Modeling and optimization of energy systems

Lecture notes

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Contents

Specific objectives

The specific objectives that have to be acquired at the end of the lecture are summarized in the following table which can be used for evaluating your progress.

Progress	Topic
	Energy conversion system model
OOOOOO	Definition of the system boundaries
OOOOOO	What is a state variable, what are the degrees of freedom of a thermodynamic state
OOOOOO	What is a constitutive equation and how a thermodynamic model works
OOOOOO	Define the process units
OOOOOO	State the energy and the mass balances of a unit
OOOOOO	State the modeling equations of a unit
OOOOOO	State the assumptions of a model. Be able to explain the level of detail and complexity trade-off
OOOOOO	Realize a degree of freedom analysis, define the specifications, what are dependent and independent variables
OOOOOO	Solve a unit model using a sequential approach, be able to explain the pro and cons of the sequential approach
OOOOOO	Explain the solving methods that can be used in a sequential solving approach
OOOOOO	Solve a unit model using a simultaneous approach, be able to explain the pro and cons of this approach. What are the more important conditions for using a simultaneous approach. How does it compare with sequential approach. How to solve a simultaneous model.
	Solve a Flowsheet
OOOOOO	Analyze the degrees of freedom of a flowsheet
OOOOOO	Apply the Motard method to define a sequence to solve a sequential modular simulation problem. What are the difficulties of the sequential approach.
OOOOOO	Numerical methods for solving the sequential problems
OOOOOO	State a simultaneous solving problem for flowsheeting, what are the necessary conditions and the difficulties of using a simultaneous approach
OOOOOO	Numerical methods for solving simultaneous problems.
OOOOOO	Pro and cons of simultaneous and sequential approaches
	Thermo-economic objective functions
OOOOOO	Different type of thermo- economic optimization problem
OOOOOO	Estimate the investment of a process flowsheet and annualize the investment
OOOOOO	Formulate a thermo-economic objective function: operating cost, efficiency, investment, total cost, environmental impact, life cycle impact.

Progress	Topic
	Optimization problems
OOOOOO	Define the different possible use of optimization in process flowsheeting
OOOOOO	State a problem of parameter identification
OOOOOO	What is the data reconciliation
OOOOOO	How to analyze the redundancy of a system: overspecification, missing measurements, just calculable systems.
OOOOOO	Stating an optimization problem: black box, simultaneous, hybrid methods
OOOOOO	Pro and cons of the different approaches
OOOOOO	Describe the different methods to solve optimization methods, what are the pro and the cons of each of them
OOOOOO	Solving an unconstrained optimization problem
OOOOOO	Solving a multi-variable unconstrained optimization problem
OOOOOO	Solving a multi-variable constrained optimization problem
OOOOOO	Solving a MILP optimization problem
OOOOOO	Solving a problem using heuristic methods
OOOOOO	Stating a multi-objective optimization problem
OOOOOO	Choosing a optimization solving method

Preface

These notes have been written on the basis of the following documents:

- 'Techniques de modélisation et d'optimisation des systèmes énergégtiques', B. Olsommer and M.R. von Spakovsky, LENI-STI-EPFL, 1997
- 'Simulation et optimalisation statistique des systèmes industriels', B. Kalitventzeff and G. Heyen, Université de Liège, 2000
- 'Méthodes d'analyse et de synthèses énergégtiques des procédés industriels, F. Maréchal, Université de Liège, 1997

Additional information can be found in:

- R. Turton. Analysis, Synthesis, and Design of Chemical Processes. Prentice Hall, Upper Saddle River, N.J, 3rd ed edition, 2009.
- L. Puigjaner and G. Heyen. Computer Aided Process Engineering Vol. 1 and 2. Wiley-VCH, Weinheim, 1st ed edition, 2006.
- G. Ulrich and P. Vasudevan. A Guide to Chemical Engineering Process Design and Economics a Practical Guide. CRC, Boca Raton, Fla, 2nd ed edition, 2003
- I.C. Kemp. Pinch analysis and process integration: a user guide on process integration for the efficient use of energy. Butterworth Heinemann, 2007. `https://www.dawsonera.com/abstract/9780080468266`.

Please inform the authors of any mistakes, i.e spelling errors, and improvements suggestions.

Chapter 1

Introduction

In this chapter the basic notions for the modeling and optimization of energy conversion systems are introduced: systems, models, state variables and degrees of freedom.

1.1 Introduction

This course deals with the modeling and the optimization of industrial energy systems. An industrial energy system may refer to a whole process, a part of a process or set of processes that generate through energy conversion other forms of energy or consumer goods. These processes are for example:

1. Processes for the production of electricity: today over 80% of the world's electricity generation is achieved through thermal conversion of the energy resource.
2. Energy conversion processes: for example heat pumps, hydrogen production processes, biomass or coal gasification.
3. Chemical and petrochemical processes.
4. Food industry processes.

From a thermodynamic point of view, the common point between these processes is the transformation of raw materials into products and by-products through a set of operations (Figure 1.1). In a general way, this system can be described considering that the conversion of raw materials and energy occurs through a set of interconnected equipments:

- heat exchangers, evaporators, condensers
- distillation columns, cyclones, filters, absorbers
- boilers
- gas turbines, motors
- compressors, turbines
- reactors, reformers, ...

Each equipment unit performs its tasks through series of transformations of thermodynamic states: heat exchange, separation, reaction,... The different operations can be strongly integrated in one single unit. For an engine, for example, chemical reactions (combustion and production of pollutants), diffusion and mixing, heat exchange and expansion occur simultaneously. From a system point of view, it is possible to gather the production units in different sub-systems. The main operations will be grouped in sub-systems called processes, which will often rely on production supports: water, solvent, catalysis... The preparation, treatment, distribution and recycling of the production supports constitute as well sub-system (process) of the main system:

- hot water network
- filters, filters clean-up
- catalyst regeneration
- packaging, bottles washing, ...

In industrial processes, the thermodynamic state changes are achieved through the energy supply from outside the system. Consequently, this energy needs to be converted and distributed in an appropriate form for the required transformation. It will be in different forms: electric, mechanic, thermal,... The operations of the transformation of energy resources into useful energy are grouped in a sub-system called energy conversion that includes:

- boilers
- gas turbines, combustion engines, electric motors
- steam distribution, steam turbines
- heat pumps, refrigeration cycles
- hot oil network,...

In such transformations, the resources (i.e feedstock and energy) are not fully converted into the final products and by-products, but are also present in the emissions and in the losses. The waste produced by the process is often treated, and, if possible, recycled before being disposed, for the protection of the environment, but also for economical reasons. The system will therefore include several sub-systems for waste treatment, including:

- waste water treatment
- elimination of solvents residuals
- sieving and filtration systems
- gas treatment systems: scrubbers, filters, catalytic systems,...

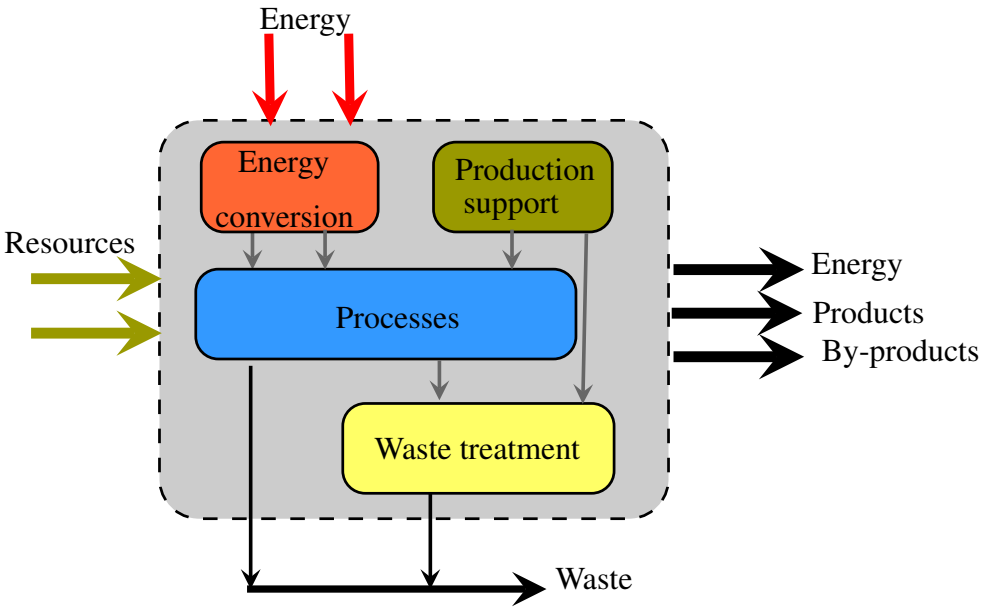


Figure 1.1: Integrated energy system.

All these transformations follow the first principle of thermodynamic (i.e. energy conservation) and the second principle of thermodynamics (i.e. transformations occur with an increase in entropy in an isolated system). The entropy can be seen as a measure of disorder. The economic indicator defining the performance of the plant, can be expressed by:

Profits = Incomes-Operating costs-Investments

where the incomes are the results of the sale of all products and by-products, the operating costs represent the expenses relative to the operation of the plant (i.e. the purchase of raw materials, energy and production supports, the cost of emissions and waste, the costs of maintenance and taxes), and the investments are the financial means required for the purchase of all the equipments. These costs need to be expressed in a coherent monetary unit (for example CHF (2014)/year).

Besides the economic performance, which is highly dependent on the economic position of the investor and the socio-economic context, the engineers use different performance indicators that rely on thermodynamic values defining the state of the process. Some examples are the energy efficiency (ratio energy in the products/energy input), the mass conversion (ratio kg of products/ kg of raw material) and the exergy efficiency (ratio exergy in the products/exergy drawn from the resources). The evaluation of these indicators allows the engineers to better understand the energetic and exergetic aspects of the processes they investigate, and to propose improvements with the objective of increasing the performance. More details about the notion of exergy are provided in [3, 14].

Nowadays, there are challenges related to the sustainable development of our society, besides the economic challenges related to the profitability of an industrial process. The manufacturers need to try to maximize the performances of their production units, in order to satisfy the constraints of the Kyoto agreements, which aim at reducing and stabilising the CO_2 emissions. Consequently, the target is to maximize both the efficiency and the economic profits.

In this context, the engineers develop on the one side increasingly complex energy conversion concepts, which are based on more and more advanced technologies such as fuel cells. On the other side, engineers try to exploit the full potential of the existing systems to improve their performances, both in terms of energy conversion efficiency and of emissions reduction. The complexity of the implemented systems, and the optimal use of purchased raw materials and energy, has led to the development of highly integrated energy systems which aim at the maximum conversion of the exergetic input. Some examples are fuel cell systems and integrated gasification and combined cycles. In the field of electrical energy production, the current tendency is to promote the use of renewable energy sources (e.g. biomass, waste) or of low quality resources (e.g. coal). However, these options also face difficulties: resource variability, pollution risks, risk of failure, etc.. Moreover, co-generation systems gain more and more importance. Co-generation systems satisfy the thermal energy demand in an exergetic optimal way by transforming the fuel in high-quality energy before using the degraded energy in the form of useful heat.

Regarding all these difficulties, modeling and optimization tools play an essential role for mastering the design, behavior and operation of such systems. The objective of energy systems **modeling** is to describe the systems behavior and the influence of the different parameters on the performance, by applying computer-aided process engineering tools. The modeling tool computes the thermodynamic states of the various input and output streams, as well as those internal to the plant. Consequently, the overall performance of the system can be calculated, as well as the performance of each process unit (i.e equipment). In the perspective of decision-making, the modeling tool allows evaluating the impact of decisions on the performance without recurring to the experimental testing, which may be very expensive. The modeling tool is very useful to evaluate decisions concerning the system design, because, in this case, an experimental system does not exist.

The aim of the **optimization** is to identify the best decisions to be taken in order to improve the performance of the system. Modeling is an essential step prior to the optimization, as it allows to compute

the system's performance. Nowadays, optimization tools are used all along the life of an industrial energy system, from its design to its decommissioning:

- In research and development (R&D), engineers use modeling and optimization to identify the best experimental operating conditions, to conceive the experimental set-up, to exploit the results, to estimate the change of scale (passing from a pilot plant to an industrial system), etc.
- For the process design, modeling and optimization tools are applied to determine the best configuration, the optimal size of the equipments and the best operating conditions, to conceive the control system and the optimal strategy of operation, to estimate the environmental impact, and to evaluate safety and reliability aspects.
- During the process installation, modeling tools are used to verify the performance and the specifications.
- The process operation is continuously optimized. This is done by first predicting and monitoring the process and equipments performance, and then by adapting the specifications (planning, predictive maintenance, online optimization, model-based control, etc.).
- Modeling and optimization tools are also used to optimize the investments for the plant upgrading: retrofit study, capacity increase, etc.
- Finally, modeling tools are applied to conceive the decommissioning of the plant in the most appropriate way.

1.2 Modeling

A model has to calculate and characterize the transformations of thermodynamic states that take place in the process. Therefore, the process behavior and its operating limits has to be transcribed into a mathematical model. Considering the energy system as a whole, the mathematical model is an 'operator' transforming the inputs into output values (Figure 1.2).

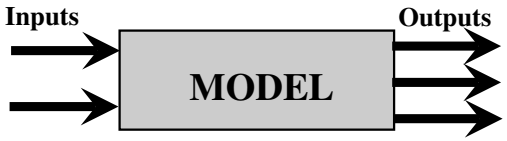


Figure 1.2: Model= mathematical transformation.

For the modeling, a distinction must be made between the materials inputs, and the information inputs. A material input can be an information output, because it is the result of the model resolution. For example, the amount of fuel entering a system, which can be calculated to satisfy a given heat demand. The model inputs are the specifications: the demand that the system must satisfy, the raw materials and resources properties, the characteristics of the environment (e.g. ambient temperature and pressure, economic data, cooling water temperature, etc.) and the market specifications (e.g. products quality and by-products emission limit, etc.). The outputs are the products, emissions and wastes (e.g. different forms of degraded energy and pollutants), the operating costs, the equipment size, etc.. In addition to the values that characterize the system's performance, the model will also compute the values of the variables that characterize the state of the system. The mathematical model of the system can be represented by Eq. 1.1 where X_{output} is the value of the output variables and X_{input} the value of the input variables. The complexity is that it is not easy to get an explicit form for the model which will be described in a general way by a system of equations to be solved as Eq. 1.2, where X_{state} are the variables characterizing the State of the system. The variables X_{output} are a subset of the variables X_{state}.

$$X_{output} = F(X_{input}) \tag{1.1}$$

$$F(X_{input}, X_{state}) = 0 \tag{1.2}$$

Conceptually, an industrial energy system can be represented as a set of interconnected boxes like in Figure 1.3. The interconnections represent streams that link boxes between them. Each box, namely a process unit, represents a mathematical operator (model) which transforms the state of the connected flows. This mathematical operator represents the thermodynamic transformations by the physical and chemical phenomena that occur in the unit. The mathematical operator represents thus the mass and energy balances, as well as the mathematical formulation of the thermodynamic transformation taking place in the unit: heat transfer, mass transfer, chemical reaction, expansion, compression, etc. Each connection between two units defines a stream whose state allows to characterize the material and/or energy it transfers from one unit to another. In an energy system, different types of streams can be differentiated:

- Material streams representing the flow of material in the pipes
- Thermal streams representing heat transfers
- Mechanical streams that represent the work
- Electrical streams that represent the transfer of electric power
- The flow of information may be used to represent the control loops

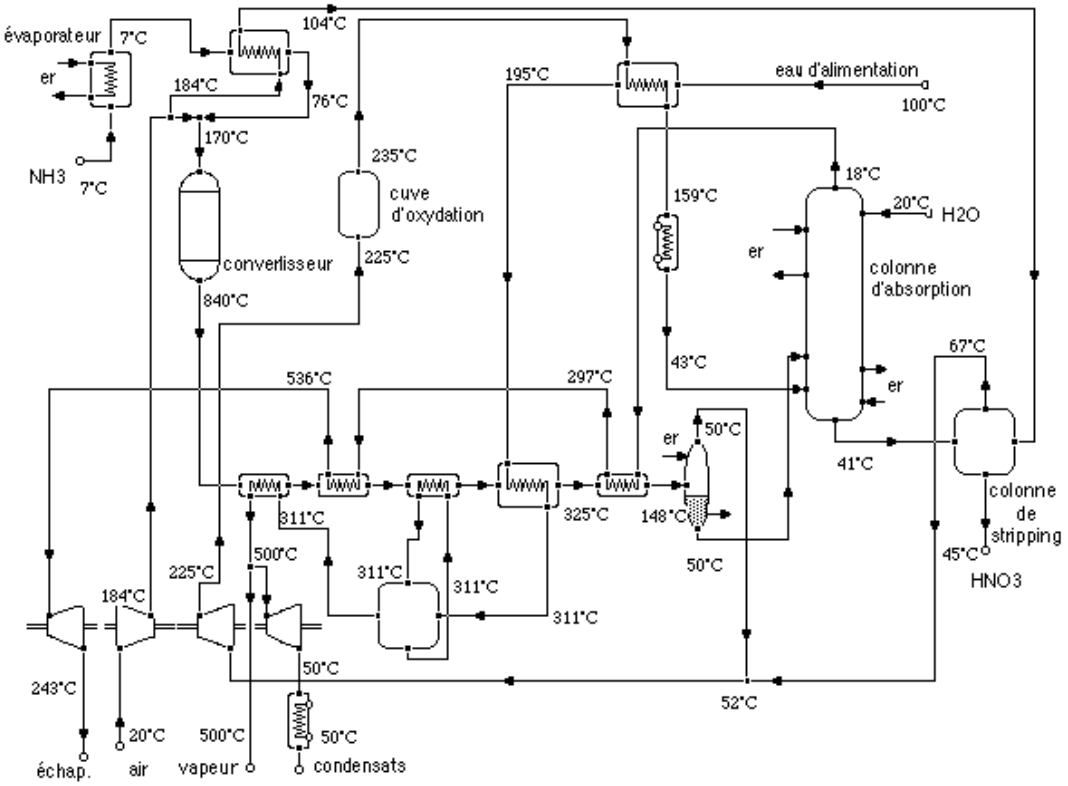


Figure 1.3: Flowsheet of the nitric acid process.

The model of such a system will include three types of relationships:

1. Transfer relations representing the transfer of information between units and therefore the way in which the units are interconnected. These relationships define for example that the compressor outlet stream enters the heat exchanger that follows.
2. Modeling equations, which mathematically represent the mass and energy balances, as well as the physical and chemical transformations that take place in the unit.
3. Thermodynamic binding relations that link state variables between them and characterize the material stream.

1.3 The model

A model is a set of interconnected modules (units). Each module is characterized by the equations that model in a generic way its operation; these equations are called modeling equations. A unit can schematically be represented by Figure 1.4.

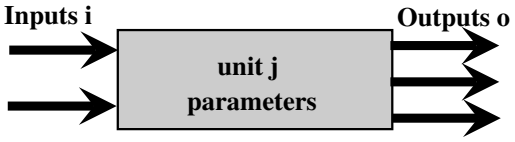


Figure 1.4: Schematic representation of a unit.

The modeling equations constitute a set of equations $F(X_{state}) = 0$ categorized into different groups:

- Mass balances
- Heat balances
- Sizing equations / performance equations
- etc.

The modeling equations of unit j define a subset of the matrix $F(X_{state}) = 0$:

$$F_j(X_{state,j}) = 0 \tag{1.3}$$

with:

$X_{state,j} = (m_{ij}, P_{ij}, h_{ij}, m_{oj}, P_{oj}, h_{oj}, par_j)$

m_{ij}	flow of the input stream i of the unit j
P_{ij}	pressure of the input stream i of the unit j
h_{ij}	molar enthalpy of the output stream o of the unit j
m_{oj}	flow of the output stream o of the unit j
P_{oj}	pressure of the output stream o of the unit j
h_{oj}	molar enthalpy of the output stream o of the unit j
par_j	parameters of the unit j

The connection of two units defines the variables X_{state} which are shared by the units (d_{ij}=d_{ok} if the input stream i of the unit j is the output stream o of unit k). By describing the interconnections between units, a set of equations and variables that describe the system modelling are obtained. The number of modelling equations n_e is lower than the number of state variables X_{state} n_v. The difference between the number of state variables and equations is called *degrees of freedom DoF* :

$$DoF = n_v - n_e \tag{1.4}$$

In order to define the state of the system, the DoF has to be determined. To do this, n_{DOF} equations are added. These equations are divided into two sets: specification equations and set point equations.

The **specification equations** n_s define the conditions that the system must satisfy:

- External conditions: fuels characteristics , ambient temperature, market conditions, etc.
- State of the equipments of the installation: fouling of heat exchangers, expansion efficiency, characteristic curves of pumps and compressors, etc.
- Requirements that the process must satisfy: mechanical power of the turbines, temperature at the heat exchanger outlet, etc.

The state of the system's elements are determined by parametric identification based on one or several sets of measurements that have been rendered consistent by a validation calculation. Based on an appropriate definition of the state variables, the specification equations can be written in the simple form Eq. 1.5.

$$S(X_{state}) = 0 s_i(X_{state}) : x_i - v_{si} = 0, \forall i = 1, ..., n_s \tag{1.5}$$

with:

$S(X_{state})$	vector of specification equations
$s_i(X_{state})$	element i of the vector S that defines the specification i
x_i	state variable corresponding to the specification i
v_{si}	value of the specification i
n_s	number of specifications

The **set point equations** relate to the variables which the engineer can manipulate to optimize the process performance. The value of the set point results from the engineers instructions. These variables are called decision variables n_c. The number n_c represents the actual number of degrees of freedom of the process. Like the specification equations, the set point equations take the form of Eq. 1.6:

$$C(X_{state}) = 0 c_i(X_{state}) : x_i - v_{ci} = 0, \forall i = 1, ..., n_c \tag{1.6}$$

with:

$C(X_{state})$	vector of set point equations
$c_i(X_{state})$	element i of the vector C that defines the set point i
x_i	state variable corresponding to the set point variable i
v_{ci}	value of the set point i
n_c	number of set point variables

To be computable, the system must satisfy Eq. 1.7. This condition is necessary but not sufficient, because in addition the equations $F(X_{state})$, $S(X_{state})$ and $C(X_{state})$ have to be independent.

$$n_{dof} = n_c + n_s \tag{1.7}$$

In addition to the knowledge of the state variables, the values of some indicators may also be needed. These values are determined by equations known as **performance equations/linking equations**. Each of these equations is an additional variable. The system of equations which sets linking variables defines a square system that can be calculated once the value of X_{state} is known. This set of equations can include, for example, the calculation of the efficiency or of the profit.

1.4 State variables

1.4.1 State variables of material streams

The transfer of material/mass is characterized, on the one hand, by the extensive variables (e.g. partial flow or flow) and, on the other hand, by intensive variables (e.g. composition). To characterize the transfer of energy, several variables can be used: pressure, temperature, total enthalpy, mass or molar enthalpy, entropy, etc.

From a thermodynamic point of view, a stream of n_x substances will be completely characterized by fixing the value of n_e extensive variables (with $n_e \geq 1$) (e.g. flow), and $2 + n_x - n_e$ intensive variables. Then the other variables can be calculated based on the thermodynamic state equations. For example, a steam flow (mono-substance fluid) is fully characterized by fixing its flow and two intensive variables which characterize its thermodynamic state: for example the entropy and pressure. By the thermodynamic relations, other state variables can be calculated based on the value of the two chosen variables.

It should be noted that the choice of the independent variables defining the thermodynamic state of a fluid has to ensure that:

1. The variables are independent (i.e. choose at least 1 extensive variable).

2. The thermodynamic equations allow to represent the thermodynamic state in a bi-univocal way. The choice of the temperature and pressure as state variable to represent the thermodynamic state of water is not valid if a phase change takes place (see Figure 1.5). At the saturation pressure, the same temperature corresponds to several enthalpy states (between liquid and saturated vapor) corresponding to different vapor fraction values. If a phase change occurs, it is therefore necessary to fix in addition to the temperature another variable, either the vapor fraction, or the enthalpy, in order to determine the thermodynamic state.

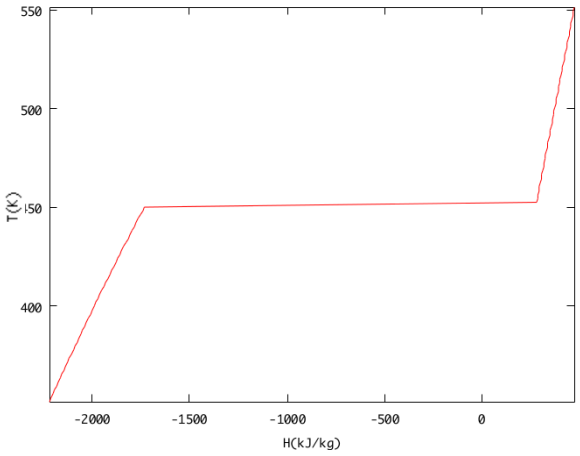


Figure 1.5: Temperature-Enthalpy diagram of water.

1.4.2 State variables of thermal streams

A thermal stream (heat stream) is characterized by the amount of energy that is transferred. It is commonly expressed per unit of time thus defining the transferred power. In some cases, the stream may be characterized by its temperature level, although this definition is is only indicative and cannot be generalized.

1.4.3 State variables of mechanical streams

A mechanical stream is characterized by the power and the speed of rotation of the shaft.

1.4.4 State variables of electrical streams

An electricity stream is by analogy characterized by its intensity and its tension and or power.

