below for the **X-axis**, **Y-axis** or **Image Quality** tabs are indicated.



Titles, Legends and Labels

Title format and Label format

For the **Title format** or **Label format**, select **Plain text** (the default) or **LaTeX formatted text**.



For **LaTeX formatted text** you can use the LaTeX math text to enter text. See ADD_LABEL_TEXT and Plot Labels for more details.

Show legend

Select the **Show legend** check box to include a legend on the plot. By default no legend is displayed.

Legend phase caption style

For the **Legend phase caption style**, choose **None**, **All**, **Constitution description** or **Ordering description**.

▶ About Legend Styles

Retain labels



Graphical Mode only.

By default the **Retain labels** check box is selected. Plot labels are kept (retained) when plots are updated. It can be applied globally or locally to individual plots.

Show header



Console Mode only.

Click to select the **Show header** check box to display the basic details about the plot along the top. This includes the date and time the plot is generated, the database used and the properties.

Axis label format

Click the **X-axis** and **Y-axis** tabs to edit these settings.

Choose either **Plain text** or **LaTeX-formatted text**.

Axis label font

Click the **X-axis** and **Y-axis** tabs to edit these settings.

Click the **Modify** button to the right of the window to select a **Font name**, **Style**, **Size** and **color**.

Choose or enter a **Tick mark length** (**3** is the default). The defaults are to have the **Tick marks outside the chart** and to **Show tick labels**. Click to clear the check boxes as required.

Tick label font

Click the **X-axis** and **Y-axis** tabs to edit these settings.

Click the **Modify** button to the right of the window to select a **Font name**, **Style**, **Size** and **color**

Fonts and Background Colors

Title font, Legend font, Label font, Header font

To change various attributes for the **Title**, **Legend**, **Label** and **Header** , click **Modify** to edit the **Font Name**, **Style**, **Size** and **Color**.

Legend background color, Background color, Canvas color, Border color

To change various background color attributes, click **Modify** to choose a color or enter a specific color.

Lines and Grids

Show grid

Click to select the **Show grid** check box to include a grid on the plot. By default no grid is displayed.

Show every Nth tieline



Tielines are only applicable to phase diagrams.

Choose an integer value ranging from 0 to 99.

Color option (plot lines)

For the for plot line colors, choose a **Color option** from the list: **Legacy**, **Printer friendly**, **JFree chart**, **Pastel**, **Medium dark**, **Bright dark**, **Vivid** or **Earth**.

This option is also available for specific plot lines. To change the color of an individual plot line double-click it in the **Results** window and use the color palette to define it or enter a specific color.

Border width

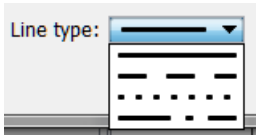
Choose a plot **Border width** between **1** (thin, the default) and **10** (thick).

Line width

For the plot line width, choose a **Line width** from the list. These options are also available for specific plot lines. To change an individual plot line width double-click it in the **Results** window.

Line type

This option is only available for individual plot lines. To change an individual plot line type double-click it in the **Results** window and choose a **Line type** from the list.



Data Points, Anchors and Numbers

Show anchor

Click to select the **Show anchor** check box. By default, an anchor between the label and the plot point is displayed.

Show data points

Click to select the **Show data points** check box to display the data points on the plot lines. This option is also available for specific plot lines. To show data points on an individual plot line double-click it in the **Results** window and select the check box.

Data points marker size

Choose the **Data points marker size** between **1** (small) and **10** (large). The default is 3.

Number of decimals

Choose the **Number of decimals** to display in the plot. The default is 2.

Numeric format

Choose the **Numeric format** to display in the plot **Auto**, **Decimal** or **Scientific**.

Plot Area Size

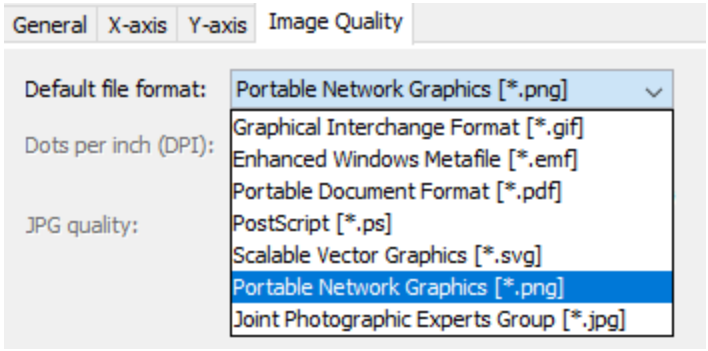
Plot area size

The **Fit the plot area size to the enclosing window** option is selected by default.