1.4.5 Variables of unit models

The parameters of models are variables that describe the operation of the unit, for example the operating pressure, pressure loss, mechanical power, the heat exchange area, etc. The definition of these parameters is linked to the modeling equations. Their choice may have a considerable impact on the model resolution.

1.4.6 Which state variables to use?

State variables are required for the model calculation. Due to the number of degrees of freedom of the concerned state, it is important to choose the independent variables and those that will be calculated by the thermodynamic model. If the choice of the variables is completely free for the model establishment the following criteria are recommended to make the best choice.

Choice of an intensive variable rather than extensive variable

Molar or mass quantities are preferred to total quantities, using only one flow rate quantity. This is justified by the fact that the thermodynamic quantities are calculated in molar values. This allows to avoid the degeneration of the thermodynamic state when the flow is zero. The calculation of the temperature on the basis of the total enthalpy may be impossible when the flow is zero. In this case, the equation is undetermined, which is not the case with the molar enthalpy, even if the state does not exist.

Make sure that the variables represent the state in bi-univocal way

Although the thermodynamics are developed as a function of the temperature and pressure, the choice of the molar enthalpy will be preferred to that of temperature in the case of a mono-substance fluid. The temperature does not completely characterize the saturation and an additional variable (the vapor fraction) must be given to calculate the enthalpy. On the other hand, the molar enthalpy and pressure perfectly characterize the enthalpy content of the stream. The choice of the molar enthalpy is thus justified.

The total enthalpy is calculated by Eq. 1.8:

$$H_i = h_i \cdot \dot{m}_i \tag{1.8}$$

and the temperature by 1.9:

$$T_i = f(h_i, P_i, x_i) \tag{1.9}$$

The function $f(h_i, P_i, x_i)$ corresponds to a thermodynamic calculation of the equilibrium in fixed molar enthalpy, pressure, and composition.

Chapter 2

Thermodynamic properties

This chapter introduces the principles for the calculation of the thermodynamic properties of a stream. The key elements are the constitutive equations.

2.1 Introduction

The thermodynamic models allow to represent a set of thermodynamic properties of a stream with n_c compounds based on the knowledge of $n_c + 2$ state variables. Thermodynamic relationships are represented by equations of state which are generally expressed in terms of mass or molar magnitudes. These are mathematical expressions of the well-known diagrams from the thermodynamics: T-s, h-s, p-v, etc. diagrams.

Typical thermodynamic properties calculated by the thermodynamic model (i.e. constitutive equations) are:

- Density, specific volume (v)
- Enthalpy (h), entropy (s), specific heat (cp)
- Viscosity, thermal conductivity, diffusion coefficients, surface tension
- Phase equilibrium (L-V, L-L, L-L-V)
  - Saturation point, dew point
  - Heat of vaporization
  - Saturation pressure
  - Phase distribution coefficients
- Chemical reactions
  - Heat of reaction
  - Equilibrium constants

The thermodynamic models mathematically represent the properties and interaction forces. The thermodynamic properties are related to the energy storage mode in molecules. The different types are:

- Binding energy between atoms
  - Heat of reaction
  - Heat of formation

  - Equilibrium constant

- Energy of the molecules
  - Translation: perfect gas
  - Rotation and vibration properties defining the contributions to cp, enthalpy and entropy

- Interactions between molecules
  - Attraction and repulsion between the molecules which are represented by the equations of state. These allow to calculate the mixing properties by introducing corrections to perfect gas law and which are important for calculating the transport properties and the phase changes.

The properties of the mixtures are determined on the basis of the thermodynamic properties of pure substances. These are obtained from literature. For well-known substances, such as water, air and CO_2, the data have been compiled and very precise empirical equations have been established. For others, general equations are developed based on a limited number of properties and on the observation that for similar substances the properties are identical in reduced coordinates. The properties that should be provided for a substance are:

- Critical properties: temperature, pressure, density
- Acentric factor
- Boiling temperature and enthalpy of vaporization
- Fusion temperature and enthalpy
- Enthalpy and the free enthalpy of formation

Correlations can be used to estimate the values of the missing parameters based on these data. One should however be aware that for a substance the specific values are better than those obtained with the correlations. Most modeling software offer thermodynamic models and a database of substance properties. For example, NIST (`http://webbook.nist.gov`) or DIPPR `http://www.aiche.org/dippr`).

When using these databases for the development of a model, one has to verify the sources of the data from the database and if necessary verify that the validity range (temperature, pressure and concentration) corresponds to the one of the model. This is very important because in some cases, correlations with high exponents are used which can lead to undesirable reverse answers.

2.2 Enthalpy calculation

The equations for calculating the enthalpy of a mixture are given here as an example. For the calculation of the energy balances, the enthalpy of a gas must be assessed on the basis of the temperature and pressure. For an ideal gas, the following formulas are used.

2.2.1 Gas enthalpy

$$H^g_{id}(T,P,x_i) = \sum_i \Delta H_i(T^o) + \int_{T^o}^{T} \left(\sum_i x_i \cdot Cp_i(T) \right) \cdot dT$$

$$Cp_i(T) = a_i + b_i \cdot T + c_i \cdot T^2 + d_i \cdot T^3$$

It should be noted that the ideal gas enthalpy does not depend on the pressure.

2.2.2 Liquid enthalpy

The liquid enthalpy is assessed based on the gas properties and on the vaporization enthalpy which can be assessed with the Watson formula. The temperatures are expressed in Kelvin and the enthalpy of vaporization is calculated with regard to a reference with an known vaporization enthalpy and temperature. In most cases, the reference temperature is the boiling temperature. The scale exponent 0.38 can be used as approximation if the exponent of the substance is unknown.

$$\Delta H_{vap_i}(T) = \Delta H_{vap_i}(T_i^b) \cdot \left(\frac{T_i^{crit} - T}{T_i^{crit} - T_i^b} \right)^{0.38}$$

The enthalpy of the liquid is given by:

$$H_{id}^l(T, P, x_i) = \sum_i \Delta H_i(T^o) + \int_{T^o}^{T} \left(\sum_i x_i \cdot Cp_i(T) \right) \cdot dT - \sum_i \Delta_{vap_i}(T)$$

2.2.3 Enthalpy of liquid-vapor mixture

If the vapor fraction α is known, the enthalpy of the liquid-vapor mixture is calculated by the sum of the enthalpy of the liquid and the vapor. The enthalpy of the liquid $H_{id}^l(T, P, x_i^l)$ and of the vapor $H_{id}^g(T, P, x_i^g)$ are calculated for different liquid and vapor compositions obtained from the liquid-vapor equilibrium calculation.

$$H_{id}^{l-v}(T, P, x_i) = \alpha \cdot H_{id}^g(T, P, x_i^g) + (1 - \alpha) \cdot H_{id}^l(T, P, x_i^l)$$

2.3 Liquid-vapor equilibrium calculation

The thermodynamic model is composed of:

- Equations: f(variables, parameters)=0, mass and energy balance, equilibrium conditions
- Coherent choice of thermodynamic laws (equations of state or correlations) setting the model validity range and of the necessary data.

Example of state equation: Soave equation. The Soave equation of state is given by:

$$P = \frac{RT}{V - b} - \frac{a(T)}{V \cdot (V + b)}$$

with
$a = a_c \left[1 + (0.48 + 1.574\omega - 0.176\omega^2)(1 - \sqrt{T_r})\right]^2$
$a_c = 0.42748 \frac{(RT_c)^2}{P_c}$
$b = 0.08664 \frac{RT_c}{P_c}$

Several auxiliary variables are defined $Z = \frac{PV}{RT}$, $A = \frac{a \cdot P}{(RT)^2}$ and $B = \frac{b \cdot P}{RT}$. The values of Z are solution of the equation $Z^3 - Z^2 + (A - B - B^2) \cdot Z - A \cdot B = 0$. With these variables, the fugacity coefficient can be calculated:

$$ln\varphi = Z - 1 - lnZ - \int_{\infty}^{V} \frac{Z - 1}{V} = Z - 1 - ln(Z - B) - \frac{A}{B} ln \frac{Z + B}{Z}$$

2.3.1 Equilibrium conditions

The partial fugacities of the mixture constituents i at T and P must be equal in the two phases: $f_i^L = f_i^V$. These variables are generally expressed by the fugacity coefficient (φ) for the vapor phase and the activity coefficient (γ) and the reference fugacity f^* for the liquid phase:

$$\varphi_i \cdot y_i \cdot P = \gamma_i \cdot x_i \cdot f_i^{*L}$$

The equilibrium coefficient K_i is defined by the ratio of the mole fraction in the vapor phase y_i and in the liquid phase x_i:

$$K_i = \frac{y_i}{x_i} = \frac{f_i^{*L} \cdot \gamma_i}{P \cdot \varphi_i}$$

knowing that

$$\varphi_i = \varphi_i(T, P, \bar{y}, \bar{\Theta_\varphi})$$
$$\gamma_i = \gamma_i(T, P, \bar{x}, \bar{\Theta_\gamma})$$

with:

$\bar{x}$ and $\bar{y}$	vectors of molar fractions
$\bar{\Theta_\varphi}$ and $\bar{\Theta_\gamma}$	vectors of parameters

The number and the values of the parameters depend on the choices made for physical-chemical laws. Therefore K_i can be written as: $K_i = f(T, P, \bar{x}, \bar{y}, \bar{\Theta})$.

Remember that f_i^{*L} is the fugacity of the constituent i (pure liquid) at the temperature and pressure of the mixture or the reference fugacity. This term only depends on T and P. This is the symmetric convention. If the constituent does not exist in the liquid state, i.e. if it is noncondensable, the reference is the infinite dilution state. This is the asymmetrical convention. At moderate pressure:

$$f_i^{*L} = f_i^{*LS} \cdot exp\left[\frac{v_i^s \cdot (P - P^s)}{RT}\right]$$
$$f_i^{*LS} = P_i^S \cdot \varphi_i^{*S} \tag{2.1}$$

with:

f_i^{*LS}	fugacity of pure substance at saturation at the temperature of the mixture
φ_i^{*S}	fugacity coefficient of saturated vapor under the same conditions
P_i^S	saturated vapor pressure of component i (calculated using the vapor equation of state)

If the pressure of the system is chosen as a reference, these relations are not modified. If the reference state of the liquid is chosen to be that of the pure substance at pressure P^r and at the temperature of the system:

$$f_i^{*LR} = P_i^{*LS} \cdot \varphi^{*S} \cdot exp\left[\frac{v_i^s \cdot (P^r - P^s)}{RT}\right]$$
$$f_i^{*L} = f_i^{LR} \cdot exp\left[\frac{v_i^L \cdot (P - P^r)}{RT}\right] \tag{2.2}$$

The molar volume of the liquid is generally considered to be independent of pressure, which justifies the approximations made in the formulas above. In addition, this hypothesis is found implicitly when calculating φ for the component i. The advantage of choosing the reference pressure equal to 0 is that the two phases have the same reference state. If the reduced temperature ($T_r = T/T_c$) of the component i is greater than 1, the saturation pressure cannot be calculated, an extrapolated value must be taken or the fugacity of the liquid has to be calculated in another way. This case is not treated here (i.e. asymmetric convention). It can therefore be assumed that the relationship: $K_i = f(T, P, \bar{x}, \bar{y}, \bar{\Theta})$ is known. It is useful to remember that there are various approximations that represent a set of possible behaviors for the vapor and liquid phase. Figure 2.1 summarizes these opportunities.

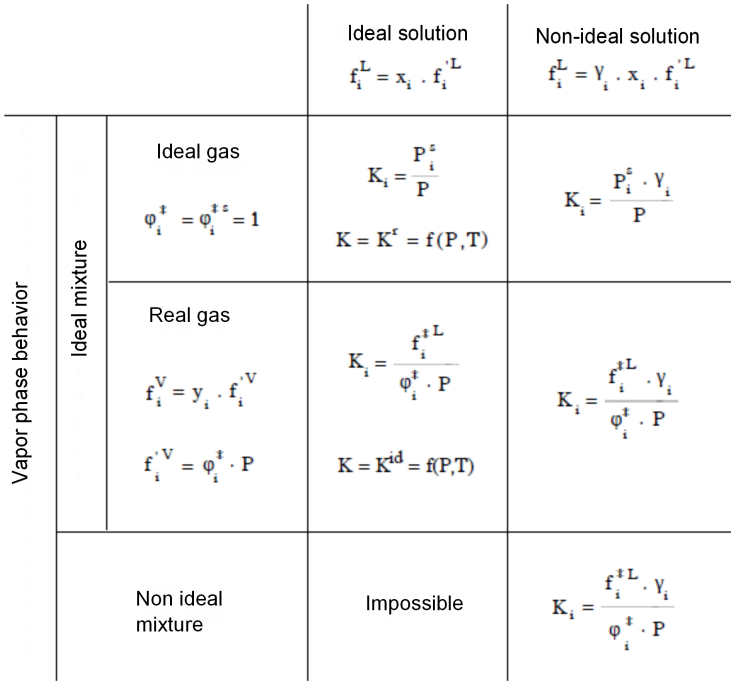


Figure 2.1: Vapor and liquid phase approximations.

The fugacities of the pure component in the mixture conditions T and P are noted $f_i^{'L}$ and $f_i^{'V}$ for the liquid and vapor phase respectively. Note that K^r (Raoult) and K^{id} (Ideal) are independent of the phases compositions and that they give a fairly good approximation of the K values.

2.3.2 Liquid-vapor equilibrium model: Specifications

The equilibrium equations are written:

$$K_i = f(T, P, \bar{x}, \bar{y}, \bar{\Theta}) \quad with \quad i = 1, .., n \tag{2.3}$$

The parameters $\bar{\Theta}$ are determined based on laws that define the partial fugacities of components. The relations defining K_i are:

$$\begin{aligned} y_i &= K_i \cdot X_i \quad with \quad i = 1, .., n \\ x_i &= \frac{y_i}{K_i} \quad with \quad i = 1, .., n \end{aligned} \tag{2.4}$$

The material balances are written according to the two equations below:

$$\begin{aligned} x_i &= \frac{z_i}{1 + \alpha \cdot (K_i - 1)} \\ y_i &= \frac{K_i \cdot z_i}{1 + \alpha \cdot (K_i - 1)} \end{aligned} \tag{2.5}$$

These equations are derived from the equations $F \cdot z_i = V \cdot y_i + L \cdot x_i$ with $\alpha = V/F$ the vapor fraction ($1 - \alpha = L/F$ the liquid fraction). The variables F, V and L are, respectively, the number of moles contained in the whole system, in the vapor phase and in the liquid phase. The corresponding molar fractions are z_i, y_i, which have to satisfy:

$$\sum x_i - 1 = 0 \qquad (2.6)$$
$$\sum y_i - 1 = 0$$

One of these two equations may be replaced by:

$$\sum x_i - \sum y_i = 0 \qquad (2.7)$$

The data of equilibrium problems involve the variables F and z satisfying the relation $\sum z_i = 1$. Considering that $F = 1$ (one mole of mixture) and that z_i has been normalized, $V = \alpha$ and $L = 1 - \alpha$. A count of the equations and variables leads to Table 2.1.

Equations	Numbers	Variables	Numbers
2.3	n	T,P,x	2n+2
2.4	n	y	n
2.5	n	K_i	1
2.6	2	α	-
Total	3n+2	Total	3n+3

Table 2.1: L-V equilibrium: variables and equations.

However, considering the sum of the equations Eq. 2.4 and Eq. 2.5, one realizes that the 2 equations Eq. 2.6 are not independent. Only one of them should be retained or only the equation Eq. 2.7. This normality equation is denoted $S(VAR) = 0$. The notation "VAR" refers to one of the previously considered variables, for example P, T, α, etc. The equation $S(VAR) = 0$ designs any of the equations Eq. 2.6 or 2.7. The count is therefore:

(3n+1) equations and (3n+3) variables

Furthermore, one can calculate any state function (the one that is considered the most often in the liquid-vapor equilibrium is the enthalpy H) either for a constituent i in the system or in one of the two phases, either for all of these. For example:

$$H = \alpha \cdot \sum_i x_i \cdot H_i^V + (1 - \alpha) \sum_i x_i \cdot H_i^L \qquad (2.8)$$

These equations introduce as many new variables as there are equations. Finally:

(3n+2) equations and (3n+4) variables

It will thus be necessary to establish two additional specifications. According to the choice that is made, one distinguishes the equilibrium calculations (or partial vaporization: flash):
at fixed T and P
at fixed P and α, special cases: the calculations of the dew T ($\alpha = 1$) and bubble T ($\alpha = 0$))
at fixed T and α, special cases: the calculations of the dew P ($\alpha = 1$) and bubble P ($\alpha = 0$))
at fixed P and H
at fixed P and S

2.3.3 Solving the model equations: Moderate pressure

Analysis of the incidence matrix

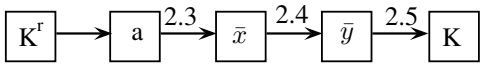
In the incidence matrix, the lines represent the equations, while the columns represent the variables. The non-zero elements of the incidence matrix are those for which the variable i is involved in equation j. The following table represents the incidence matrix for the equilibrium calculation of two components:

Inc. Eq.	K_1	K_2	x_1	x_2	y_1	y_2	α	P	T	H
2.3	X		X	X	X	X		X	X	
		X	X	X	X	X		X	X	
2.4	X		X		X					
		X		X		X				
2.5	X		X		X		X			
		X		X		X	X			
2.6			X	X	X	X				
2.8			X	X	X	X	X	X	X	X

Note that only the relationship Eq.2.8 allows to calculate H. The residual system 2.3-2.6 forms a irreducible matrix $(3n+1)\cdot(3n+3)$. The resolution of such a system of non-linear equations will quickly become problematic (for example, if n>5). Several methods exist of course to solve such problems (Newton-Raphson, Marquardt, etc.), but they require an iterative procedure and are subject to many imponderabilities (dependence on the initial point, relaxation, etc.). In addition, partial derivatives have to be calculated and the matrices (Jacobian for example) have to be defined on the basis of the problem to be addressed.

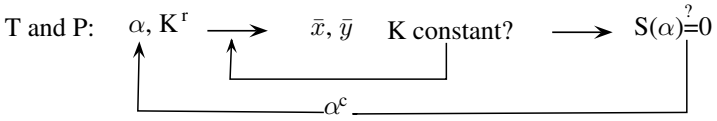
Calculation algorithms

Therefore, it can be investigated if the dimension of the problem of (3n+1) equations can be reduced. To do this, the problem at given T and P is chosen (EFA). As previously stated, the coefficient K of the component i can be approximated by: $K^r(T,P)$ or $K^{id}(T,P)$ and consequently, if α is approximated, $x(\bar{x})$ can be computed by the relation Eq. 2.5, $y(\bar{y})$ by Eq. 2.4 and finally the coefficients K of each constituent by Eq.2.3. This procedure is schematically represented here:



The simplified notation is: $K^r, \alpha \rightarrow \bar{x}, \bar{y} \rightarrow K^r$

The notation $\bar{x}, \bar{y}$ is used because depending on the type of problem, the first or the second expression of Eq.2.4 and 2.5 have to be applied. The variables K depending in general on $\bar{x}$ and $\bar{y}$, an iteration over K is needed to check that the normality condition is satisfied and α has to be modified accordingly. There are two nested loops of convergence as illustrated here:

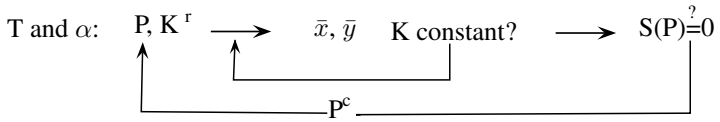


The expression $S(\alpha) = 0$ corresponds to $\sum_i x_i - \sum_i y_i$ obtained for a value α when the value of K is converged. This value and eventually others are used to determine the adjusted value of α satisfying the condition of Eq. 2.6. The remaining questions are:

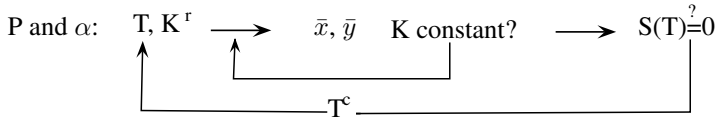
- How can the adjusted value of α be calculated to promote the convergence?
- Can the convergence of K also be promoted?
- Are all the constraints satisfied, for example $0 < \alpha < 1$?
- Is the form S(VAR)=0 ($S(\alpha) = 0$) always the same in all cases?
- Which convergence tests can be performed?

These questions will be addressed after having set the simplified iteration schemes for other equilibrium calculation types.

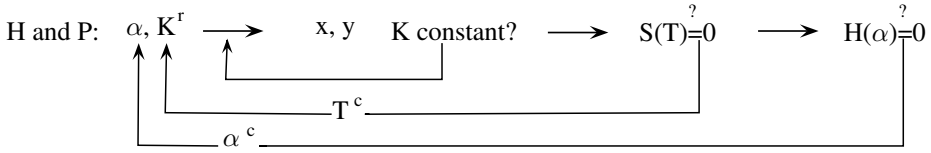
Consider the case where T and α are given (ETA)



And for P and α fixed (EPA):



The following case is different because it involves the enthalpy (EPH). Looking at the incidence matrix, it is noted that it is necessary to go through an auxiliary variable. There is a choice between α and T. These variables can be reversed afterwords.



The condition $H(\alpha) = 0$ is described in such a way that the enthalpy of the system is the one which has been imposed and called H_d: $H(\alpha) = H(T, P, \bar{x}, \bar{y}, \alpha) - H_d = 0$.

If an equilibrium has to be solved at fixed T and H, the resolution would be similar to the previous one; i.e. iterations over the pressure (at the condition that the enthalpy depends on pressure, which is not the case for ideals and perfect gases).

Convergence criterion, resolution and acceleration

Based on the PT mode, the difficulties which might arise are first described. There is a choice between three expressions for $S(\alpha)$:

$$
\begin{aligned}
S_1(\alpha) &= \sum_i x_i - 1 = \sum_i \frac{z_i}{1+\alpha(K_i-1} - 1 \\
S_2(\alpha) &= \sum_i y_i - 1 = \sum_i \frac{K_i \cdot z_i}{1+\alpha(K_i-1} - 1 \\
S_3(\alpha) &= \sum_i x_i - \sum_i y_i = \sum_i \frac{(1-K_i) \cdot z_i}{1+\alpha(K_i-1} - 1
\end{aligned}
\tag{2.9}
$$

For given values of K_i, these three functions evolve as shown in Figure 2.2.

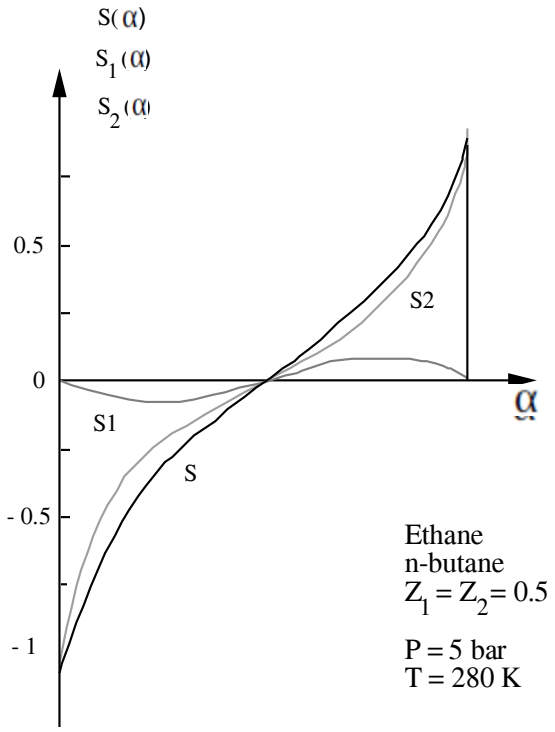


Figure 2.2: L-V equilibrium calculation.

In this case, the S function is unimodal and is therefore preferred. If S_1 or S_2 is selected, there are two solutions and with some resolution methods the solution tends towards $\alpha = 0$ or $\alpha = 1$. To find the solution of $S(\alpha) = 0$ the Newton method, the 'regula-falsi' method, the Wegstein method or even a parabolic interpolation method can be used. Some convergence methods may lead to a value of α outside the domain $0 < \alpha < 1$. Before accepting the value provided by the convergence algorithm, this value has to be tested, if $\alpha \leq 0$ then $\alpha = 0$ or if $\alpha \geq 1$ then $\alpha = 1$. The convergence tests are of two types:

$$
\begin{aligned}
\left|S(\alpha^{k+1}) - S(\alpha^k)\right| &< \epsilon_1 \\
\left|\alpha^{k+1} - \alpha^k\right| &< \epsilon_2
\end{aligned}
$$

These two tests have to be satisfied before completing the calculation. Finally, the promotion of the convergence of the inner loop must cover each K_i. Experience shows that iterations on this loop converge

quickly by simple substitution. One has to be more careful in the case of highly non-ideal systems where very complex equations of state are used (Soave, NRTL, UNIQUAC,...). It will be necessary to use methods like Marquardt or Broyden that will be described later.

2.4 Importance of the correlations coefficients validity limit

To illustrate the importance of the validity range of the correlations, one has to look at the shape of the equation for the calculation of the enthalpy:

$$\begin{aligned} H^g_{id}(T,P,x_i) &= \sum_i x_i \cdot \Delta H_i(T^o) + \int_{T^o}^{T} \left(\sum_i x_i \cdot Cp_i(T) \right) \cdot dT \\ Cp_i(T) &= a_i + b_i \cdot T + c_i \cdot T^2 + d_i \cdot T^3 \\ H^g_{id}(T,P,x_i) &= \sum_i x_i \cdot \Delta H_i(T^o) \\ &+ \sum_i x_i \cdot \left\{ a_i \cdot (T - T^o) + \frac{b_i}{2} \cdot (T^2 - (T^o)^2) + \frac{c_i}{3} \cdot (T^3 - (T^o)^3) + \frac{d_i}{4} \cdot (T^4 - (T^o)^4) \right\} \end{aligned}$$

This equation takes the form of the curve in Figure 2.3 with the coefficients values taken from literature [20]. It can be noted that this formula leads to a decrease of the enthalpy with the temperature, which does not represent the actual behavior of the fluid. Having noticed this anomaly, the authors proposed other values for the coefficients which represent more adequately the enthalpy at high temperature. It should be noted that the two correlations give quite different results and that correlation 1 is aberrant.

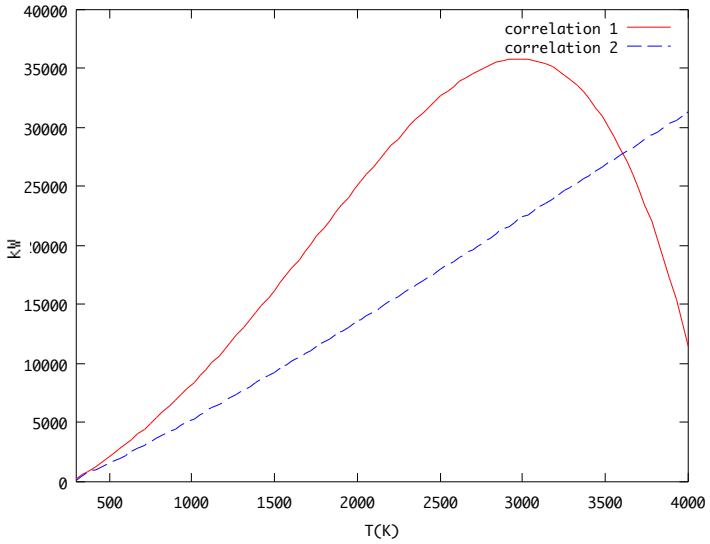


Figure 2.3: Enthalpy calculation based on the correlations [20].

Chapter 3

Unit models

This chapter explains what a is process unit model and how it is solved. As an example the unit models of several equipments are illustrated.

3.1 Introduction

The first step of developing a process model (Figure 3.1) is to define the set of equations that describe the process behavior. This model is established from a list of basic equipments (process units) that are interconnected. The equations system $F(X)$ of the modeling equations is generated from the units and their interconnections. Each unit brings its list of equations, which is called unit model. The role of the engineer who uses a flowsheeting software is to choose the unit models and assemble them. In this chapter, the common unit models used in energy systems are described (knowing that this list is not exhaustive).

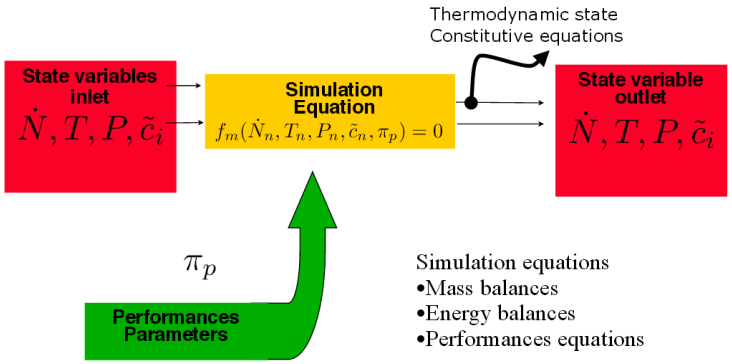


Figure 3.1: Process unit model.

These equations are implemented in a traditional manner in most commercial flowsheeting software, ASPEN, HYSYS, gProms, Belsim, etc. Depending on the unit type, the equations are therefore generated automatically and it is not necessary to define them. However, it is useful to know the principles that are used in order to verify the pertinence of the model used.

During the models development, the form of the equations and the choice of the variables that are involved are very important, because they determine the model robustness and the resolution method. The use of optimization techniques imposes also a compromise between the level of detail of the model and the complexity of the implemented equations.

3.2 Types of models

A model consists of a set of equations involving a set of state variables. A unit is represented schematically in Figure 3.2.

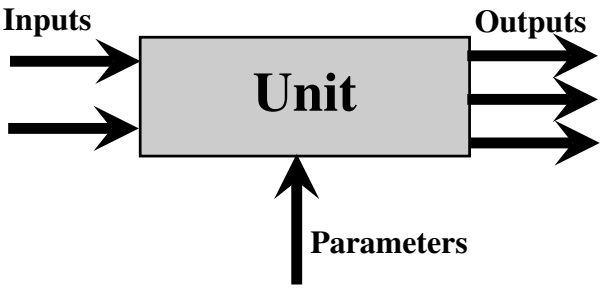


Figure 3.2: Unit model.

Equations: n_e

material balances	n_c
energy balance	1
impulsion balance	n_i
models equations	n_m
specifications	n_s

Variables: n_v

state	$N_x = (N_{OUT} + N_{IN}) \cdot (n_c + 2)$
parameters	n_p
internal variables	n_t

The generic term of the balance equations is:

Accumulation=In-Out+Generation-Consumption

In this chapter, only stationary models are treated. In this case, the accumulation term is equal to zero. The number of degrees of freedom is equal to $n_{DOF} = n_v - n_e$ and represents the number of variables or the number of additional equations that are necessary for calculating the unit. The simplest form of the additional equation is the set-point or the specification ($x_i = x_i^{spec}$). The incidence matrix (Figure 3.3) is used to identify the number of degrees of freedom. In this matrix, the lines represent the equations and the columns the variables. In the incidence matrix an non-zero element is written if the variable i (column i) is involved in the equation j (line j). In this matrix the specification equations are represented by a line with a single non-zero element. In order to calculate the unit there are two necessary conditions:

- The incidence matrix must be square: as many equations as variables.
- The equations have to be independent. It must be possible to swap the rows and columns so that a non-zero element appears on each diagonal element of the matrix.

If these two conditions are met, it means that the matrix can be inverted, and the elements on the diagonal are selected as a pivot (see Gaus-Newton's method and LU decomposition). To solve the model the matrix has to be invertible. Consequently, the value of the pivot must not become zero during the procedure of the matrix inversion. In the latter case, the problem is said numerically singular.

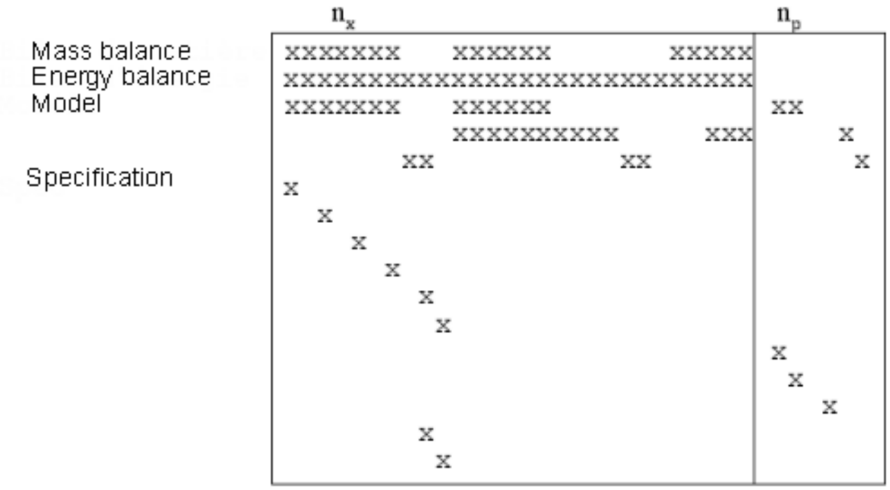


Figure 3.3: Example of an incidence matrix.

3.3 Model resolution

Two strategies for solving a model can be applied: the simultaneous resolution or the sequential resolution.

3.3.1 Simultaneous resolution

For a simultaneous resolution, all the model equations and the specification equations are written. This produces a system of n_e non-linear equations and n_v variables (state variables, parameters and internal variables) to be solved by a suitable method (see Chapter Model resolution). The mathematical expression is given by:

$$\begin{aligned} M(X_x, X_p) &= 0 \\ S(X_x, X_p) &= 0 \quad \Longrightarrow F(X) = 0(N_e x N_v) \\ IN(X_x) &= 0 \end{aligned}$$

with:

$M(X_x, X_p) = 0$	Model equations
$S(X_x, X_p) = 0$	Specification equations
$In(X_x) = 0$	Specification equations of the inputs
$F(X) = 0$	System of equations to be solved
X_x	State variables of input streams
X_p	Parameters and internal variables of the model
N_e	Number of equations
N_v	Number of variables

Example: Turbine model

Figure 3.4 illustrates the turbine model. The suffix **s** represents the specified values. The objective of this model is to calculate the mechanical power and the state of the output stream, knowing the flowrate, temperature, pressure and input compositions, the isentropic efficiency of the turbine and the outlet pressure.

The model equations are:

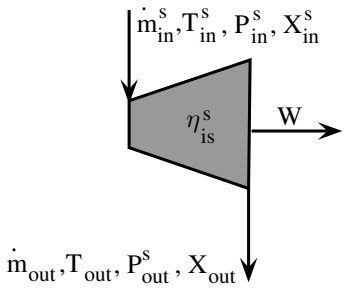


Figure 3.4: Example: Turbine model.

$\dot{m}_{out} - \dot{m}^s_{in} = 0$	Mass balance
$x^j_{out} - x^{j,s}_{in} = 0 \; \forall j = 1, ..., n_c$	Mass balance (composition)
$h_{in} - h(T^s_{in}, P^s_{in}, X^s_{in}) = 0$	Constitutive equation: Enthalpy of the input
$s_{in} - s(T^s_{in}, P^s_{in}, X^s_{in}) = 0$	Constitutive equation: Entropy of the input
$h^{is}_{out} - h(s_{in}, P^s_{out}, X_{out}) = 0$	Isentropic expansion equation
$h_{out} - h_{in} + \eta^s_{is} \cdot (h_{in} - h^{is}_{out}) = 0$	Isentropic efficiency equation
$T_{out} - T(h_{out}, P^s_{out}, X_{out}) = 0$	Linking equation: Calculation of output temperature
$W_{out} - \dot{m}^s_{in} \cdot (h_{in} - hout) = 0$	Energy balance

To these equations, the specification equations are added (inputs and model specifications):

Inputs	
$\dot{m}_{in} - \dot{m}^s_{in} = 0$	Input flowrate
$x^j_{in} - x^{j,s}_{in} = 0$	Input composition
$T_{in} - T^s_{in} = 0$	Input temperature
$P_{in} - P^s_{in} = 0$	Input pressure
Model	
$P_{out} - P^s_{out} = 0$	Output pressure
$\eta_{is} - \eta^s_{is} = 0$	Isentropic efficiency

3.3.2 Sequential resolution

The principle of the sequential resolution is to associate to each variable the equation that allows to solve it and to determine the resolution sequence. In this approach, the resolution sequence is determined in such a way that the equations can be solved successively, one after another. This approach is similar to the sequence of pivoting, while inverting the matrix of equations, solving for each pivot elimination a non-linear equation. For this approach, the resolution is formulated explicitly wherever possible. To calculate the i^{th} variable of the model, this translates to Eq. 3.1 where $f^*_i(x_j)$ is a non-linear expression representing the i^{th} equation.

$$x_i = f^*_i(x_j) \qquad \forall j = 1, ..., i-1 \tag{3.1}$$

In this approach, the sequence's resolution depends on the sequence of the matrix pivoting and so on the list of specifications. In a sequential approach, the input streams are considered as specified, whenever it is possible. Then a set of specifications representing an operation mode of the unit model is chosen.

Example: Turbine model

For the turbine model given by:

$$
\begin{array}{lcl}
\dot{m}_{out} & = & \dot{m}^s_{in} \\
x^j_{out} & = & x^{j,s}_{in} \\
h_{in} & = & h(T^s_{in}, P^s_{in}, X^s_{in}) \\
s_{in} & = & s(T^s_{in}, P^s_{in}, X^s_{in}) \\
h^{is}_{out} & = & h(s_{in}, P^s_{out}, X_{out}) \\
h_{out} & = & h_{in} + \eta^s_{is} \cdot (h_{in} - h^{is}_{out}) \\
T_{out} & = & T(h_{out}, P^s_{out}, X_{out}) \\
W_{out} & = & \dot{m}^s_{in} \cdot (h_{in} - hout)
\end{array}
$$

the incidence matrix becomes:

```
mout   x
xout    x
Hin      x
Sin       x
Houtis  x xx
Hout     x xx
Tout    x   xx
W        x  x x
```

Turbine example: sequential versus simultaneous approach

The main difference between the two resolution strategies is the fact that for the sequential resolution it is necessary to define a new resolution sequence when the operating mode changes. For the turbine example, if the specifications are changed and the flowrate has to be calculated for a given mechanical power, and an output pressure (Figure 3.5) a new resolution strategy has to defined, which involves a reformulation of the model equations and of the resolution sequence.

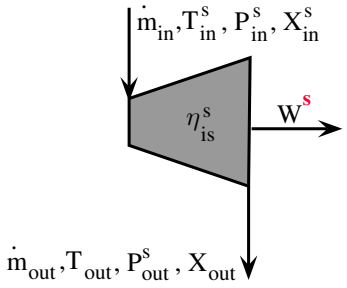


Figure 3.5: Example: Turbine model - New calculation mode.

The modified turbine model is given by:

$$
\begin{array}{lcl}
x^j_{out} & = & x^{j,s}_{in} \\
h_{in} & = & h(T^s_{in}, P^s_{in}, X^s_{in}) \\
s_{in} & = & s(T^s_{in}, P^s_{in}, X^s_{in}) \\
h^{is}_{out} & = & h(s_{in}, P^s_{out}, X_{out}) \\
h_{out} & = & h_{in} + \eta^s_{is} \cdot (h_{in} - h^{is}_{out}) \\
T_{out} & = & T(h_{out}, P^s_{out}, X_{out}) \\
m_{in} & = & \frac{W^s}{h_{in} - hout} \\
\dot{m}_{out} & = & \dot{m}_{in}
\end{array}
$$

Another resolution method is to not change the resolution sequence and use an iterative loop for the promotion of convergence (Figure 3.6): the model calculates the mechanical power and it changes the value of the flowrate until the mechanical power is equal to the specified value. This second approach has the advantage of not having to rewrite the resolution sequence. However, it has the disadvantage of an iterative loop which may be costly in terms of calculation time.

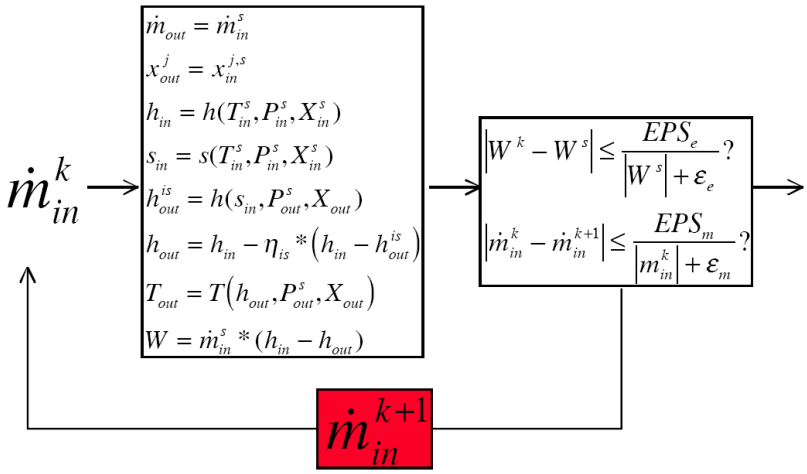


Figure 3.6: Iterative loop.

For the simultaneous resolution, only the specification equations have to be modified and the models equations remain unchanged. The difference also appears if one wants to make the model more accurate by using empirical equations (Eq. 3.2) to calculate the efficiency rather than considering it as constant.

$$\eta_i s = a \cdot \tau + b \cdot \dot{m}_i n \cdot \bar{\nu} + c \cdot (\dot{m}_i n \cdot \bar{\nu})^2 + d \tag{3.2}$$

with:

τ	compression ratio
$\bar{\nu}$	average volume (mass basis)
a, b, c, d	characteristics of the studied unit

For the simultaneous strategy, the equations defining the efficiency are added to the model equations with in this case, the definition of additional internal variables (τ, $\bar{\nu}$). At the level of the specifications, the specification setting the isentropic efficiency as a constant is replaced by the specification of parameters of the empirical expression.

The corresponding model is:

$$\dot{m}_{out} - \dot{m}_{in}^{s} = 0$$
$$x_{out}^{j} - x_{in}^{j,s} = 0$$
$$h_{in} - h(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) = 0$$
$$s_{in} - s(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) = 0$$
$$h_{out}^{is} - h(s_{in}, P_{out}^{s}, X_{out}) = 0$$
$$\tau \cdot P_{out} - P_{in} = 0$$
$$\bar{\nu} - \frac{\nu(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) + \nu(T_{out}, P_{out}^{s}, X_{out})}{2} = 0$$
$$\eta_i s - a \cdot \tau + b \cdot \dot{m}_i n \cdot \bar{\nu} + c \cdot (\dot{m}_i n \cdot \bar{\nu})^2 + d = 0$$
$$h_{out} - h_{in} + \eta_{is} \cdot (h_{in} - h_{out}^{is}) = 0$$
$$T_{out} - T(h_{out}, P_{out}^{s}, X_{out}) = 0$$
$$W - \dot{m}_{in}^{s} \cdot (h_{in} - hout) = 0$$

with the specifications:

$$\dot{m}_{in} - \dot{m}_{in}^{s} = 0$$
$$x_{in}^{j} - x_{in}^{j,s} = 0$$
$$T_{in} - T_{in}^{s} = 0$$
$$P_{in} - P_{in}^{s} = 0$$
$$P_{out} - P_{out}^{s} = 0$$
$$a - a^{s} = 0$$
$$b - b^{s} = 0$$
$$c - c^{s} = 0$$
$$d - d^{s} = 0$$

For the same model but with a sequential resolution approach, it is no more possible to find a resolution strategy 1 variable / 1 equation. In fact, the calculation of the average mass volume requires the mass volume of the output which can only be calculated if the outlet temperature, and therefore the isentropic efficiency, are known. It is thus necessary to introduce an iterative resolution loop.

$$\dot{m}_{out} = \dot{m}_{in}^{s}$$
$$x_{out}^{j} = x_{in}^{j,s} \qquad \forall j$$
$$h_{in} = h(T_{in}^{s}, P_{in}^{s}, X_{in}^{s})$$
$$s_{in} = s(T_{in}^{s}, P_{in}^{s}, X_{in}^{s})$$
$$h_{out}^{is} = h(s_{in}, P_{out}^{s}, X_{out})$$
$$\tau = \frac{P_{in}^{s}}{P_{out}^{s}}$$
$$\bar{v} = \frac{v(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) + v(T_{out}^{k}, P_{out}, X_{out})}{2}$$
$$\eta_{is} = a * \tau + b * \dot{m}_{in} * \bar{v} + c * \left(\dot{m}_{in} * \bar{v}\right)^{2} + d$$
$$h_{out} = h_{in} - \eta_{is} * \left(h_{in} - h_{out}^{is}\right)$$
$$T_{out}^{k+1} = T\left(h_{out}, P_{out}^{s}\right)$$
$$\left|T_{out}^{k} - T_{out}^{k+1}\right| \leq \frac{EPS_{T}}{\left|T_{out}^{k}\right| + \varepsilon_{T}} ?$$

← NO YES

↓

$$W = \dot{m}_{in}^{s} * \left(\left(h_{in} - h_{out}\right)\right.$$

A brief comparison of the two resolution approaches is given in Table 3.1.

	Simultaneous	Sequential
Problem statement	incidence matrix implicit	DOF analysis required
Robustness	unique solving scheme	specific solving procedure bounds, if-then-else
Calculation modes	required	numerical noise at flowsheet level if iterative scheme

Table 3.1: Simultaneous versus sequential resolution approach.

3.4 Unit models examples

Turbine and compressor

The unit model of the turbine or compressor simulates one stage of expansion (or compression). A multi-stage turbine is therefore represented by a succession of stages of expansions and splitters to represent the draw-offs. The model of the expansion (or compression) stage is based on the isentropic expansion (compression) equation Eq. 3.3 (Figure 3.7).

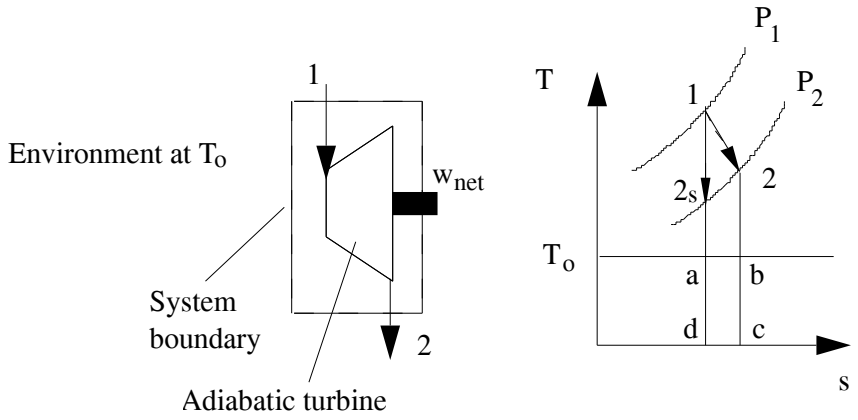


Figure 3.7: Expansion model of a turbine and isentropic expansion.

$$\begin{aligned} W &= \dot{m} \cdot (h_{in} - h_{out}) \\ h_{in} - h_{out} - \eta \cdot (h_{in} - h^{is}_{out}(P_{in}, h_{in}, P_{out})) &= 0 \end{aligned} \tag{3.3}$$

with:

h_{in}	molar enthalpy at expansion stage inlet
h_{out}	molar enthalpy at expansion stage outlet
P_{in}	pressure at expansion stage inlet
P_{out}	pressure at expansion stage outlet
η	isentropic efficiency of expansion
$h^{is}_{out}(P_{in}, h_{in}, P_{out})$	molar enthalpy from isentropic expansion between h_{in}, P_{in} and P_{out}

This equation is written as function of the intensive variables (molar enthalpy and pressure). It can therefore be evaluated even when the flowrate that passes through the turbine is zero. The efficiency and the compression ratio, as well as the expression of the volume flowrate limit can be expressed in terms of other variables through characteristic curves. These curves allow to represent the behavior of a turbine or compressor when the operating conditions vary. In the case where the unit does not exist (process design), a constant isentropic efficiency is chosen for each stage of expansion (average expansion ratio: 3) or a correlation based on market analysis is used [17]. The use of a correlation to set the efficiency must be treated with caution, it has to be ensured that operating conditions are similar. The choice of the value depends on the type of turbine. Typical values can be found in [5].

Steam distribution (header)

In integrated energy systems, steam can be produced in different boilers or turbines, and then be distributed to various users: turbine, processes, district heating network, etc. The steam distribution is provided through a network of pipes that is maintained at a given pressure level. Each pressure network is called *header* whose role is to collect and distribute steam. The header model assumes that the pressure of all output streams is identical. Pressure losses in the pipes between two production or draw-off points

are neglected.

An important feature of an header is that the flowrate through portions of the pipes is unknown and may be reversed depending on the value of the feed and draw-offs flowrates. These are in fact defined by optimization and according to the demands that have to be satisfied. This is illustrated in Figure 3.8. When the turbine is running, the two inlets of the header are mixed (point 3) to power the turbine. The input 2 is a splitter. On the other hand, when the turbine is not running, the input 2 becomes a mixer and the thermodynamic state of the draw-off 1 can be totally different.

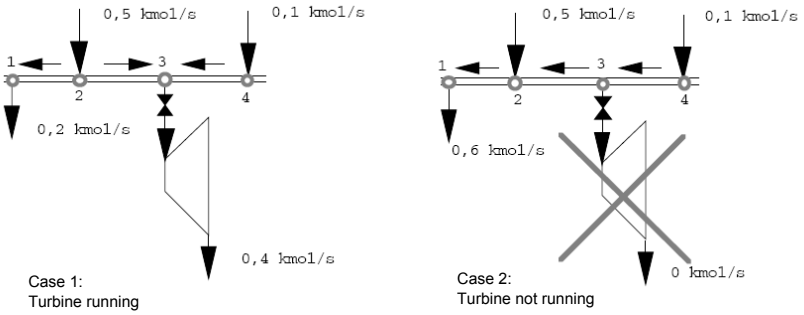


Figure 3.8: Steam header characteristics.

The model developed to simulate the header allows to calculate changes of the flow direction of the concerned fluid. The change of the flow direction between two headers is also calculated. In this case, the pressure drop that depends on the flowrate between two headers defines the pressure of the two headers (Figure 3.9). The difficulty of modeling such a situation is that, despite the fact that the number of degrees of freedom remains the same, the number of equations generated at each node (point of connection of a flow on the header) changes (Figure 3.10).