Click **Define the plot area size** to enter a **Plot area height** and **Plot area width (not applicable to triangular plots**. The units are pixels and the size is kept as the size on the screen (96 dpi).

Image Quality

Click the **Image Quality** tab to access the settings below.



Choose a **Default file format**: **Portable Network Graphics .png** (the default),**Graphical Interchange Format .gif**, **Enhanced Windows Metafile .emf**, **Portable Document Format .pdf**, **PostScript .ps**, **Scalable Vector Graphics .svg**, or **Joint Photographic Experts Group .jpg**.

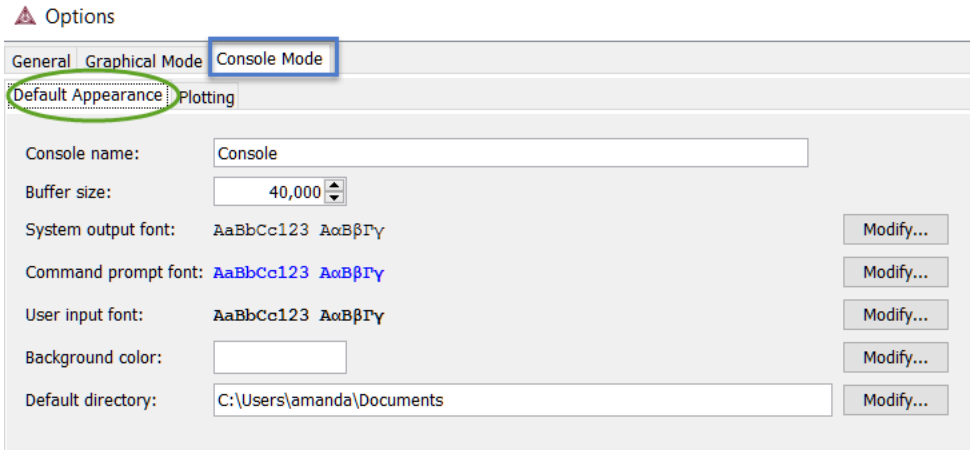
The following settings are only available for .png and .jpg file formats.

To change the resolution of a *.png or *.jpg image, click to clear the **Use default resolution** check box. Then enter a numerical value in the **Dots per inch (DPI)** field.

For .*jpg files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.

Global Settings: Console Mode Default Appearance

To open this window, from the main menu select **Tools → Options**. To change the name, buffer size, fonts and colours for a specific Console window, right-click the label for that particular Console and select **Properties**.



Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button.

Console name

The default is `Console` or enter another name to display.

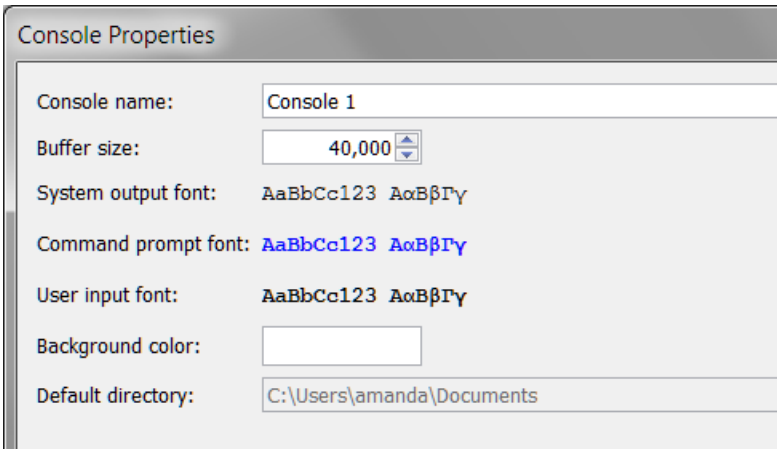
Buffer size

The default buffer size is 40,000.

In Console Mode, sometimes the output overflows the window text buffer. This is how to increase the buffer size.

1. Right-click the Console tab header in the Console window (if this is the first Console tab, it is labeled **Console 1**).

2. Click **Properties**, and increase the **Buffer size** in the Console Properties window.



System output font

Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.

Command prompt font

Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.

User input font

Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.

Background color

Click **Modify** to open the **Select Color** window to choose a background color for the Console Mode window where you enter commands.

Default directory

Set the default directory file path to where the various file types are saved.