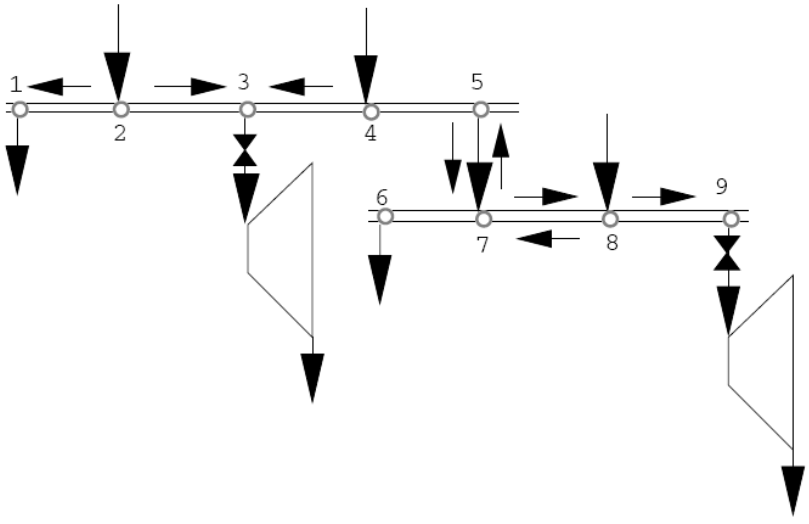


Figure 3.9: Direction change between two headers.

If the flow of stream 2 (Figure 3.10) goes from left to right, the node is a splitter whose simulation introduces the following 3 equations:

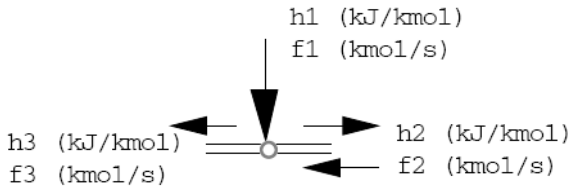


Figure 3.10: Simulation of splitter or mixer.

1 Mass balance
$f_1 - f_2 - f_3 = 0$
2 Model equations
$h_2 - h_1 = 0$
$h_3 - h_1 = 0$

On the other hand, if the flow of stream 2 goes from right to left, the node is a mixer whose simulation introduces the following 2 equations:

1 Mass balance
$f_1 + f_2 - f_3 = 0$
1 Energy balance
$f_3 \cdot h_3 - f_1 \cdot h_1 - f_2 \cdot h_2 = 0$

If during iteration, the flows are such that the type of the node changes, the calculation can be solved by a simultaneous approach, since the equation type and the variables involved in the equation change.

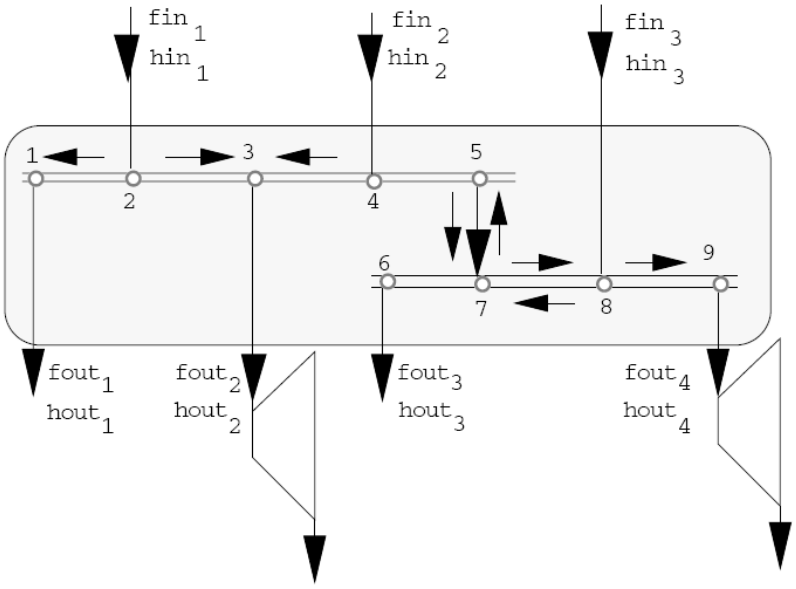


Figure 3.11: Modelling of a set of interconnected headers.

A system such as the one reported in Figure 3.11 is difficult to manage by the two resolution approaches. With the sequential approach, it is necessary to adjust the resolution sequence on the basis of the flowrates and thus compute the nodes either in the form of a mixer or of a splitter. With a simultaneous approach, it is necessary to choose a hybrid approach combining the simultaneous and the sequential approach.

For the system reported in Figure 3.11 all the interconnected headers are considered as a set of units with respect to the flowrates and pressures, and as a single unit to calculate the energy balance. The following algorithm can be used:

- The energy balances being linear, they are satisfied for each iteration, insofar as negative flowrates are accepted.
- Determine the type of each node: splitter or mixer, for known flowrate.
- Determine a calculation sequence for the nodes that allows to calculate the enthalpy content of the output streams of the system.
- Generate the model equations of the header from the calculated molar enthalpies (Eq. 3.4).

$$h_{c,i}(f_{in,j}, h_{in.j}) - h_{out,i} = 0 \qquad \forall i = 1, ..., n_{out} \tag{3.4}$$

with:

$h_{c,i}$	the molar enthalpy calculated for output i of the system calculated on the basis of the flowrates and enthalpies of the inputs
$f_{in,j}$	the flowrate of the inlet stream j
$h_{in,j}$	the molar enthalpy of inlet stream j
$h_{out,i}$	the molar enthalpy of the output stream i (in the state variables list)

In this case, although the calculation order of the various nodes may change during iteration, the equations definition remains identical. By this representation, discontinuities in the derivatives of the equations are not deleted when switching from one type to another. However, in order to reduce the value of these discontinuities, the derivatives of $h_{c,i}$ are calculated by numerical perturbation of $f_{in,j}$ and $h_{in,j}$. It has to be noted that the equations is again written as a function of the molar enthalpy, and the equations can therefore be evaluated even when the flowrate is zero.

Heat exchanger

In industrial energy systems, heat exchangers often include phase change transformations: condenser and evaporator of a heat pump, pre-heating heat exchangers by vapor condensation, condenser at condensing turbine outlet, etc. The simulation model of the heat exchanger has therefore to take into account phase changes. In this case, the conventional formula Eq. 3.5 resulting from the assumption of constant *cp* can no longer be applied.

$$Q = U \cdot A \cdot \Delta T_{lm} \tag{3.5}$$

with:

Q	heat load
U	mean heat transfer coefficient
A	exchange area of the exchanger
ΔT_{lm}	log mean temperature difference between hot and cold streams

In the case of a phase change, the heat exchanger can be modeled by considering a succession of zones (Figure 3.12) in which the *cp* of the two fluids can be considered constant and the formula Eq. 3.5 can be applied. The sizing equation is highly non-linear and non-continuously differentiable Eq. 3.6.

$$A_i - \sum_{k=1}^{n_{zi}} \frac{Q_{ik}}{U_{ik} \cdot \Delta T_{lm,ik}} \tag{3.6}$$

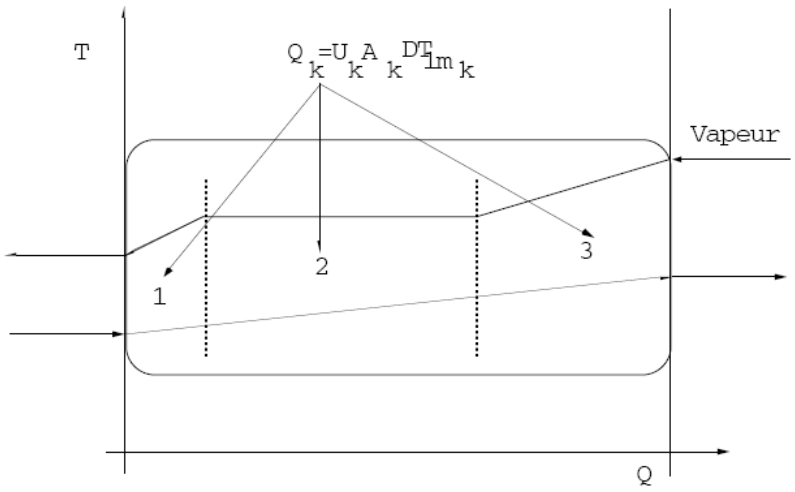


Figure 3.12: Heat exchanger representation: several zones in series.

with:

A_i	surface of heat exchanger i
Q_{ik}	thermal load of the zone k of heat exchanger i
U_{ik}	heat transfer coefficient in the zone k
$\Delta T_{lm,ik}$	log mean temperature difference between hot and cold streams in zone k of the heat exchanger i
n_{zi}	number of zones defined by linear sections of the H_T diagram of the hot and cold streams in heat exchanger i

Although it is relatively easy to implement this type of model in a sequential approach in which the input and output variables are set, this formulation is much more complex in the case of a simultaneous approach. The application of this formulation in a simultaneous approach requires many developments:

- Use of a *smooth approximation* technique as applied by [9] to attenuate the discontinuity of the derivatives.
- Calculation of the boundary conditions (the residue and derivatives) in the case of degeneration of the equation when the *cp* are equal.
- Iterative calculation of the residue when the surface is specified; the enthalpy of the output stream is calculated for the specified surface and the equation Eq. 3.7 is generated. This approach is more stable than the one using the residual from the equation, particularly because of the strong non-linearity of equation Eq. 3.7, leading to temperatures crosses in the exchanger during iteration. By calculating the molar enthalpy of the output stream, the heat exchanger is always calculated for feasible conditions, which makes the problem easier to solve.

$$h^c_{out} - h_{out} = 0 \tag{3.7}$$

with:

h^c_{out}	molar enthalpy of the output stream calculated iteratively based on the specified area
h_{out}	molar enthalpy of the output stream in the state variables list

- Calculation by linearization of extreme conditions: zero flowrate, temperature cross, etc. This feature is very important because it is precisely in the extreme operating conditions that the optimization will pick the optimum. It is not acceptable that the numerical search of the optimum

stops when a residual cannot be evaluated. If the situation has no physical significance, one should give a value to the residual and the path (which depends on the calculation of derivatives) to the feasible domain.

In the heat exchanger model, pressure drop calculation relationships (depending on the flowrate and temperature) and correlations for the calculation of heat transfer coefficients have also to be added. It has to be noted that in the case of the simulation of existing units, correlations can generally not reproduce the measured performance. It is therefore necessary to consider an unknown parameter (representing the fouling factor and the degree of crossed flows) which will be identified based on the performance test measurements.

The simulation of condensers and evaporators is done by adding the condition of saturation of the output stream. This constraint is computed by algorithms of the resolution method that introduces a linking equation Eq. 3.8.

$$h_{out} = h_{calc}(P, \alpha, x_i) \tag{3.8}$$

with:

h_{out}	molar enthalpy at the outlet
P	pressure at the outlet
α	vapor fraction
x_i	molar fraction of compound i at the outlet
h_{calc}	molar enthalpy calculated for fixed P and α

Valve

The valve is an adiabatic expansion. The pressure drop in the valve depends on the flowrate and is given by the conventional equation for the pressure drop calculation.

Radiative exchange

The radiative exchange is calculated by the following formula Eq. 3.9. The pressure drop across the heat exchanger is expressed as a function of the flowrate.

$$Q = G\dot{S} \cdot \sigma \cdot (T_{out,f}^2 \cdot T_{ad}^2 - T_p^4) \tag{3.9}$$

with:

$T_{out,f}$	outlet temperature of the flue gas
T_{ad}	adiabatic combustion temperature
G	factor of geometry of the oven
S	exchange surface
σ	Stefan-Boltzmann's constant $5,6697 \cdot 10^{-8} W/m^2/K^4$
T_p	average temperature of the reception area calculated by: $T_p = \frac{T_{in}-T_{out}}{2} + 70$
T_{in}	inlet temperature of the stream to be heated
T_{out}	outlet temperature of the stream to be heated

Liquid-Vapor separator

The vapor-liquid separator model (Figure 3.13) separates the stream into two saturated streams, one liquid and one vapor stream. The equations of the liquid-vapor separator model are:

Mass balance	$F \cdot z_i = L \cdot x_i + V \cdot y_i$
Energy balance	$F \cdot H_f = V \cdot H_v(T, P, y_i) + L \cdot H_l(T, P, x_i) + Q$
Liquid composition	$\sum x_i = 1$
Vapor composition	$\sum y_i = 1$
LV equilibrium	$y_i = x_i \cdot K_i(T, P, x_i, y_i)$

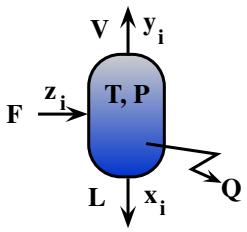


Figure 3.13: Liquid-Vapor separator.

K_i is the ratio of the molar concentrations of the substance i in the vapor and liquid phases that is calculated to get for each substance the same fugacity in the vapor and liquid phase.

Combustion

In the combustion model, illustrated in Figure 3.14, a generic fuel formed of carbon (C), hydrogen (H) and oxygen (O) (subscripts denote the atomic composition of the fuel) is burned with an oxidant containing oxygen (O_2), nitrogen (N_2) and water (H_2O).

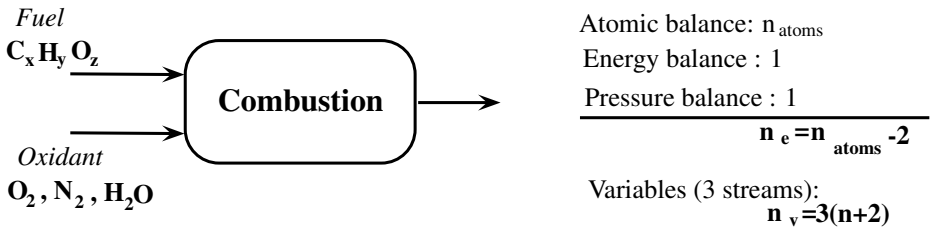


Figure 3.14: Combustion model.

Assuming complete combustion, the following equations are used to calculate the composition of the flue gas (N_2, CO_2, H_2O and O_2). The energy balance allows to calculate the adiabatic combustion temperature.

$$xC + xO_2 \rightarrow xCO_2$$

$$yH + \frac{y}{4}O_2 \rightarrow \frac{y}{2}H_2O$$

$$\dot{m}^{O_2}_{fumées} = \dot{m}_{air} * x^{O_2}_{air} + \dot{m}_{fuel} * (z - x - \frac{y}{4})$$

$$\dot{m}^{CO_2}_{fumées} = \dot{m}_{fuel} * x$$

$$\dot{m}^{N_2}_{fumées} = \dot{m}_{air} * x^{N_2}_{air}$$

$$\dot{m}^{H_2O}_{fumées} = \dot{m}_{fuel} * \frac{y}{2} + \dot{m}_{air} * x^{H_2O}_{air}$$

$$\dot{m}_{fuel} * (h_i^{f0} + \int_{T^\circ}^{Tin} .C_{pi} dT) + \dot{m}_{air} * (\sum_i x^i_{air} h_i^{f0} + \int_{T^\circ}^{Tair} \sum_i x^i_{air} .C_{pi} .dT) = \sum_i \dot{m}^i_{fumées} h_i^{f0} + \int_{T^\circ}^{T_{ad}} \sum_i \dot{m}^i_{fumées} .C_i$$

Complex unit model

A complex unit such as a boiler is calculated by connecting different basic models (Figure 3.15).

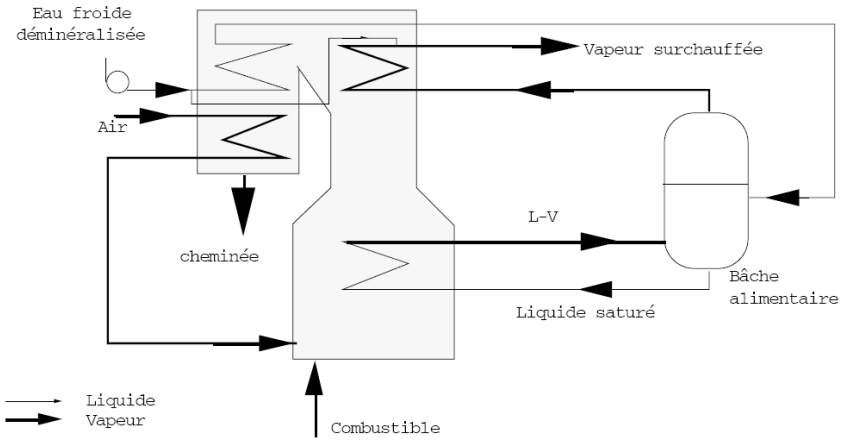


Figure 3.15: Scheme of a boiler.

The set of interconnected basic models is given in Figure 3.16. It has to be noted that superheating is often performed in several super-heaters and that these may be calculated by radiative or convective exchange depending on their location and the fumes temperature.

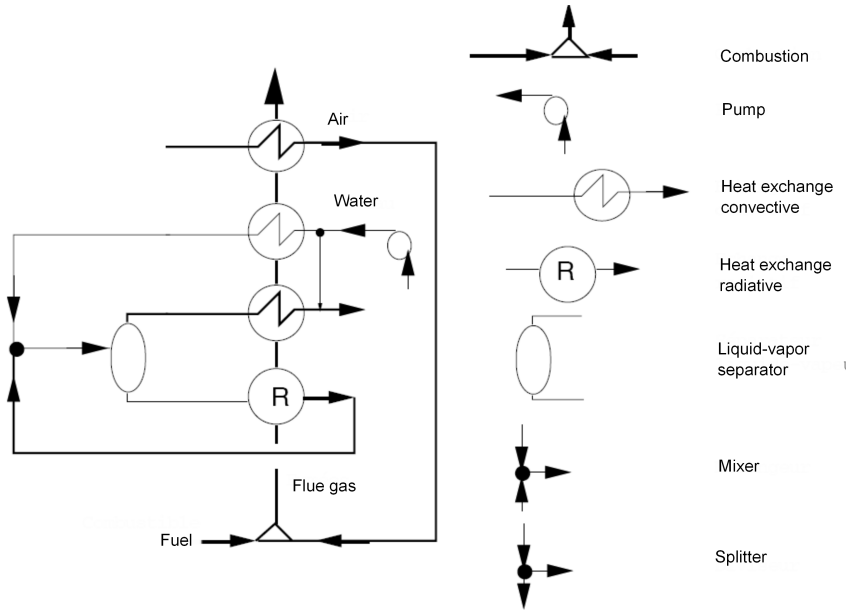


Figure 3.16: Simulation model of the boiler by assembly of unit models.

The set of equations of a gas turbine model are illustrated in Figure 3.17.
This model is considered in the global system of a combined cycle consisting of the gas turbine, the fuel compressor, the recovery boiler, the steam turbine and the condensing unit (Figure 3.18).

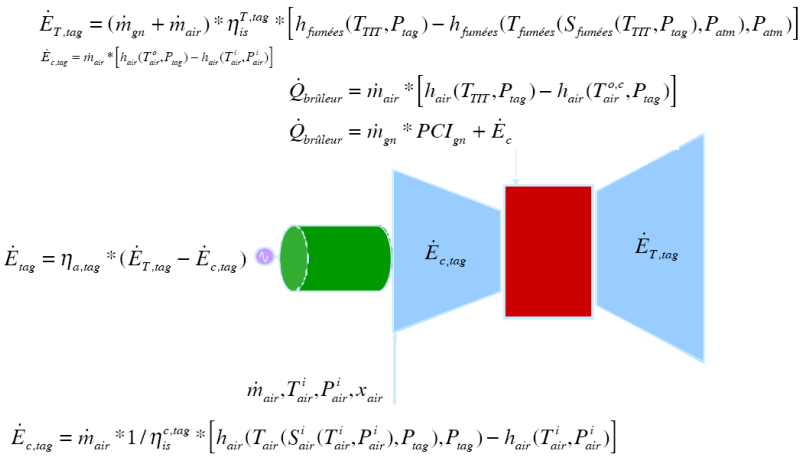


Figure 3.17: Gas turbine model.

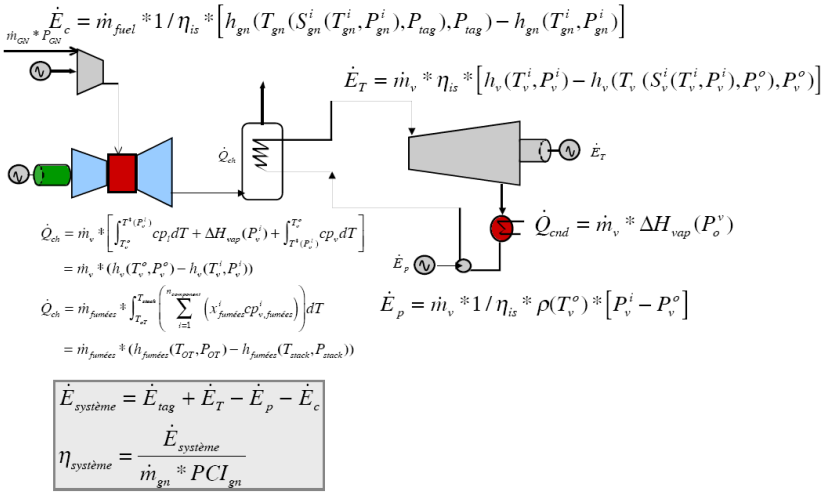


Figure 3.18: Combined cycle model.

Chapter 4

Model resolution: Sequential approach

To solve simulation problems a sequential approach is most commonly applied. The objective of this chapter is to present the sequential modular method and to introduce a way to address the problem of handling recycling loops (the Motard method).

4.1 Flowsheet resolution

There are mainly two resolution methods to solve models of integrated energy systems, namely the modular sequential and the simultaneous approach. The main problem of a sequential approach is how to deal with recycling. Additional information can be found in literature [23, 2].

4.2 Sequential modular method

The simulation of a system (i.e. set of equipments) is considered. It is assumed that a model (i.e. calculate the state of the output if the input is known) is available for each process unit.

The static simulation of chemical systems systematically induces convergence problems. Consider the very simple diagram of Figure 4.1 representing a small part of a chemical process. To be able to solve the equations related to a unit, the unit input stream has to be known. However, if there are loops, all the input streams are not known: to calculate the heat exchanger HE1, stream 1 and 2 must be known. Stream 2 depends successively on streams 10, 8, 5 and 6, 4. Consequently, stream 4 and 6 are required for stream 2. However, stream 4 is obtained by the resolution of the heat exchanger HE1. To solve this problem, a tear has to be made, that is, one must estimate one of the streams and then calculate all the units of the series and finally use a method of convergence promotion in order to obtain a better estimate of the quantities on the stream that is cut/teared. For example, if stream 2 is teared, the heat exchanger HE1 can be calculated, then the reactor, the exchanger HE2, the separator and the splitter. Thus new values are obtained for stream 2 and convergence has to be reached on stream 2 after iteration. If a more complex system is considered, it is not obvious to directly determine the stream to be cut, in such a way that the number of tears and the convergence problem are minimized.

4.2.1 The Motard method

A method for determining the minimum number of tears has been developed by Motard [2]. This method is illustrated here based on an example. Figure 4.2 represents a system consisting of 6 units interconnected directly or through recycling or by-pass. Each arrow represents a directed stream from a certain size (matter, energy,...) that should be determined. For each unit, there is a model that can be solved to compute the output stream based on the inputs. It is assumed that the system is in steady-state conditions, meaning that there is no accumulation. If there is a chemical transformation (in a reactor for example), it is necessary to introduce a virtual stream expressing the amount of product formed and the

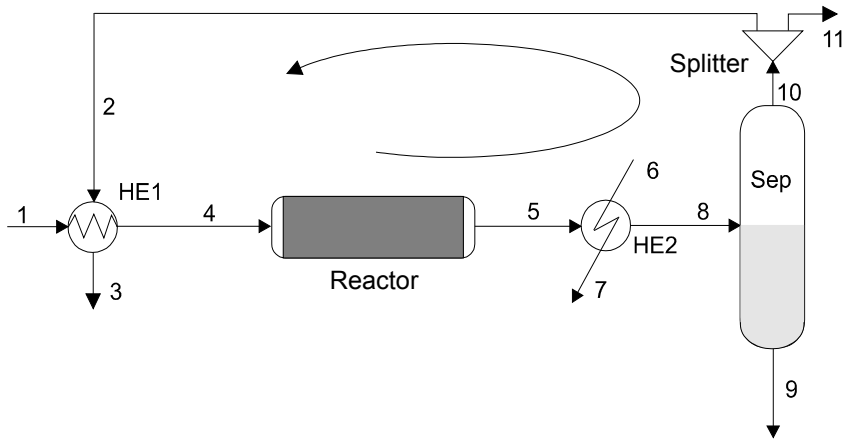


Figure 4.1: Example of a process with recycling.

amount of reagents consumed. This case will not be considered explicitly.

First, the notion of dual graph is introduced and some systematic rules, which allow to solve the system by organizing the calculation sequence in an optimal manner, are presented.

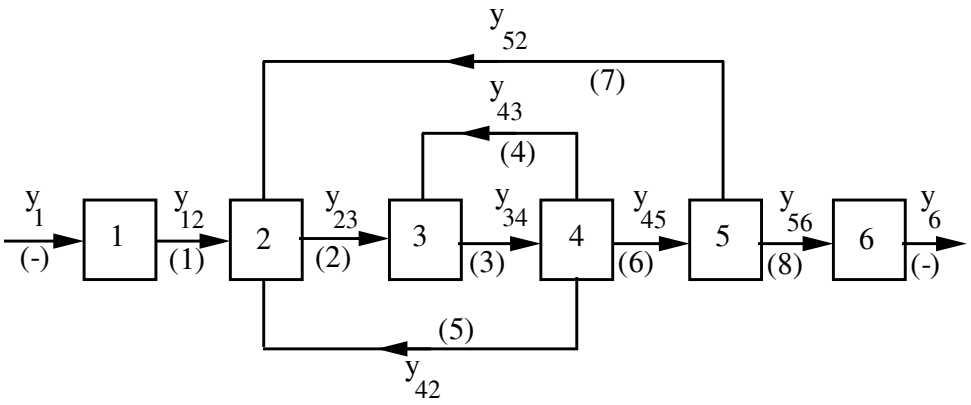


Figure 4.2: Dual graph of a system.

The dual graph

The dual graph is established from the system flowsheet. The big difference between these two types of graphs lies at the level of the meanings of the branches and nodes. Branches (nodes) of the flowsheet become the dual graph nodes (branches). Figure 4.3 shows the relationship between a flowsheet and a dual graph.

Figure 4.3: Flowsheet (left) and dual graph (right).

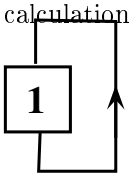
Rules of the Motard algorithm

A general rule is to:

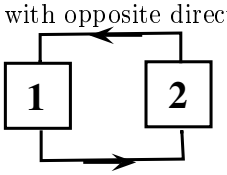
Tear the stream occurring in the largest number of cycles

To find this stream in a systematic way, the dual graph representation of the flowsheet is considered and the following rules have to be applied:

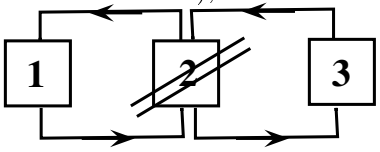
1. Remove the streams that have no predecessor.
2. Replace the streams that have only one predecessor by their predecessor.
3. Open loops by tears when a stream depends on itself (these are the loops on a single node). The calculation of stream 1 involves an iterative calculation loop and so a tear.



4. Open loop by tearing when a stream predecessor depends on his predecessor (Tear parallel streams with opposite direction).



5. Tear streams with the highest number of predecessors. If two loops involve a single node (i.e. the same stream), this one should be teared. In fact, two loops are thereby cut by a single tear.



A teared stream has no predecessor. Guess the value and restart in point 1.

Remarks:

- The last rule is rarely applied, because the others are usually sufficient.

- When a rule is applied, one has always to start from the 1st rule to continue.

These rules allow the decomposition of the flowsheet before the simulation. They allow to determine and locate the minimum number of tears so that the calculation of the units can be sequential and iterative.

These rules are applied here to identify the tears for the system given in Figure 4.2. From the graph the following Table 4.1 can be set.

Stream	Stream predecessor
1	-
2	1, 5, 7
3	2, 4
4	3
5	3
6	3
7	6
8	6

Table 4.1: Motard algorithm: Streams' predecessors table.

According to rule 1, stream 1 is deleted because it has no predecessor. Hence, Table 4.1 becomes Table 4.2:

Stream	Stream predecessor
2	5, 7
3	2, 4
4	3
5	3
6	3
7	6
8	6

Table 4.2: Motard algorithm: Streams' predecessors table (rule 1).

Applying rule 2, the streams 4, 5, 6 are replaced by their single predecessor (stream 3). Table 4.2 becomes Table 4.3:

Stream	Stream predecessor
2	3, 7
3	2, 3
4	3
5	3
6	3
7	3
8	3

Table 4.3: Motard algorithm: Streams' predecessors table (rule 2).

Applying rule 2 again, the stream 7 is replaced by its predecessor stream 3. As stream 2 has already stream 3 as predecessor there is no need to write it twice. Table 4.3 becomes Table 4.4.
In the same way, stream 2 is replaced by its predecessor stream 3. As stream 3 exists already as a predecessor of stream 2 there is no need to rewrite it. Hence the final table becomes Table 4.5.
It is obvious that it is not necessary to recopy the table every time. Generally, the successive corrections are made to the first table (Table 4.1) (possibly in color) until obtaining this final Table 4.5. It can be noticed that all streams have stream 3 as predecessor stream (except stream 1 which did not).

Stream	Stream predecessor
2	3
3	2, 3
4	3
5	3
6	3
7	3
8	3

Table 4.4: Motard algorithm: Streams' predecessors table (rule 2).

Stream	Stream predecessor
2	3
3	3
4	3
5	3
6	3
7	3
8	3

Table 4.5: Motard algorithm : Final streams' predecessors table.

Now let's look at the application of the Motard rules through the dual graph. The first dual graph is obtained from the first flow table (Table 4.1). Attention: here the numbers represent the streams.

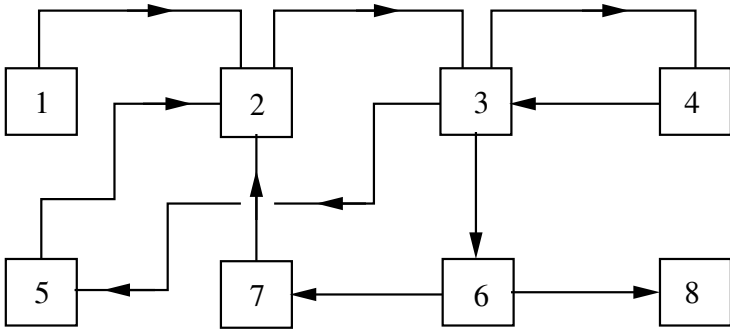


Figure 4.4: Initial dual graph for the system illustrated in Figure 4.2.

Applying the rules, the dual graph successively changes according to the Tables 4.2-4.5 as shown in Figure 4.5.

The last graph, as well as Table 4.5, show that all the streams have stream 3 as predecessor, even the stream 3. Consequently, there is an own loop on the stream 3 and **stream 3** has to be **teared**. All the other streams disappear by applying rule 1 because if stream 3 is deleted, the others have no predecessor. Then, the iterative process starts as illustrated in Figure 4.6.

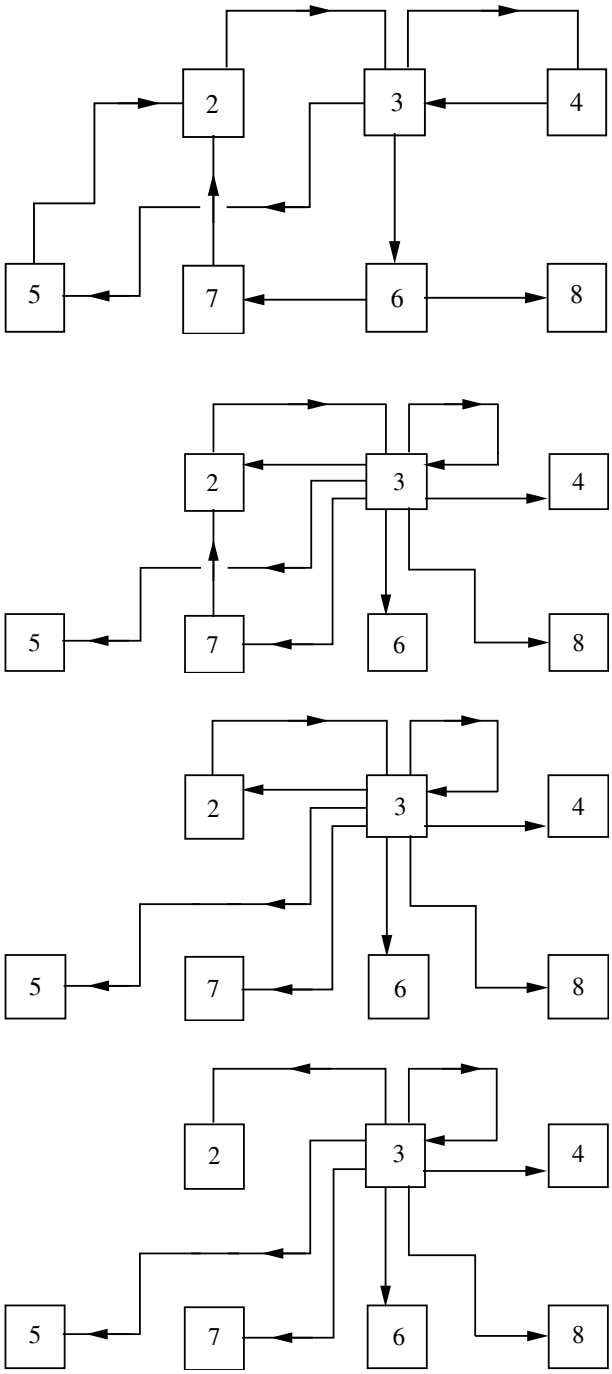


Figure 4.5: Evolution of the dual graph: Motard algorithm applied for the system illustrated in Figure 4.2.

Let's consider a single stream description variable (for example flow rate) and give stream 3 a first value a. The streams 4, 5 and 6 can then be calculated. Stream 7 ($7{=}f_6(6)$) can then be calculated. At this time, the streams 2 ($2{=}f_1(1,5,7)$) and 3 ($3{=}f_2(2,4)$) can also be calculated. Note as a' this new value of stream 3. If $a' \neq a$, we start again the calculation with a' or rather with a new a that is a function of a' (e.g.: $a = a'$, a' is renamed a) until:

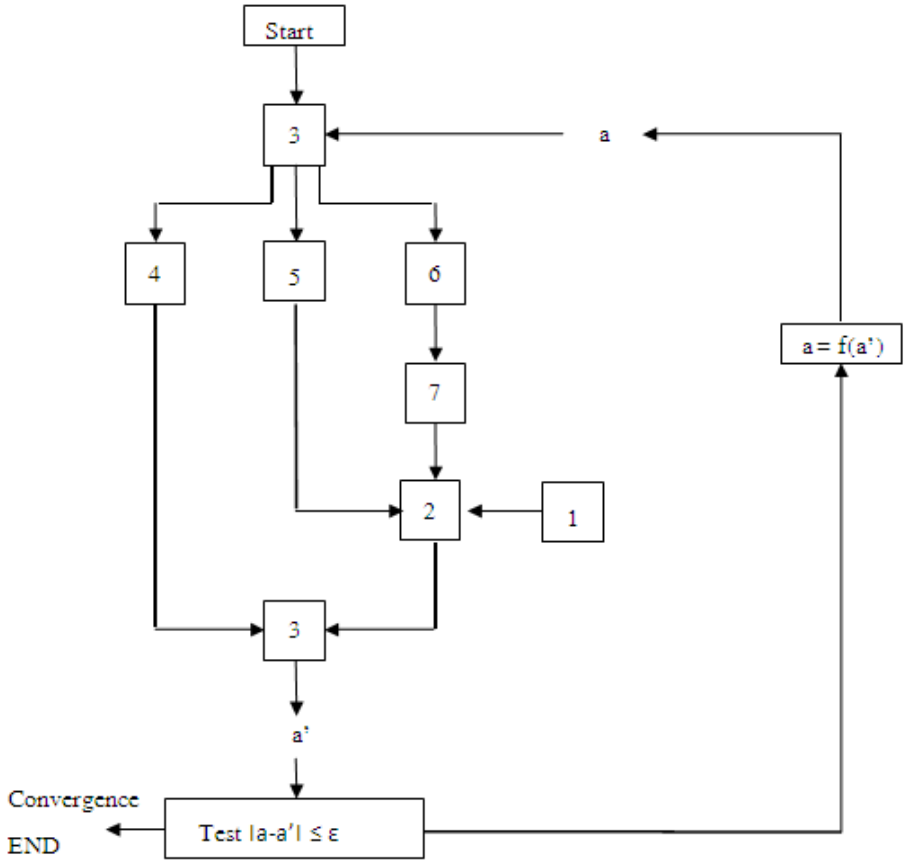


Figure 4.6: Iterative process for the sequential resolution.

$|a = a'| \leq \epsilon$ with ϵ fixed. After convergence the value of stream 3 is found and all the other streams can be determined.

Remarks :

- A less cost-effective solution would be, for example, to tear streams 4, 5 and 7. A sequential calculation would have been obtained, but there would have been a more complicate iterative process.
- Obviously, the presented theory does not mean that one should not make first all possible eliminations when they are easy to achieve.

Let's now process a more complex case for which the flowsheet and dual graph are given below (Figure 4.7). The Motard algorithm is applied in Table 4.6.

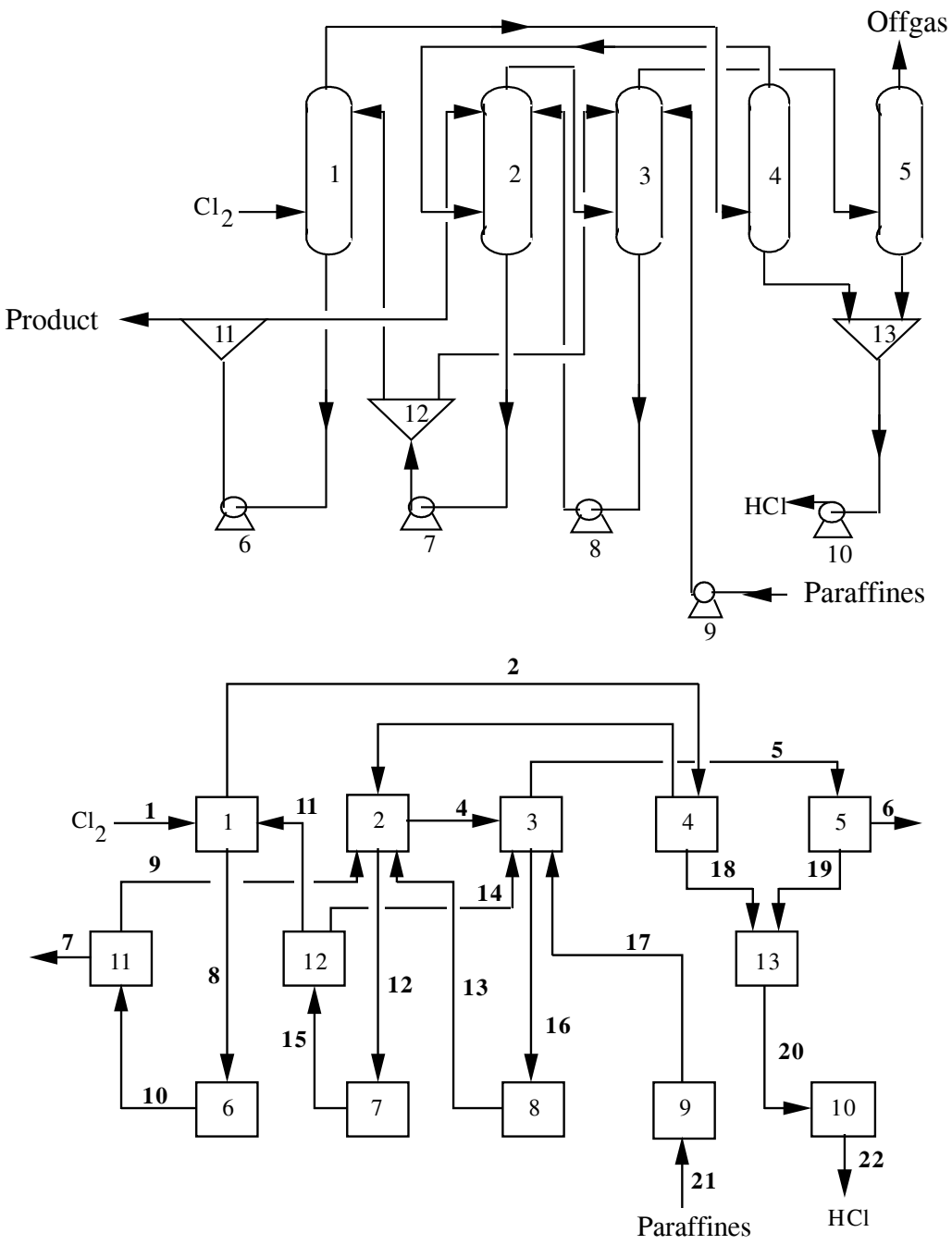


Figure 4.7: Flowsheet and dual graph of a distillation process.

There is a loop to find the stream 4, accompanied by a convergence test, as well as a loop on the stream 12. It is a calculation where two loops of convergence are nested, a step forward to 12 can be made when 4 is converged. The calculation scheme is shown in Figure 4.8.

Stream 1 and 21 are inputs and streams 22, 6 and 7 outputs. It has to be noted that all the intermediate calculations that are not necessary (streams 6, 19, 20, 22) are not performed each time but only when convergence is reached. Stream 17 is calculated knowing the input stream 21. A vector a of input data (T, P, partial molar flow) is chosen for the stream 12, and stream 15 is calculated which gives streams 14

Stream	Stream predecessor					
1	-	-	-		-	
2	1, 11	15	12		-	
3	2	15	12		-	
4	3, 9, 13	13, 15	12, 16		16	Tear 4
5	4, 14, 17	4, 14	4, 12		4	
6	5	5	5		4	
7	10	15	12		-	
8	1, 11	15	12		-	
9	10	15	12		-	
10	8	15	12		-	
11	15	15	12		-	
12	3, 9, 13	13, 15	12, 16	Tear 12	-	
13	16	16	16		16	
14	15	15	12		-	
15	12	12	12		-	
16	4, 14, 17	4, 15	4, 12		4	
17	21	-	-		-	
18	2	15	12		-	
19	5	5	5		4	
20	18, 19	18, 19	18, 19		4	
21	-	-	-		-	
22	20	20	20		4	

Table 4.6: Motard algorithm table for complex distillation process.

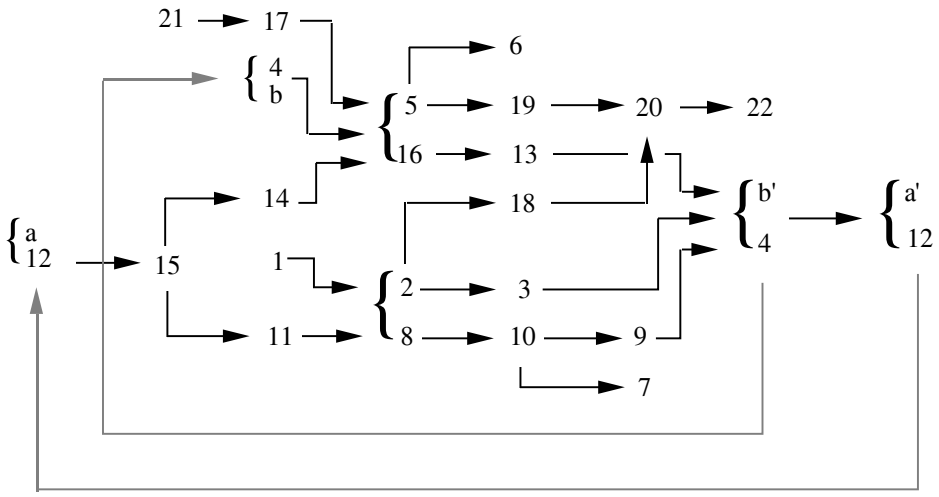


Figure 4.8: Calculation scheme for complex distillation process.

and 11. Stream 11 and the input stream 1 provide streams 2 and 8, based on stream 2 stream 3 (and 18) is found, while streams 10 then 9 (and 7) are found based on stream 8. For stream 4 a vector b is chosen (17 and 14 being known). Based on stream 4, stream 16 (and 5) are calculated and then stream 13. Then streams 9, 13 and 3 allow to calculate $4 = b'$. Test on $b' = b$, new values for b etc. until convergence of the loop on stream 4. Stream $12 = a'$ (from 13, 3, 9) is calculated; test on $a' - a$, new values for a, etc. until convergence of the loop on stream 12. Finally the streams 6, 18, 19 and 20 are calculated.

Choice of tears. The application of the Motard rules allows to determine the minimum number of tears that are necessary to solve the system. However, sometimes to reduce the computation time, it is interesting to make one or two additional tears or move the location of the tear along a loop. Finally, several types of tears/cuts are defined, according to the number of unknown variables:

- Total cuts (need to find n partial flowrates, T and P)
- Mass cuts (only the total flowrate is unknown)
- Thermal cuts (only the temperature is unknown)

To solve the system illustrated in Figure 4.9, a tear has to be added. Each stream can be represented by a vector containing the state variables, the specifications, the quantities of matter: for example a vector F containing: T, P, $\dot{M}$, x_i. Which stream has to be cut? If stream 2 is teared, the temperature, composition and possibly the pressure are initially not known. Therefore, a *total cut* has to be made on the stream to solve the system. However, between stream 1 and the input stream, the total flowrate and the compositions do not change, and the pressure is defined by the pressure drop. The only parameter that changes is the temperature. Consequently, it is sufficient to perform a *thermal cut*. This will facilitate the calculation as an iteration over one single variable has to be done. This highlights the important difference between total and partial cuts (compositions or temperature, etc.). Before making a cut, it should therefore be systematically evaluated whether there is no way to perform a partial cut, which will be always interesting from a calculation time prospective.

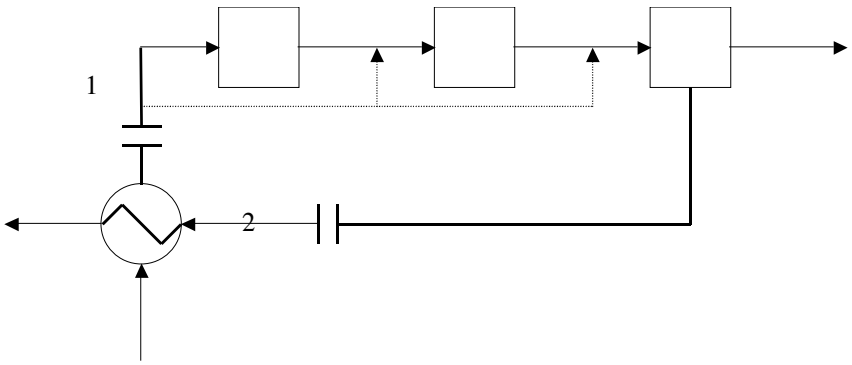


Figure 4.9: Example: mass and thernal cut.

Chapter 5

Optimization methodology

In this chapter the various forms of an optimization problem (mathematical definition) are highlighted and the different strategies that can be adopted to solve the optimization problem are presented. The key questions that are addressed are: What is an optimization method? How can models be used to state an optimization problem? How is a solving strategy defined for an optimization algorithm? What are the advantages and drawbacks of the different solving strategies?

5.1 Mathematical definition of the optimization problem

The optimization problem consists in determining the optimal values of the decision variables allowing to reach a given objective $f_{obj}(X_{state}$. The objective can be, for example the minimum operating costs. The optimization problem is defined by the following generic form:

$$\min f_{obj}(X_{State})$$

with	$f_{obj}(X_{State})$	Objective function
	$X_{State} = \{X_{Flows}, X_{Parameters}, Y_{decision}\}$	Variables
subject to	$F(X_{State}) = 0$	Model equations
	$S(X_{State}) = 0$	Specification equations
	$G(X_{State}) \geq 0$	Inequality constraints

The inequality constraints mathematically represent the acceptable limits of the considered variables. They can be classified into different categories:

- Operating limits: these are defined in the equipment specification sheets. For existing equipment, operating limits can be contractual values that delimit the responsibility of the equipment manufacturer. These limits are part of the exploitation authorization.
- Regulations: environmental constraints or constraints with regard to the exploitation authorization. For example, the emissions of certain pollutant are regulated and have to satisfy concentration and quantity limits. In process design, these limits may represent either current conditions or future conditions to be satisfied by the new facility.
- Technology limits and heuristics: during the design of a new facility or the renovation of an existing one, the operating limits (pressure, temperature, flowrate, power) of the new equipments are defined to represent the characteristics of the equipments that are commercially available. These constraints represent the limits of the materials or of the construction techniques.
- Numerical limits: when the model uses correlations to model the equipment or to compute the objective function, it is necessary to incorporate the validity limits of these correlations in the

optimization calculation in order to ensure the pertinence and accuracy of the solutions. The numerical limits also represent the validity limits of the models, whether unit models or even constraints regarding the system configuration. For example, the inequality constraints prohibiting the reversal of the flow direction is introduced if this inversion is not explicitly foreseen in the developed model. It is also important to consider the validity limits of the thermodynamic methods used to evaluate the thermodynamic properties of fluids, indeed, if the validity range is not respected some values may become inconsistent.

The inequality constraints can be divided into two categories:

1. *Soft constraints* that may be violated during the resolution. These constraints must be satisfied in the optimization procedure but their satisfaction or not has no impact on the calculation of the model: e.g. emission limit, maximum flowrate,...

2. *Hard constraints* that cannot be violated during the calculations otherwise the numerical calculation crashes. These constraints must be satisfied in any assessment of the model and should be treated appropriately to prevent failures in the iterative convergence procedure: e.g. flow direction inversion.

The strategies for solving optimization problems can be classified according to the level of integration between the optimization method and the model resolution. The common strategies discussed in detail hereafter are:

- Black box approach
- Simultaneous approach
- Two levels approach (hybrid approach)

5.1.1 Black-Box approach

In the black box approach the model and the optimization method are considered as two independent entities (Figure 5.1). The optimization method sends a set of decision variables values to the model and receives in return the value of the objective function(s) and the inequality constraints. It is therefore assumed that the model includes a robust resolution procedure that is able to calculate the objective function for any values of the decision variables.

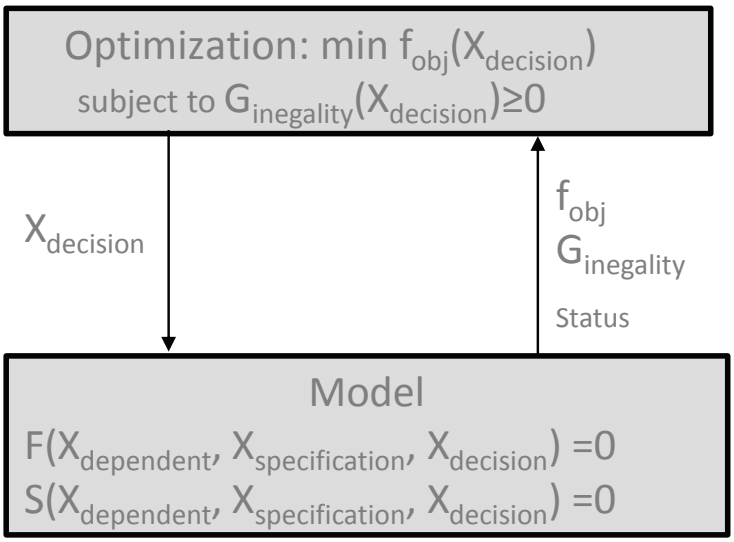


Figure 5.1: Black box approach.

Optimization method

The black box approach allows the use of almost all types of optimization algorithms. It is suitable both for direct methods (without calculation of derivatives), indirect methods (with calculation of derivatives) and heuristic methods (genetic algorithms, simulated annealing) or even graphic approaches. The method becomes heavier when the optimization method requires the calculation of derivatives. For non-heuristic methods, the optimum search is based on the assumption that the model is unimodal, i.e. there is only one single value of the objective function for a given set of decision variables.

Advantages

The main advantage of this method is its simplicity and robustness. It is essentially based on the quality of the model. It also allows to develop a model for which an efficient, reliable and robust resolution method has been developed.

The model may be discontinuous and contain conditional programming: if such conditions... then... , which is far more difficult with the simultaneous method.

Each model calculation result corresponds to a feasible operating point and can therefore be used for evaluation.

The number of variables considered by the resolution algorithm is the number of decision variables, which may be relatively limited even in the case of calculation of large systems.

Disadvantages

The black box approach is based on the quality of the model and will have difficulties to solve problems with inequality constraints. In the resolution procedure, checks have to be implemented and the status of the calculation results has to be verified. This allows the optimization algorithm to receive the information if the values returned by the model are consistent and correspond to a significant point.

This method is heavy in computation time, especially when iterative calculations are required to solve the model.

The success and effectiveness of the method highly depends on the model robustness and its ability to find a solution for each set of decision variables: when the model respond is that it has no solution, this does not mean that the internal procedures have not found any solution but that there is actually no solution. Time should be spent at the level of the model and its initialization when iterative procedures are used.

The calculation of the inequality constraints is relatively difficult. Only soft constraints can be treated easily. Hard constraints can only be treated by including them at the level of the decision variables. Which means that a prior knowledge of the optimum location with regard to these hard constraints is needed and that the model and its resolution have to be programmed on the basis of the probable activation of these constraints.

The model is developed for the calculation of the chosen objective function. If the model is to be used for another purpose, it has to be reprogrammed. This method is therefore not very convenient when the developed model is to be used throughout the life of the installation where the same model has to be used to optimize the design, then carry out performance monitoring and finally optimize the operating conditions according to the market demand. As all the decision variables vary from one case to another, the model, if it is used in a black box approach, should be modified accordingly.

The black box method is highly dependent on the accuracy of the model resolution algorithms since it is based on the value of the objective function for a given set of variables.

It should be noted that the choice of a black box approach has no real impact on the choice of the model resolution method: the model of a black box approach can be solved by a simultaneous resolution.

5.1.2 Simultaneous approach

In the simultaneous approach, the optimization problem and the model are solved simultaneously (Figure 5.2). This implies the use of non-linear and constrained optimization algorithms that use most of the time indirect methods based on the calculation of derivatives. In the simultaneous approach, the model is not in charge of the resolution of the model equations. The model calculates the value of the modeling and specification equations (for given the state variables). While, it is the optimization algorithm that is responsible for calculating the value of all the state variables in order that satisfy the modeling and specification equations, for checking the inequality constraints and for minimizing the objective function.

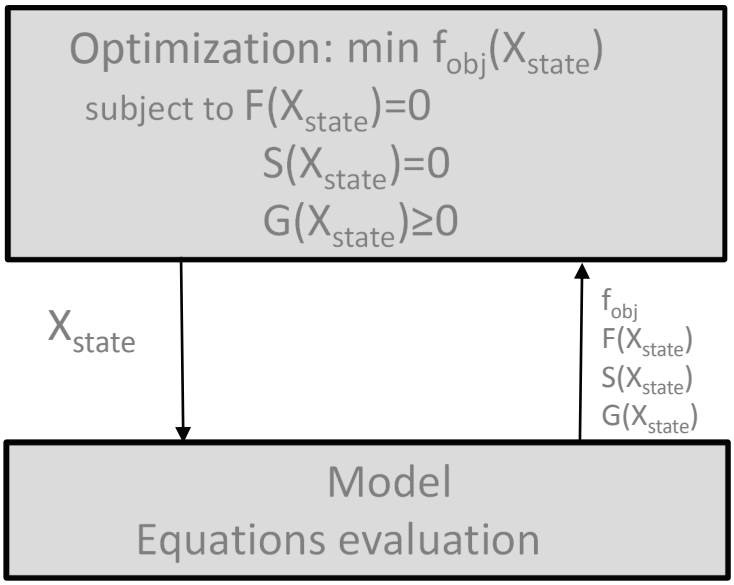


Figure 5.2: Simultaneous approach.

Optimization methods

In the case of a simultaneous approach, the optimization algorithms are constrained non-linear algorithms which must be able to deal with large systems. For these methods, feasible and infeasible path methods are distinguished, depending on whether they first seek to solve the system of equality equations and then follow an optimization path to reach the optimum or whether they seek to simultaneously satisfy the equality constraints and optimality conditions (see Optimization courses).

Advantages

The advantage of the simultaneous methods is the flexibility at the level of the problem definition: the model defines a list of equations to solve and the optimization algorithm is in charge of the resolution. It is therefore particularly well suited for efficient resolution algorithm. Especially, when the model is able to calculate the derivatives analytically. This approach is particularly appropriate if using software developed for process modeling and optimization (gProms, GAMS and AMPL programming languages). These software use a programming language specifically developed for the development of optimization model and implicitly incorporate the calculation of derivatives and the use of advanced optimization techniques.

The computation time of the simultaneous method is significantly reduced compared to the back box method. This approach is thus interesting for on-line optimization systems, for which the previous solution will be used as starting point for the new calculation.

It is possible to easily use continuation methods to assist in the resolution of strongly non-linear problems.

Simultaneous approaches, being based on methods using derivatives, have as an advantage the possibility to use all the information generated at the solution point, Lagrange multipliers, parameters' sensitivity, ..., the analysis of the incidence matrix verifying that the problem is well-posed.

Simultaneous approaches allow to easily change the problem formulation, without having to change the model definition and to choose the list of dependent variables.

Disadvantages

The effectiveness of the simultaneous methods is strongly linked to the initial values of the state variables. Therefore, a good initialization is required based on direction information from the derivatives values, prior to the resolution strategy. If the prior initialization is well made, the resolution of the problem is easy. The initialization is done before the optimization procedure in contrast to the black box approach where a good initialization is required at each evaluation.

The simultaneous resolution procedure provides feasible points only at the end of the procedure. In the case of non-convergence, the calculations are made not exploitable, while in the black box approach all calculated points represent a system state.

Iterative procedures for the evaluation of equations are avoided as much as possible in the simultaneous approach. Indeed, any iterative calculation causes a precision loss which affects not only the residues value but also the value of the derivatives.

Simultaneous approaches cannot easily handle conditional simulation problems. Only the cases where the condition does not determine the optimum position can be easily considered in a simultaneous optimization approach. When the optimal solution is conditioned by the decision, it will be necessary to include integer variables and therefore to consider conditions, such as constraints, as part of the whole optimization problem.

5.1.3 Two levels approach

The two levels approach has been developed to combine the advantages of the black box and simultaneous approach. The principle of two levels or hybrid approach is to solve part of the model as a black box and to charge the optimization algorithm with part of the specification equations (Figure 5.3).

In the two levels approach, the resolution of a sub-system of the equations at the level of the model aims to allow a fast and robust resolution that eliminates some of the variables ($X_{dependent}$) and part of the equations of the overall problem. The resolution algorithm is in charge of solving the reduced problem. This approach is similar to a reduced gradient approach, however, in this case, the reduction is performed into the resolution strategy, while in the reduced gradient approach, it is the result of a mathematical manipulation of the linear or quadratic approximation of the optimization problem.

The two level approach requires non-linear constrained optimization algorithms. Consequently, heuristic optimization algorithms cannot be used.

This approach combines the advantages of both approaches, however it has also some disadvantages: mainly at the level of the heavy programming and the derivatives calculation. For an efficient hybrid approach, derivative chaining (analytical calculation) has to be possible, which allows to calculate the derivatives unit by unit by perturbation of only the relevant variables.

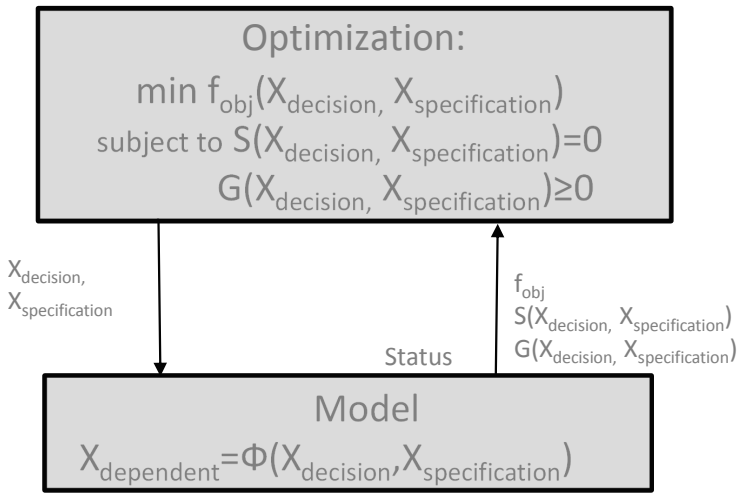


Figure 5.3: Two levels approach.

This approach is mainly used in cases where the resolution of the model needs iterative calculations and the accuracy of the derivatives calculation is strongly dependent on the precision of the internal iterative calculations. Remember that the calculation of the derivatives by perturbation is often done by a forward calculation Eq. 5.1:

$$\frac{\delta f}{\delta x_i} = \frac{f(X + \Delta x_i) - f(X)}{\Delta x_i} \tag{5.1}$$

For this calculation, the calculation precision of $f(X)$ must be significantly better than the value of the perturbation $f(X + \Delta x_i) - f(X)$, so that the derivative measures the sensitivity of the function to the variation of x_i and not the noise associated with the lack of precision in the iterative procedure.

5.2 Model resolution

Whether it's in the black box approach or in the two levels approach, the techniques that can be used to solve the model have to be studied. As explained in detail in Chapter 4, two methods can be applied: the sequential modular approach and the equation solver (simultaneous) approach.

Most simulation software are based on modular sequential approaches. The process model is decomposed into standard building blocks corresponding to the main types of unit operations. Simulation libraries provide routines to model the behavior of these units based on the mass and energy balances and some empirical equations. The units are resolved in a sequential manner by following the path of matter and energy in the process: the outputs of the units are calculated from the inputs and the parameters. Recycling and control loops are solved iteratively starting with values estimated for the teared stream (Section 4.2). Mathematical blocks are used to solve the tearing equations (with the possibility of some additional equations) by matching the values estimated with the results obtained by looping through the sequence of units. Because derivatives are seldom available, the promotion of convergence is generally based on substitution or on improvements based on the largest eigenvalue or the Wegstein extrapolation. Methods similar to the Newton method, trying to iteratively build approximations of the Jacobian matrix (or first derivatives matrix), such as the Broyden method, have also been used successfully.

In the case of the simultaneous approach called equation solver, all the equations and variables are processed simultaneously by a resolution algorithm that solves the overall system.

Many studies compared the two approaches; both have advantages and disadvantages. It should be noted that the sequential approach was longtime preferred due to the computing power of computers that could

not solve large size problems with a simultaneous approach. Today this constraint does not exist anymore which explains the proliferation of the simultaneous methods. The current trend is the development of hybrid methods to take advantage of the advantages of the two approaches.

A lot of research has been done to determine the most appropriate approach to solve the simulation problems and optimization of energy systems. Kontopoulos et al. [13] came to the conclusions that the choice depends on the type of problem. The results of the comparative study are summarized in Table 5.1.

	Sequential / black box	Simultaneous
Problem statement	*	***
Recycling	*	****
Pressure handling	*	****
Initialization	****	*
Debugging	****	**
Rigorous models	****	*
Conditional simulation	***	*
Flexibility	*	****
On-line optimization	*	****
Optimization	**	****
Robustness	****	**
Total	**	***

Table 5.1: Comparison between sequential (black box) and simultaneous resolution approaches: *Not satisfactory, ** Satisfactory, *** Good, **** Very good.

Remarks:

- For the simultaneous approach, the problem statement does not require the definition of the sequence. The algorithm for the degrees of freedom identification helps to define the specifications.

- In many simulation and optimization problems of energy systems, refrigeration cycles or vapor cycles, the pressures are determined counter-current to other variables: the pressure is set at the condenser outlet and defines the pressure of previous devices through the pressure loss. This is difficult to treat in a sequential approach because the inlet pressure has to be estimated in such a way that the pressure losses will not lead to impossible calculations (ex: negative pressure).

- A good initial value of all variables is necessary for the simultaneous approach, while for the sequential approach, only the value of the variables of the tears must be well estimated. This disadvantage of the simultaneous approach is moderated when the model is used in a global method. In this case, one of the preliminary operations is the validation of the measurements, which provides a value of all variables in the simulation and optimization. This operation, however, shifts the initialization problem to the validation tool, which also uses a simultaneous approach. Flowsheeting software often have an interactive mode that allows to perform a priori initialization of the units by an approximate sequential calculation.

- Identifying the cause of a non-convergence is more difficult in a simultaneous approach than in a sequential approach. In a sequential approach, the non-convergence is associated with the resolution of a particular unit. The analysis of the sequence and of the values allows to understand more easily the cause of the problem. In the simultaneous approach, all the equations and variables are processed simultaneously. In this case it is not easy to identify the cause of the non-convergence. However, it is possible to take advantage of the information of the resolution to identify the convergence problems. It is important to be able to distinguish the true convergence problems related to the difficulties encountered by the resolution software from the convergence problems resulting from the fact that the problem is impossible and that there is no solution having a physical meaning.

- The use of a rigorous simulation model can be difficult in the simultaneous approach because of the presence of discontinuities of equations or derivatives. Moreover, the simultaneous approach cannot easily handle conditional calculations.
- The simultaneous approach is very effective and robust when an initial point is found. In a few iterations a new point is obtained by changing the value of a specification or of a set-point. The sequential approach is penalized with a heavier calculation of derivatives which penalizes the calculation time. However, both approaches are robust to calculate a new operation point from a known solution.
- Simultaneous methods are particularly well suited to address optimization problems especially when it is necessary to satisfy inequality constraints. With a suitable choice of the state variables, the inequalities will be expressed in the form of linear equations that are always satisfied during the resolution. This avoids to calculate units in impossible conditions (e.g. negative flows). In the sequential approach, the inequality constraints appear in the form of a non-linear inequality equations that will require a special treatment to avoid convergence problems. The treatment of the inequalities is highly dependent on the robustness of the resolution software.
- The calculation of recycling involves iterative computations (Motard method to identify tears (section 4.2.1)). Loops have not to be forgotten because there is no convergence criteria in the case of an implicit resolution: by calculating several times the model a simple substitution is done. However no convergence criterion is applied which certifies that the substitution has led to a stabilization of the solution. In this case, there is a significant risk to consider a system as a converged, while in reality it is not (some energy and mass balances might not be satisfied!). This cannot happen with the simultaneous approach since the resolution of the tear equation (loop) is part of the equation system to be solved.

The availability of the derivatives is another asset of the simultaneous approach for the calculation of the optimization or for the exploitation of the results. In the simultaneous approach the calculation of the Jacobian matrix is the essential information to solve the problem because it defines the search direction. The Jacobian A is the matrix of the derivatives of the equations system for which ij element is defined by Eq. 5.2

$$A_{ij}(x^k) = \frac{\delta F_i(x^k)}{\delta x_j} \tag{5.2}$$

with:

$F(x)$	modeling and specification equations
$A_{ij}(x^k)$	element ij of the matrix A at the point x^k
$\frac{\delta F_i(x^k)}{\delta x_j}$	value of the partial derivative of function F_i with respect to the variable x_j at the to the point x^k

Two aspects have to be considered:

- In general, the size and the sparsity of this matrix are very important. In the case of a steam network, the average is 4 non-zero elements per line. So it is mportant to use a sparse matrix to store the Jacobian.
- The derivatives can be calculated analytically based on the equation formulation. However, when the form of the equations is not known or is too complex (e.g. in the case of conditional simulation), the derivatives are calculated numerically by a finite-difference or a central difference approach.

$$A_{ij}(x^k) = \frac{\delta F_i(x^k)}{\delta x_j} = \frac{F_i(x^k + \Delta x_j^k) - F_i(x^k)}{\Delta x_j^k} \tag{5.3}$$

where $F_i(x^k + \Delta x_j^k)$ is the value of equation i for which a single variable j among the variables X^k at the iteration k has been perturbated by the small value $+\Delta x_j^k$

The numerical calculation of derivatives is costly in computation time since it is necessary to systematically calculate the equations for each variable of the problem. It is obvious that flowsheeting software try to perform the analytical calculation when possible, and when the numerical calculation is required, they try to do it in a smart way and avoid unnecessary calculations. In the case of the modeling of energy systems, the calculation of the derivatives of thermodynamic functions is often done numerically due to the discontinuities in the enthalpy-temperature function. Indeed, at the level of the discontinuity, the derivative has two values, the choice of the correct value depends actually on the direction/path that is chosen based on the value of the derivative to perform the iteration step.

5.3 The AGE procedure to simulate and optimize energy systems

The AGE procedure (analyze, generate, evaluate) represents a generic three-step methodology that is applied during a modeling and optimization study.

The first step, *analyze*, consists in the problem statement: choose and assemble unit models and then analyze the degrees of freedom of the system to determine the specification equations and set-points (or command variables).

The second step, *generate*, corresponds to the resolution of the equation system. This implies initializing the variables and solving the non-linear equation system.

The third step, *evaluate*, consistent in drawing a solution from the numeric result in solution. The consistency of the numerical results provided by the model are checked and the numerical values are compared with the reality and the good engineering sense. Once the model is approved, it can be used to support decision making. The *evaluate* step is also used to determine the cause of the failure in the case where the solution has not been found. In fact, the cause may be attributed either to the resolution algorithm that has not found the solution, or to the set of specifications that is inconsistent (unfeasible system).

5.3.1 Analyze: degrees of freedom identification

In the analysis step, the degree of freedom is defined after having selected the unit model and determined the interconnections. This consists in defining the set of specification and set-point equations ($S(X_{State}) = 0$ and $C(X_{State}) = 0$). The degree of freedom is defined by analyzing the structure of the incidence matrix (see previous Chapters). The principle of the algorithm is to place an item on each diagonal position of the matrix by exchanging rows and columns [8, 7].

In the case of simulation problems, the algorithm is applied to choose the specifications. If such a permutation exists, then a pivoting sequence exists for the matrix inversion, which allows to say that the problem is structurally well-defined. When such a permutation cannot be found, it means that several variables (i.e. columns) collide to occupy the diagonal position of a line. In this case, the problem is *underspecified*. The addition of an extra line (i.e. specification), which will assign one of the columns which conflicted, will allow the algorithm to continue. For a given line (i.e. equation), the list of variables that are in conflict for the diagonal place defines the list of items among which one variable has to be specified. Similarly, the application of the algorithm of the matrix inversion allows to identify the *over-specifications* (i.e. excess equations). Surplus equations that are in conflict for one variable and which belong to the set $S(X_{State})$ define a subset of specifications in which one should be deleted.

Applied to the incidence matrix of the problem, this algorithm allows to define a square matrix (m+s=n) in which it is possible to permute the rows and columns in such a way that there is a non-zero on each diagonal position. With regard to the inversion of the Jacobian matrix this means that there is at least one sequence of pivots, but this does not guarantee that the value of the pivot is non-zero. If a pivot becomes zero during the factorization, the problem is numerically singular.

The algorithm does not guarantee that a solution will be obtained. Because of the non-linearity of the mathematical model, it is not sufficient to give a value to the specifications to find a solution. The set of specifications has to be consistent so that the equations can be solved simultaneously and that at the solution the variables X_{State} are in the validity range of the model.

In the case of an optimization problem, the degrees of freedom analysis stage will only deal with the over-specifications search.

5.3.2 Generate: optimization problem resolution

The *generate* step of the procedure consists in solving the model and/or the optimization problem. Various algorithms can be used to generate a numeric result as discussed in the previous chapters. For the simultaneous approach the initialization of the variables is necessary to define a good starting point for the iterative procedure and the derivatives calculation. In the case of the simulation of an existing installation, the data reconciliation gives a good starting point for the simulation calculation.

5.3.3 Evaluate: results

Once the simulation or optimization results are generated, the third step of the procedure is: to evaluate. Therefore, the simulation tool plays a very important role because it can test the solution obtained with other specifications, to test, for example, the feasibility or the flexibility of the calculated utility and heat exchange network.

The simultaneous approach is advantageous because it is possible to change the specifications without changing the calculation sequence. Moreover this approach is particularly well suited to calculate alternatives based on a known solution. The analysis of the solution by the generation of the sensitivity matrix is another benefit of the simultaneous resolution of the equation system. The objective is to calculate the variation of the variables to a change of the specification values [16].
Suppose that the solution of simulation has been obtained by solving the system: $F(X) = 0$. The considered system has fixed integer variables. In the vicinity of the solution, the first order development by the Taylor formula is:

$$F^*(X) = F_0 + A(X^0) \cdot (X - X^0)$$

with:

$F^*(X)$	the vector of the linearized equations
F_0	the vector defined by the equations at the linearization point $F_0 = F(X_0)$
X^0	the vector of variables at the linearization point
$A(X^0)$	the Jacobian matrix of the system at point X^0

When X^0 defines the solution of the system, $F_0 = 0$ and the function $F^*(X)$ is given by:

$$F^*(X) = A(X^*) \cdot (X - X^*)$$

with X^* being the vector X such that $F(X^*) = 0$.

As the vector F(X) comprises the modeling, specification and set-point equations, the linearized system can be divided into three parts:

$$\begin{pmatrix} F^*(X) \\ S^*(X) \\ C^*(X) \end{pmatrix} = \begin{pmatrix} A_F(X^*) \\ A_S(X^*) \\ A_C(X^*) \end{pmatrix} \cdot (X - X^*) = 0$$

with:

$A_F(X^*)$	Jacobian matrix (rectangular) of the modeling equations at the solution X^*
$A_S(X^*)$	Jacobian matrix of the specification equations
$A_C(X^*)$	Jacobian matrix of the set-point equations

In this system, the modeling equations $F^*(X)$ have to be equal to zero. With a suitable choice of variables, $A_S(X^*)$ is a rectangular unitary matrix: a single non-zero item equal to 1 per line. $A_S(X^*)$ is thus independent of the values of X and can be noted A_S. The following reasoning is applied to the set-points: $A_C(X^*)$ will be constant A_C.

The specification $s_i(X)$ is written:

$$s_i(X) = x_j - x_j^S = 0$$

with:

$s_i(X)$	the specification equation i corresponding to the specification of the variable j
x_j	the variable to which relates the specification j
x_j^S	the value of the specification of the variable j

At the solution, the value taken by x_j is equal to x_j^S. A perturbation ds_j of the specification is written as:

$$s_i(X) = x_j - (x_j^S + ds_j) = 0$$

For the linearized system this yields:

$$\begin{aligned} & s_i^*(X) &=& \; x_j - (x_j^*) = ds_j \\ \text{and} \quad & S^*(X) &=& \; A_s(X - X^*) = E_i \cdot ds_j \end{aligned} \tag{5.4}$$

with E_i the vector in which only element i is 1. E_i^T represents line i of the matrix A_S.

The linearized system becomes:

$$\begin{pmatrix} F^*(X) \\ S^*(X) \\ C^*(X) \end{pmatrix} = \begin{pmatrix} A_F(X^*) \\ A_S \\ A_C \end{pmatrix} \cdot (X - X^*) = ds_j \begin{pmatrix} 0 \\ E_i \\ 0 \end{pmatrix}$$

The resolution of this linear system gives the new value of the variables X to a perturbation ds_j of the specification value of the variable j. The sensitivity of the variables to the specification of the variable j is obtained by solving the system:

$$\begin{pmatrix} A_F(X^*) \\ A_S \\ A_C \end{pmatrix} \cdot \frac{dX}{ds_j} = \begin{pmatrix} 0 \\ E_i \\ 0 \end{pmatrix}$$

with:

$\frac{dX}{ds_j}$	the vector of the variables sensitivities to the specification of the variable j
$dX = (X - X^*)$	the response to the perturbation ds_j

The solution of this system is obtained by factorization of the matrix $\begin{pmatrix} A_F(X^*) \\ A_S \\ A_C \end{pmatrix}$:

$$\frac{dX}{ds_j} = \begin{pmatrix} A_F(X^*) \\ A_S \\ A_C \end{pmatrix}^{-1} \cdot \begin{pmatrix} 0 \\ E_i \\ 0 \end{pmatrix}$$

The matrix of the variables sensitivities with regard to the specifications is calculated by:

$$\frac{dX}{dS} = \begin{pmatrix} A_F(X^*) \\ A_S \\ A_C \end{pmatrix}^{-1} \cdot \begin{pmatrix} 0 \\ A_S^T \\ 0 \end{pmatrix}$$

with $\frac{dX}{dS}$ the matrix of the sensitivities with regard to the specifications whose element i, j defines the sensitivity of the variable i to the specification j.

The matrix of the variables sensitivities with regard to the set-points is given by:

$$\frac{dX}{dC} = \begin{pmatrix} A_F(X^*) \\ A_S \\ A_C \end{pmatrix}^{-1} \cdot \begin{pmatrix} 0 \\ 0 \\ A_C^T \end{pmatrix}$$

with $\frac{dX}{dC}$ the matrix of the sensitivities with regard to the set-points whose element i, j defines the sensitivity of the variable i to the set-point j.

The calculation of these matrices requires no additional factorization. It is an additional information that directly available through the use of the simultaneous approach.

The use of the sensitivities matrices can be applied to heat exchange networks results [15]. The sensitivity calculation is also used to calculate the decoupling between manipulated and controlled variables. When the set-point is the value of the controlled variable, the system of equations describes the utilities network as a transformer which calculates the manipulated variables as a function of the set-point variables (Figure 5.4). The calculation of the sensitivity matrix gives the influence of the controlled variables on the manipulated variables.

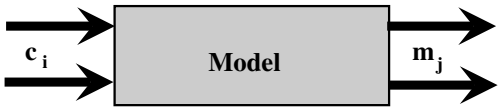


Figure 5.4: Controlled variables - manipulated variables: Transformer.

When the a set-point value influences more than one manipulated variable, there is a risk of coupling which has to be taken into account in the control strategy. Without using dynamic programming including regulators, a static study allows to quantify the coupling. By replacing in the equations system, the set of set-point equations on the controlled variables $C(X)$ by a set of specification equations on the manipulated variables $M(X)$, the model becomes an operator calculating the controlled variables (outputs) on the basis of manipulated variables (inputs) Figure 5.5.

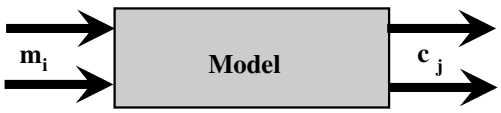


Figure 5.5: Controlled variables - manipulated variables: Operator.

The set of the manipulated variables $M(X)$ is defined by:

$$M(X) = A_M(X - X^*) = 0$$

where A_M is the matrix of the manipulated variables whose lines have only a single element with the value of 1 defining the corresponding manipulated variable.

$M(X)$ replaces $C(X)$ when the matrix $\begin{pmatrix} A_F(X^*) \\ A_S \\ A_M \end{pmatrix}$ can be inverted.

The calculation of the sensitivities matrix with respect to the manipulated variables provides the sensitivity of the controlled variables with respect to the manipulated variable m_j , the other manipulated variables being kept constant. The system operates in open loop. Element i, j of the matrix (M) is defined by:

$$m_{ij} = \left(\frac{dc_i}{dm_j}\right) mk \neq j$$

with $\left(\frac{dc_i}{dm_j}\right) mk \neq j$ the sensitivity of the controlled variable c_i with respect to the manipulated variable m_j, the other manipulated variables being kept constant.

The relative gain array (RGA) (here named matrix L) described by [4] allows to measure interactions in the process and give recommendations for the pairing of the manipulated and controlled variables. This operation allows to define the control loops of the control system (Figure 5.6) and the decoupling that has to be done between different loops.

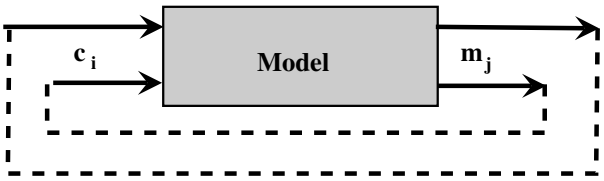


Figure 5.6: Control system.

The element ij of the relative gains array is given by:

$$l_{ij} = \frac{\left(\frac{dc_i}{dm_j}\right) mk \neq j}{\left(\frac{dc_i}{dm_j}\right) ck \neq j}$$

where $\left(\frac{dc_i}{dm_j}\right) ck \neq j$ is the sensitivity of the controlled variable c_i with respect to the manipulated variable m_j the other controlled variables being kept constant: closed-loop.

By linear algebra, the elements of this matrix can be calculated on the basis of the matrix M by multiplying terms by term the matrix M and the inverse of the transposed matrix $(M^{-1})^T$. The characteristic of the matrix L is that the sum of the elements of the rows and of the columns is equal to 1. The allocation of a manipulated variable (column) to a controlled variable (line) is achieved by choosing, for each row, the column that has the largest element in absolute value. If the value is 1, then there is no coupling between this couple and the others; if the value is close to 1, then the coupling is low; if the value is high, there is a coupling which should be taken into account to develop a control strategy (decoupling).

5.4 MINLP problems: optimization of superstructures

In process design problems the resolution algorithm has to make the choice of type yes/no. For example: choose whether or not a unit is in the superstructure. In this case, it is necessary to add to the model integer variables that represent the use or not of a unit or a flow. These variables, denoted Y, represent decisions of yes/no type:

$$\begin{aligned} y_i &= 1 \quad \text{the decision i is YES} \\ y_i &= 0 \quad \text{the decision i is NO} \end{aligned}$$

The problem becomes a mixed integer non-linear problem called MINLP (Mixed Integer Non Linear Programming). Before studying the various definitions that the optimization problem can take, the way the integer variables are considered is first presented, as well as the algorithm that can be used to solve this problem.

Specification or set-point equations with integer variables

This type of expression is used to mathematically represent the following situation: the turbine j must produce the power requested by the shaft; otherwise the mechanical power will be provided by an electric motor connected to the same shaft. Note $W_{mec,j}$ the power produced by the turbine j, $P_{mec,j}$ the power requested at the turbine j, y_j the integer variable associated with the turbine j. If $y_j = 1$ the turbine is operating and if $y_j = 0$ it does not. In this case, $P_{mec,j}$ will be produced by the electric motor. The specification equation of the power becomes:

$$W_{mec,j} - P_{mec,j} \cdot y_j = 0$$

if $y_j = 1$, $W_{mec,j} = P_{mec,j}$
if $y_j = 0$, $W_{mec,j} = 0$

All the specifications of extensive variables are treated in the same way and take the following form:

$$x_i - x_{si} \cdot y_i = 0$$

with:
- x_i the extensive variable i
- x_{si} the value of the specification of variable i
- y_i the integer variable related variable i

The value of y_i can be fixed if the specification is not a yes/no decision.

The set of specification and set-point equations is thus divided into two parts:
- $S1(X) = 0$ specifications of the intensive variables
- $S2(X, Y) = 0$ specifications of the extensive variables

The intensive variables are not subject to the same constraints: they do not depend directly on the yes/no decision, only through the balances and the modeling equations. The use of integer variables provides an additional argument in the choice of intensive rather than extensive variables to describe the state of the system. If the total enthalpy is used instead of the molar enthalpy to describe the enthalpy content of a stream and if the integer variable associated with the flow is zero, then the flowrate will be zero as well as the total enthalpy. The temperature can no longer be calculated and all the modeling equations that involve this temperature can not be assessed.

5.4.1 Inequality constraints with integer variables

Consider the example of a heat exchanger of the heat exchanger network. If the heat exchanger is used in the optimal structure ($y_i = 1$), the exchange area must be between a minimum and maximum; however, if the exchanger is not used ($y_i = 0$), its surface must be zero:

If the heat exchanger i is chosen:		$y_i = 1$ and $A_{min,i} \leq A_i \leq A_{max,i}$
If the heat exchanger i is not used		$y_i = 0$ and $A_i = 0$
with	$A_{min,i}$	the minimum surface allowed for the heat exchanger i
	$A_{max,i}$	the maximum surface allowed for the heat exchanger i
	A_i	the surface of the heat exchanger i
	y_i	the integer variable related to the use of the exchanger i

Mathematically, this is expressed by:

$$A_{min,i} \cdot y_i \leq A_i \leq A_{max,i} \cdot y_i$$

In the same way as for the specifications, the inequalities with integer variables relate only to the extensive variables. The set of inequalities $G1$ is divided into two subsets:

$G3(X,Y) \geq= 0$	defines the bounds on the extensive variables
$G4(X) \geq= 0$	defines the bounds on the intensive variables

Linking equations between integer variables

To maintain the consistency of the problem, the unit models will introduce linking equations between the integer variables, as illustrated for the unit models in Figure 5.7.

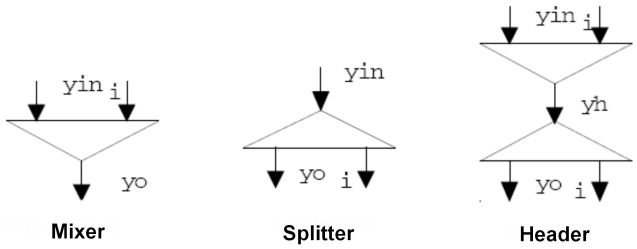


Figure 5.7: Integer variables definition for mixer, splitter, steam header.

Mixer. The mixer introduces the following equations:

$$\begin{aligned} \sum_{i=1}^{n_{in}} y_{in,i} - y_o &\geq 0 \\ y_o - y_{in,i} &\geq 0 \quad \forall i = 1, ..., n_{in} \end{aligned}$$

with:

$y_{in,i}$	integer variable associated with the input stream i
y_o	integer variable associated with the output stream
n_{in}	number of input streams

If $y_o = 0$, all the $y_{in,i}$ will be canceled by the first equation. On the other hand, if at least one $y_{in,i} = 1$, y_o must be equal to 1 to satisfy the second equation. If all the $y_{in,i}$ are zero, $y_o = 0$ verifies the first equation.

Splitter. For the splitter the equations are the following:

$$\begin{aligned} y_{in} - y_{o,i} &\geq 0 \quad \forall i = 1, ..., n_{out} \\ \sum_{i=1}^{n_{out}} y_{o,i} - y_{in} &\geq 0 \end{aligned}$$

with:

y_{in}	integer variable associated with the input stream
$y_{o,i}$	integer variable associated with the output stream i
n_{nout}	number of output streams

If $y_{in} = 0$, $y_{o,i} = 0$ according to the first equation. If one $y_{o,i}$=1, then $y_{in} = 1$ satisfies the first equation. If all the $y_{o,i}$ are zero then $y_{in} = 0$ according to the second equation.

Header. In terms of integer variables, the header is considered as a mixer followed by a splitter. The generated equations are the combination of the two previous models:

$$\begin{aligned} y_h - y_{o,i} &\geq 0 \quad \forall i = 1, ..., n_{out} \\ \sum_{i=1}^{n_{out}} y_{o,i} - y_h &\geq 0 \\ \sum_{i=1}^{n_{in}} y_{in,i} - y_h &\geq 0 \\ y_h - y_{in,i} &\geq 0 \quad \forall i = 1, ..., n_{in} \end{aligned}$$

with:

$y_{in,i}$	integer variable associated with the input stream i
y_h	integer variable associated with the header
$y_{o,i}$	integer variable associated with the output stream i
n_{in}	number of input streams of the header
n_{out}	number of output streams of the header

All these equations are introduced as a set of additional inequality equations defined by: $G5(Y) \geq 0$. This set of equations may seem superfluous since the integer variables relate to flowrates for which the integer variable is already defined by an inequality equation $f_{min,i}y_i \leq f_i \leq f_{max,i}y_i$. They are nevertheless introduced to avoid an indefiniteness in the case where the value of $f_{min,i}$ is 0.

Chapter 6

Thermo-economy

One of the main applications of the modeling of energy systems is the thermo-economic or thermo-environomic optimization. The basis of the formulation of a thermo-economic/environomic objective function will be introduced here.

6.1 Problem statement

The challenge of an integrated energy system is to transform primary energy (fuel resources) into useful energy in the form of heat or electricity (which will be sold) (Figure 6.1). In this perspective, companies invest in a set of technologies that will allow to maximize the profit. In most cases, the generated electricity will be injected in the network, while the heat will be used directly on-site by a process unit or delivered to a district heating network. The profit will be defined as the difference between the income from the sale of transformed energy (i.e. heat and electricity) and the expenses for fuel purchase, operation and labor, and installation depreciation.

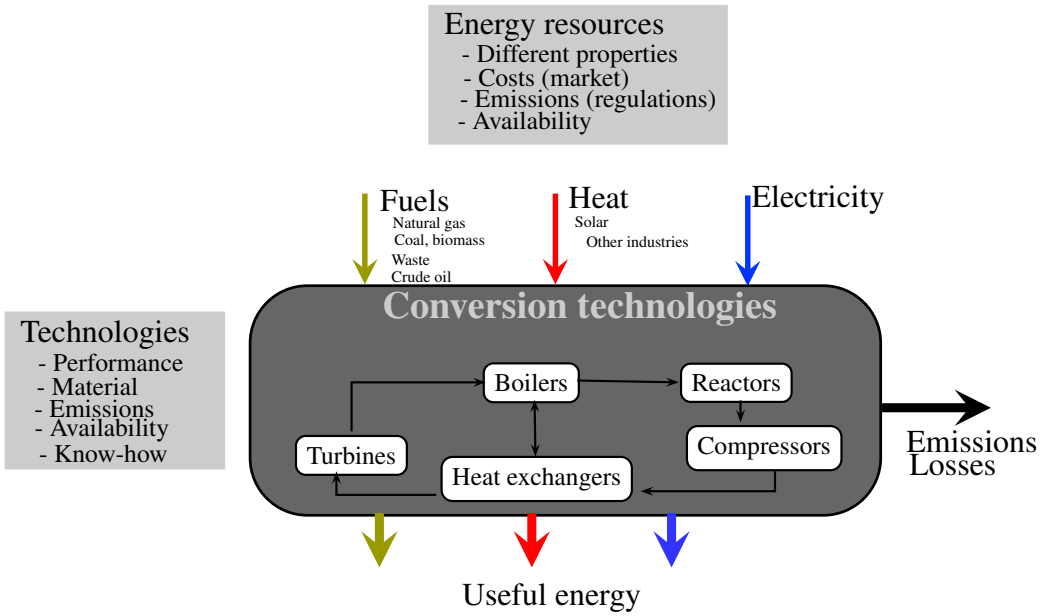


Figure 6.1: Integrated energy system.

The goal of an integrated energy system is to increase the efficiency (thermo), to decrease the costs (economic), to respect the environmental constraints and to decrease the environmental impact (environmental). As these objectives are in competition and there is a large diversity of technologies available on

the market, there is no unique solution to this problem and consequently the engineer will be faced with a thermo-economic/environomic optimization problem.

6.1.1 Definitions

The different terms of the notion 'Thermo-environomic' illustrated in Figure 6.2 are explained here.

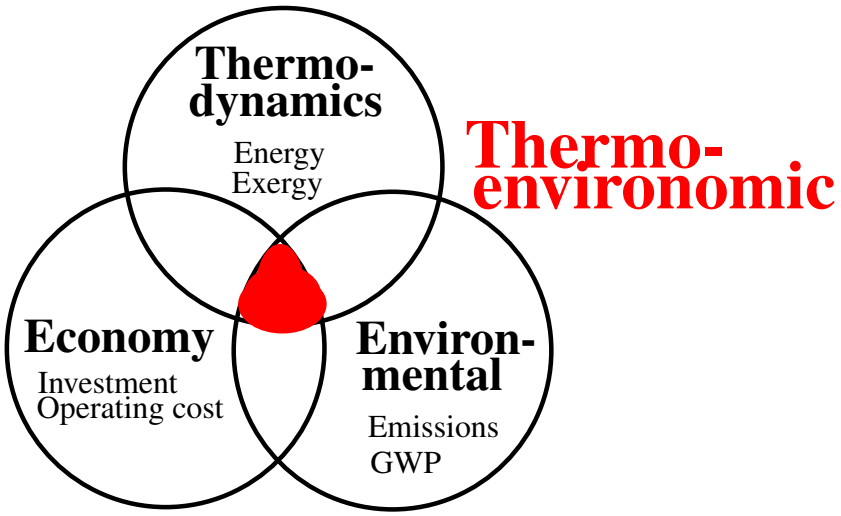


Figure 6.2: Defintion: Thermo-environomic.

Thermo

The system will be modeled by the thermodynamic phenomena taking place in the different process units, mainly the transformation of matter and energy. The model will calculate the performance of the studied system on the basis of the technical characteristics of the equipment.

Economic

The model will be used to calculate the performance of the installation which will be expressed by the economic performance. In the thermo-economic optimization, the trade-off between the operating costs resulting from the thermodynamic performance of the process and the investments to achieve these performance (purchase of equipment) will be assessed.

Environomic

In the environomic approach, the model will in addition evaluate the environmental performance of the system. The environmental performance can be defined by the emissions from the process itself, the use of raw materials, the waste treatment, or the production of the equipment. The environmental performance will be expressed in an economic form (for example CO_2 tax) to include the environmental impact of the energy system in the economic performance.

6.2 Thermo-economic performance of a process

The goal of a thermo-economic evaluation is to estimate, on the basis of the thermodynamic values calculated by the process model, the investment and its profitability. The performance is represented by the trade-off between the generated profits and the total investment costs over the lifetime of the installation.

Example: Purchase of a heat exchanger to save energy. The initial situation is illustrated in Figure 6.3.

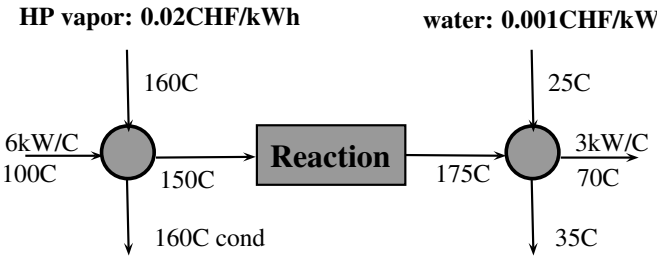
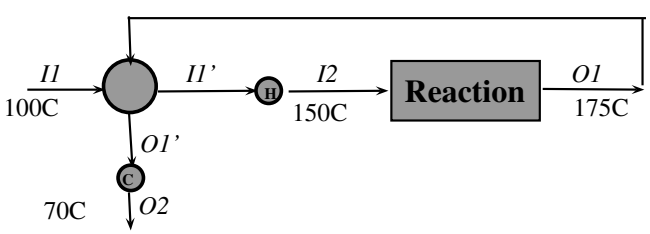


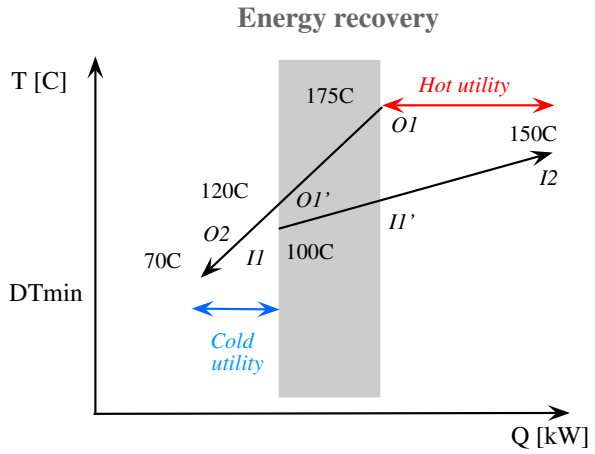
Figure 6.3: Initial process layout.

To achieve energy savings, a heat exchanger is purchased to exchange heat between the stream at the reactor inlet and the output stream (Figure 6.4).



Investment
- Heat exchanger
- Connexions/pipes
- Control

Expected benefit
- Energy savings
- Reduction of
  - cooling water consumption (C)
  - vapor consumption (H)



Heat exchanger optimal operation ?

Figure 6.4: Energy saving by heat exchange.

To evaluate the investment profitability, the following elements have to be assessed:

- Heat exchanger purchase cost
- Installation price
  - Foundation
  - Connections (pipes)
  - Control
- Funding opportunities
- Calculate the cost/benefit of the heat exchanger operation

- Energy purchase (typically lower than the case without heat exchangers)
- Maintenance

To evaluate the benefit of an energy saving project it is necessary to evaluate the compromise between the investment and the savings. Several difficulties have to be faced:

1. The investment has to be estimated with a relatively simple method. Therefore the purchase costs of the equipment, the cost associated with the installation of the equipment in the process (including the costs of foundation, connections, engineering, labor for installation, additional taxes, etc.) and the cost related to the equipment operation (for example the connection of measuring apparatus, control, safety procedures, etc...)
2. The calculation of the annual profits that will be achieved. Therefore the energy costs, the maintenance costs and the additional labor costs have to be accounted for.
3. Time scale: the investment made at the beginning of the project induces profits for a fixed period. Therefore, the money of today has to be compared with the future profits.

6.2.1 Estimation of the investment

Different investment estimation levels are distinguished depending on the required precision and the investment project maturity. The estimation of the investment costs money, the more precise the estimation the more costly it is, as shown in Figure 6.5.

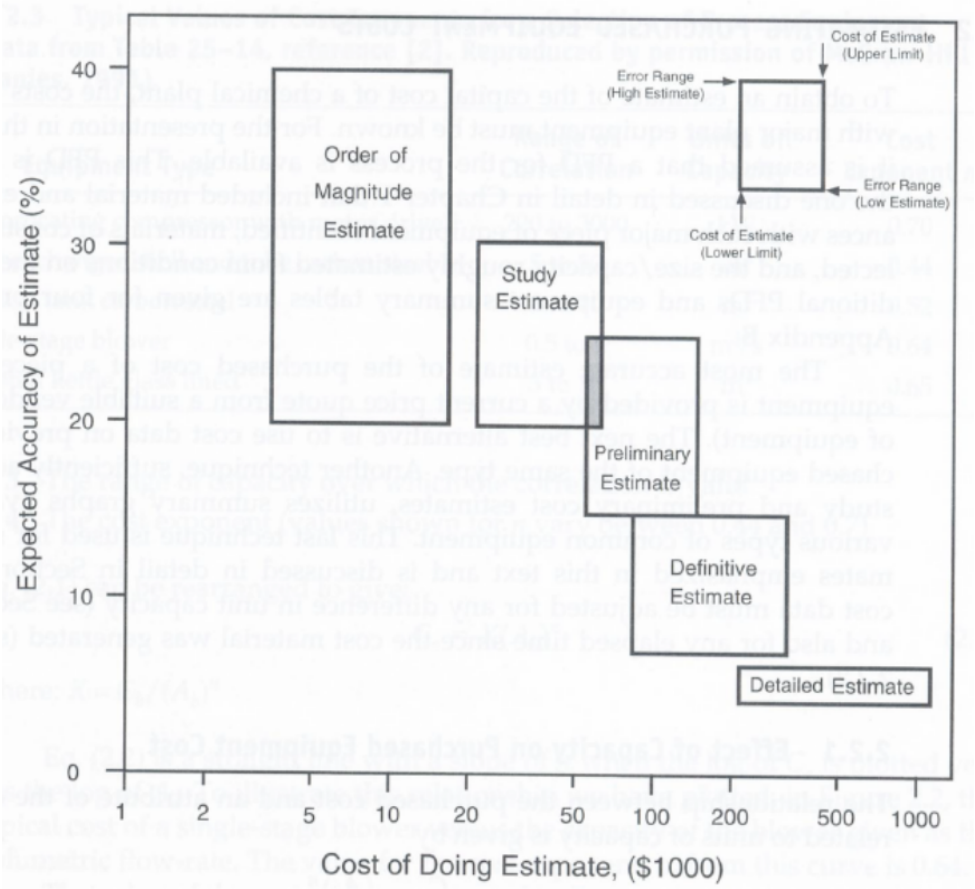


Figure 6.5: Investment estimation [21].

1. The first level corresponds to the estimation of the order of magnitude of the investment. It mainly concerns the processes or the global system. The estimation is often carried out on the basis of the production level and is obtained by comparison with an equivalent existing installation. The rule of the 6/10 is often applied.

2. The second level will be the one that is applied for energy audits and process improvement studies. Based on a PFD (Process Flow Diagram), this type of estimation requires the calculation of the size of each equipment. This level of assessment will be used to compare alternatives and identify the most promising ones.

3. The third level will be the preliminary evaluation carried out to select the best alternatives. At this level, a good investment estimation has to be done to request a budget to fund the project. At this stage a price offer will be requested for the major equipments.

4. The fourth level corresponds to the final assessment requiring a detailed calculation of the changes: dimensions of all equipment, calculation of the piping cost, costs of safety measures, taxes, etc. ...

5. Last level: detailed estimation to guide and control the project implementation. The detailed estimate is often performed by the responsible project engineers or the one who contracted the project.

For the thermo-economic optimization, a rough estimation of the investment is normally made since in the majority of cases, the list of technologies that must be used is not yet known.

If only little information is available, the investment (i.e. the purchase cost) C_p can be evaluated by equation Eq.6.1 estimating the investment on the basis of the investment of a similar facility $C_{p,ref}$ considering a scale factor of 0.6. A is the equipment attribute, for example the area for an heat exchanger.

$$\frac{C_p}{C_{p,ref}} = \left(\frac{A}{A_{ref}}\right)^{0.6} \tag{6.1}$$

With regard to the equipment purchase, the first step will be the definition of the operating conditions, the choice of the most suitable type, the calculation of the equipment size and the choice of the appropriate material. It should be noted that these choices are not independent from one another. More information can be found in [22, 21, 1, 18].

The cost estimation methods result from statistical analysis of market studies. The methods are based on the manufacturing cost of standard equipments that are then corrected to take into account the operating conditions (e.g. temperature and pressure influence). In addition to the equipment purchase cost, the costs of the equipment installation have to be added to get the installed cost (ready to start). The installed cost differs from the purchase cost by a factor of 3-4. The installed cost includes:

- Additional materials required for installation
- Foundations and piping costs
- Labor and engineering work
- Cost for the integration with other equipments
- Equipments and adaptation of control and security systems
- Taxes and royalties
- Purchase of land

To evaluate the installed cost on the basis of the purchase cost a global factor F (known as Lang factor or bare module factor) can be applied to the total cost of purchase of the equipment (Eq. 6.2). The factor depends on the plant type (i.e material that is processed, operating pressure).

$$C_i = F \cdot \sum_{i=1}^{n_e} C_{p,i} \tag{6.2}$$

with:

$C_{p,i}$	Purchase cost of equipment i
n_e	Number of equipments
C_i	Installed cost
F	Lang factor
	F=4.74 liquid processing
	F=3.1 solid processing
	F=3.63 solid-liquid processing

The estimate of the installed cost can be expressed in a canonical way. The effect of the pressure and material can be expressed by Eq. 6.3. For heat exchangers, for example, the installed cost can be evaluated by Eq. 6.4 including the effect of pressure, material choice and reference index. The values of the various parameters of this equation are taken from [21] (Figure 6.6).

$$F = B_{1,i} + B_{2,i} \cdot F_{M,i} \cdot F_{P,i} \tag{6.3}$$

$$C_i = C_{p,i} \cdot (B_{1,i} + B_{2,i} \cdot F_{M,i} \cdot F_{P,i}) \cdot \frac{I_t}{I_{t,ref}} \tag{6.4}$$

with:

$C_{p,i}$	Heat exchanger purchase cost
	$C_{p,i} = 10^{K_{1,i}+K_{2,i}logA_i+K_{3,i}(logA_i)^2}$
	K_j empirical constants from cost database
B_j	empirical constants computed from cost database
$F_{P,i}$	Pressure factor
	$F_{P,i} = 10^{C_{1,i}+C_{2,i}log\bar{P}_i+C_{3,i}(log\bar{P}_i)^2}$
	C_j empirical constants computed from cost database
	$\bar{P}$ pressure difference from atmospheric pressure
$F_{M,i}$	Material factor
I_t	Cost index for actual year
$I_{t,ref}$	Cost index for reference year

The cost indexes are used to calculate the current value of the investment compared to the date on which the investment estimation or the correlation has been established. The values of the index can be obtained in journals such as Chemical Engineering [6]. Two indexes that are commonly used are the Marshall & Swift Index and the CEPCI Index (Chemical Engineering Process Cost Index). Details about the CEPCI can be found in `http://www.che.com/Assets/File/CEPCI_1_01-2002.pdf`. The variation of the indexes along the years and the variation of the CEPCI along the years 2008/2009 are illustrated in Figure 6.7.

6.2.2 Investment annualization

To make an economic evaluation, the investment has to annualized. The annualization is necessary to compare the investment made today and the annual income (savings) expected over the lifetime of the installation.

Considering a period of n years and an interest rate i, the future value of the investment I^* (at the end of n years) can be estimated by Eq. 6.5.

$$I^* = I \cdot (1+i)^n \tag{6.5}$$

Correlation Coefficients for Heat Exchangers

er	K_1	K_2	K_3	C_1	C_2	C_3	B_1	B_2	A_{min} (m^2)
pe	3.0238	0.0603	0	6.4945[1]	−6.6786	1.7442	0.74	1.21	0.2
ipe	2.1138	0.9658	0	6.4945[1]	−6.6786	1.7442	0.74	1.21	10
e	3.2138	0.2688	0.07961	−0.06499[2]	0.05025	0.01474	1.80	1.50	4
lead	3.4338	0.1445	0.10790	−0.06499[2]	0.05025	0.01474	1.80	1.50	10
	3.5238	0.1916	0.09474	−0.06499[2]	0.05025	0.01474	1.80	1.50	10
oiler	3.5638	0.1906	0.11070	−0.06499[2]	0.05025	0.01474	1.80	1.50	10
all	3.7438	0.9270	0	6.4945[1]	−6.6786	1.7442	0.74	1.21	2
e	3.5738	0.4548	0	0	0	0	1.80	1.50	7
	3.6418	0.4053	0	−0.06154	0.0473	0	1.53	1.27	3.5
e	3.4088	0.6000	0.09944	−0.4045[3]	0.1859	0	0.74	1.21	.1
e	3.6788	0.4412	0	0	0	0	1.53	1.27	2
	3.8528	0.4242	0	0	0	0	1.53	1.27	15

ictors given are for 100 < P < 300 barg, for 40 < P < 100 use $C_1 = 0.6209$, $C_2 = -0.9274$, $C_3 = 0.3369$, for P < = 0

ictors given are for when shell or both shell and tube are > 10 barg, when tubes only >10 barg use 9, $C_2 = 0.04139$, $C_3 = 0$

ictors given are for when shell or both shell and tube are > 10 barg, when tubes only >10 barg use 0, $C_2 = 0.09717$, $C_3 = 0$

Figure 6.6: Parameters for estimating the installed cost of an heat exchanger [21].

Assuming that the same operation is performed for an annual income B (constant at the end of each year), the value of this constant entry at the end of the same period can be calculated. This corresponds to a sum of incomes, each bearing interest over the number of years minus one. This sum is a geometric progression defined by the analytical expression Eq. 6.6 where B^* is the annual income B after n years with an discount rate i (interest rate).

$$B^* = \sum_{r=1}^{n} B \cdot (1+i)^{r-1} = B\frac{(1+i)^n - 1}{i} \tag{6.6}$$

By combining Eq. 6.5 & 6.6, the present value V^* of an annual constant income B for n years with an interest rate i is given by Eq. 6.7.

$$V^* = \left(\frac{1}{(1+i)^n}\right) \cdot \left(B\frac{(1+i)^n - 1}{i}\right) = B \cdot \frac{(1+i)^n - 1}{i \cdot (1+i)^n} \tag{6.7}$$

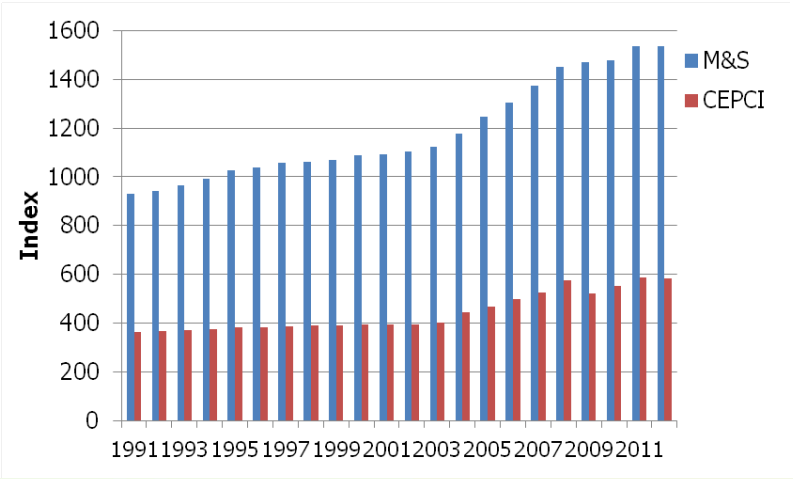
Based on this formula 6.7, the actual total cost C_{tot} corresponding to the sum of the investment made today and the operating costs over the lifetime of the equipment can be evaluated by Eq. 6.8. The annual expenditure of an investment I can then be compared with the money invested today Eq. 6.9

$$C_{tot} = I + C \cdot \frac{(1+i)^n - 1}{i \cdot (1+i)^n} \tag{6.8}$$

$$IC[CHF/year] = I \cdot \frac{i \cdot (1+i)^n}{(1+i)^n - 1} \tag{6.9}$$

with

I	initial investment
C	operating cost



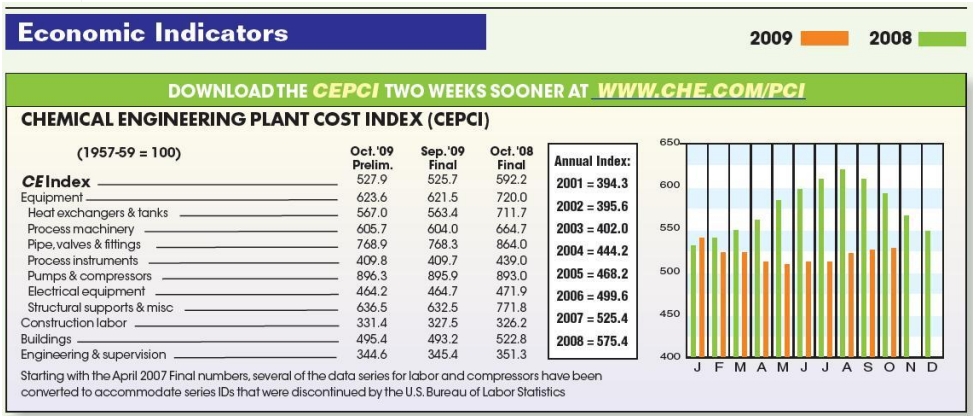


Figure 6.7: Variation of the indexes Marshall & Swift and CEPCI over the years [6].

The evolution of the annualization factor with regard to the lifetime n and the interest rate i is given in the Figure 6.8. This factor represents the equivalent lifetime if the inflation and the expected profit are accounted. It is therefore expressed in years.

6.2.3 Total cost and profit

The profit of a project corresponds to the difference between the total operating cost of the installation and the total cost after the completion of a project producing an income B over a period of n years with an investment of I. In this case, the initial investment before the project is zero and the profit over the duration of the project is expressed in discounted francs (CHF). To calculate the annual profit, the investment has to be annualized (Eq. 6.10).

$$Profit = C_{tot,o} - C_{tot} = \left[I_o + C_o \cdot \frac{(1+i)^n - 1}{i \cdot (1+i)^n}\right] - \left[(I_o + \Delta I) + (C_o - B) \cdot \frac{(1+i)^n - 1}{i \cdot (1+i)^n}\right] \quad (6.10)$$

with

I_o	initial investment before the project (I_o=0)
C_o	initial operating cost before the project
B	income from operating cost of the project
ΔI	investment of the project

Different criteria can be used to assess the profitability of a project. The pay-back time (Eq. 6.11) does not allow to compare projects with investments of different sizes. The discounted benefits (Eq.6.12)

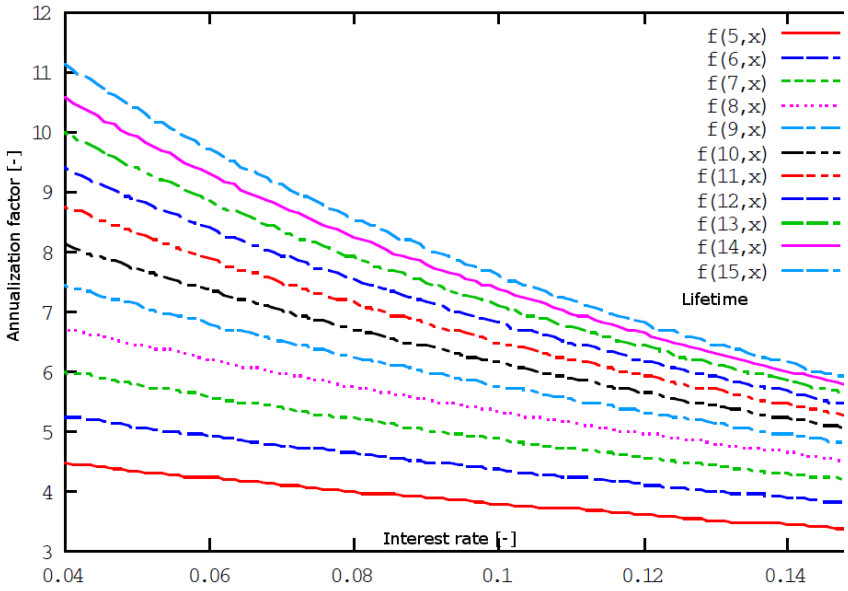


Figure 6.8: Variation of the annualization factor with regard to the interest rate and the lifetime.

and annual benefits (Eq.6.13) must also be compared with the investment. These criteria should be considered as elements of decision: go - no go. The discount rate (i.e annualization rate) i^* of the project (Eq.6.14) represents the profitability of the investment, it corresponds to the interest rate that balances the initial investment. It is therefore a good indicator of profitability. This value is unfortunately difficult to assess and require a graphic or iterative calculation. This value will be then compared to the average rate which is used either by the company that makes the investment or with the average rate for other investments in the same domain. The investment is somehow put into competition.

$$\text{Pay-back time [years]} = \frac{\Delta I}{B} \tag{6.11}$$

$$\text{Discounted benefit [CHF]} = B \cdot \left[\frac{(1+i)^n - 1}{i \cdot (1+i)^n}\right] - \Delta I \geq 0 \tag{6.12}$$

$$\text{Discounted annual benefit [CHF/y]} = B - \left[\Delta I \cdot \frac{i \cdot (1+i)^n}{(1+i)^n - 1}\right] \geq 0 \tag{6.13}$$

$$i^* \text{such as :} \quad B \cdot \left[\frac{(1+i)^n - 1}{i \cdot (1+i)^n}\right] - \Delta I = 0 \tag{6.14}$$

Analysis of the interest rate definition used in the annualization formula

The proposed analysis highly depends on the value that will be adopted for the interest rate i. This value is arbitrary but based on a few elements related to the economic context of the project. The interest or discount rate should reflect inflation, to ensure that the future value is well above the value of money in the future. It must be compared with the interest rate which could be obtained by placing the money in a bank. Investment is initially not a philanthropic operation, the investor therefore has the choice between placing the money in a bank or in a company. The interest rate therefore needs to be higher than the one given by a bank. The value that will be chosen in a company generally results from an analysis of previous investments. It should be noted that economic evaluation of projects allows to compare projects that may have fundamentally different objectives but which can be put in competition at the level of the availability of money in the company.

Typical values are: Lifetime: n = 15 years and Interest rate i = 8-9%.

6.3 Thermo-economic cost function

Generally a thermo-economic cost function will include terms related to the investment (CAPEX), the operating costs and the maintenance costs (OPEX). The annual total costs are expressed by Eq. 6.15. This formula is the result of an integral and reflects the cost in an annualized form. It represents the dynamics of the system and how it responds second-by-second to changes in the environment. It also allows to take into account investments which would be spread over the lifetime of the project. If it can be assumed that the investment is recorded at the time of the commissioning of the installation and that operation is stationary, the formula Eq. 6.15 simplifies and it is possible to define the thermo-economic formulation in terms of annual cost (CHF/year). For practical reasons, this formulation can also be adapted to take into account changes by considering the annual operation of the installation as a succession of stationary states. For example, when evaluating a heating system which depends on the ambient temperature. For a continuous process the formulation is given by Eq. 6.18.

$$C_{tot} = \int_0^{t=n_i} \tau_i(t) \cdot CO(t) \cdot dt + \sum_{i=1}^{n_e} I_i(t) \tag{6.15}$$

with

$t = 1y$	integral over one year
$\tau_i t$	annualisation rate
$CO(t)$	operating cost at time t [CHF/s] (Eq. 6.16
i	interest rate
n_i	lifetime of equipment i
n_e	number of equipments
I_i	investment of equipment i

$$\begin{aligned} CO(t) &= \sum_{i=1}^{n_{in}} \dot{m}_i(t) \cdot P_i^p(t) + \sum_{j=1}^{n_{out}} \dot{m}_j(t) \cdot P_j^s(t) + \dot{E}_{in}(t) \cdot c_{e,in}(t) \\ &- \dot{E}_{out}(t) \cdot c_{e,out}(t) + M(t) + MP(t) \end{aligned} \tag{6.16}$$

with

n_{in}	number of resources (fuels, feedstocks) purchased
$\dot{m}_i(t)$	flowrate of resource i at time t [kg/s]
$P_i^p(t)$	purchase cost of resource i at time t [CHF/kg]
n_{out}	number of products (fuels, feedstocks) sold
$\dot{m}_j(t)$	flowrate of product j at time t [kg/s]
$P_j^s(t)$	sales price of product j at time t [CHF/kg]
	negative if emission which is taxed or waste to be treated
$\dot{E}_{in}(t)$	electricity input at time t [kW]
$c_{e,in}(t)$	electricity purchase cost at time t [CHF/kWh]
$\dot{E}_{out}(t)$	electricity output at time t [kW]
$c_{e,out}(t)$	electricity selling price for exportation to grid at time t [CHF/kWh]
M(t)	annual maintenance cost at time t [CHF/s]
MP(t)	man power cost at time t [CHF/s]

$$C_{tot}[CHF/y] = CO \cdot n_h + \sum_{i=1}^{n_e} \frac{1}{\tau_i} I_i \tag{6.17}$$

$$C_{tot}[CHF/y] = OPEX + \frac{1}{\tau} CAPEX \tag{6.18}$$

with

$\frac{1}{\tau_i}$	annualisation rate $\frac{i(1+i)^n_i}{(1+i)^n_i-1}$
n_h	annual operating time [h/y] (8000-8760h/y continuous operation)
CO	operating cost [CHF/h] (Eq. 6.19
$OPEX$	yearly operating cost [CHF/y]
i	interest rate
n_i	lifetime of equipment i
n_e	number of equipments
I_i	investment of equipment i
$CAPEX$	total investment cost

$$\begin{aligned} CO &= \sum_{i=1}^{n_{in}} \dot{m}_i \cdot P_i^p + \sum_{j=1}^{n_{out}} \dot{m}_j \cdot P_j^s + \dot{E}_{in} \cdot c_{e,in} - \dot{E}_{out} \cdot c_{e,out} \\ &+ M + MP \end{aligned} \tag{6.19}$$

with

n_{in}	number of resources (fuels, feedstocks) purchased
$\dot{m}_i$	flowrate of resource i [kg/h]
P_i^p	purchase cost of resource i [CHF/kg]
n_{out}	number of products (fuels, feedstocks) sold
$\dot{m}_j$	flowrate of product j [kg/h]
P_j^s	sales price of product j [CHF/kg]
	negative if emission which is taxed or waste to be treated
$\dot{E}_{in}$	electricity input [kW]
$c_{e,in}$	electricity purchase cost [CHF/kWh]
$\dot{E}_{out}$	electricity output [kW]
$c_{e,out}$	electricity selling price for exportation to grid [CHF/kWh]
M	annual maintenance cost [CHF/y]
MP	man power cost [CHF/y]

Pollutant	Tax	Avoidance cost	Damage repair cost	Reference
CO_2	12-60	159-227	51-1310	Switzerland
NO_x	8800	-	13800-32270	Sweden

Table 6.1: Example of cost of emissions (in CHF/tonne).

6.4 Environomic cost function

The objective of the environomic cost formulation is to add in the economic objective function terms that allow to take into account the environmental impact of the facility. It is possible to use different formulations with regard to the amount of pollutants emitted by the installation. The first approach is to consider the different pollutants emitted by the facility and associate it with a specific cost. This approach is based on the principle of a tax that is proportional to the amount emitted. The environmental cost term CE or $ENVEX$ is given by Eq. 6.20 taking into account all sources of emissions and discharges from the installation. The objective function becomes Eq. 6.21.

$$CE = \sum_{j=1}^{n_{out}} \dot{m}_j \cdot \left(\sum_{i=1}^{n_j^{pollutants}} x_{i,j} \cdot T_i \right) \tag{6.20}$$

with

n_{out}	number of emissions types
$\dot{m}_j$	flowrate of emission j
$n_j^{pollutants}$	number of pollutants in stream j
$x_{i,j}$	fraction of pollutant i in stream j
T_i	tax for pollutant i [CHF/kg]

$$C_{tot}[CHF/y] = CO \cdot n_h + CE \cdot n_h + \sum_{i=1}^{n_e} \frac{1}{\tau_i} I_i(t) \tag{6.21}$$

The definition of the value T_i is of course difficult. One can consider that this factor represents the price that allows to restore the initial state of the environment in which the facility is located. Different approaches may be proposed, the simplest is the one that is based on the values of applicable taxes. For example, in Switzerland a CO_2 tax of 15CHF/t_{CO2} was introduced in 2008, the tax was increased to 36CHF/t_{CO2} in 2010 and is foreseen to increase to 60CHF/t_{CO2} in 2014 and to around 100-120CHF/t_{CO2} in 2020 (Confédération Suisse 2012 `www.bafu.admin.ch`). These values have to be compared with another approach that would use the avoidance cost or the estimated cost of repair of the damage created by the pollutant (Table 6.1).

To be accurate this approach should be extended to include the impact of the production of raw materials, the production of equipment and the use of products generated by the process. This is done in the life cycle assessment LCA method that is standardized in ISO 14040 &14044 [11, 12]. LCA consists of four main steps: the goal and scope definition, the life cycle inventory (LCI), the impact assessment LCIA and the interpretation. It is important to note that for this evaluation average statistical values will be combined with values obtained from the model. Therefore, one should ensure that the orders of magnitude allow to represent the impacts on which it is possible to act by changing the design of the installation [10]. In this case, the environomic contribution can be expressed by Eq. 6.22 and the objective function will be Eq. 6.23.

$$CE = n_h \cdot \left(\sum_{j=1}^{n_{out}} \dot{m}_j \cdot \left(\sum_{i=1}^{n_j^{pollutants}} x_{i,j} \cdot T_i \right) + \sum_{r=1}^{n_{in}} \dot{m}_r \cdot \left(\sum_{i=1}^{n_r^{pollutants}} x_{i,r}^* \cdot T_i \right) \right) + \frac{1}{n_a} \sum_{e=1}^{n_{eq}} S_e \cdot \left(\sum_{i=1}^{n_{pollutants}} x_{i,e}^+ \cdot T_i \right) \quad (6.22)$$

$$C_{tot}[CHF/y] = CO \cdot n_h + CE + \sum_{i=1}^{n_e} \frac{1}{\tau_i} I_i(t) \quad (6.23)$$

with

n_h	annual operating time [h/y]
n_{out}	number of emissions types
$\dot{m}_j$	flowrate of emission j
$\dot{m}_r$	flowrate of resource r
$n_j^{pollutants}$	number of pollutants in outlet stream j
$n_r^{pollutants}$	number of pollutants in inlet stream r
$x_{i,j}$	fraction of pollutant i in stream j
$x_{i,r}^*$	emission of pollutant i per unit of resource r [kg/kg]
n_a	lifetime of installation
S_e	size of equipment e
n_e	number of equipments
$x_{i,e}^*$	emission of pollutant i for the equipment e per unit of size
T_i	tax for pollutant i [CHF/kg]

In order to take into account the geographical location, one has to consider the fact that the pollutant emitted at a given location can have a different impact when it is issued to another location. In a heavily polluted environment, an additional issue for example can lead to unacceptable pollution levels and should in this case lead to a much greater cost. This can be expressed by Eq. 6.25. This inequality constraint will limit emissions both in terms of quantities and in terms of concentrations. These values are in this case included within the limits to obtain permits to operate the facility.

$$n_h \cdot \sum_{j=1}^{n_{out}} \dot{m}_j \cdot x_{i,j} \leq q_i^{max} \qquad \forall i = 1, ..., n^{pollutants} \quad (6.24)$$

$$x_{i,j} \leq x_{i,j}^{max} \qquad \forall i = 1, ..., n^{pollutants} \forall j = 1, ..., n^{out} \quad (6.25)$$

Chapter 7

Data reconciliation

This chapter introduces the concept of data reconciliation and validation of an industrial process. The major topics that are addressed are: how to calibrate models (use all the information available while respecting the fundamental equations of thermodynamics), place measurements, virtual sensors by process models, correct the values of the measurements (data reconciliation), identify parameters, etc.

7.1 Introduction

The process data are the basis on which rely any control and any assessment of its performance. The data reliability is very important when they are intended for the process monitoring (control, identification, ...). Therefore,consistent data is needed to accurately represent the process and correctly identify the parameters prior to the simulation, optimization or the revamping of a large factory.

The data validation or reconciliation is a very important task that turns the available data in a coherent set defining the state of the process. Today, computers are used to ensure the control of processes. Thus, there is a large number of data, gathered and stored, which can be systematically validated using an ad hoc program increasing the data accuracy and ensuring their coherence.

7.1.1 Sources of measurement errors

Process measures are never consistent. The main reasons are:

- There are disturbances due to the instability of the process even if the control system is very effective. Certain conditions (such as weather) cannot be controlled.
- Measurement devices are not always reliable. Instrumental biases may not be compensated adequately; measuring devices may be defective.
- The readings of the measures and manipulations (laboratory testing) can introduce errors.
- The experimental point can be influenced by undesirable elements and the measure does not correspond to the expected variable (bad position of a thermocouple, influence of the flow distribution in a heat exchanger, effect of a condensate in a vapor stream, dirt on a measuring device).
- Accidents may change the expected balances of a process (losses, bursting of a heat exchanger, heat loss,...).

7.1.2 Definition of a process state

To set the state of an industrial facility, many measures of variables describing the system such as temperature, pressure, flowrate, composition, etc., have to be made. When the number of measures is less than a given threshold (called number of specifications), it is not possible to define the state of the system

(see previous Chapters). Eventually, the state of a subsystem can be defined. As far as these measures are selected carefully and that their number equals the number of specifications, the mass and energy balances can be used to calculate the other variables of the system. In such circumstances, a systematic measurement error, even if minimal, can bias, sometimes dramatically, the calculations of the other variables of the system (i.e. introduce great errors). As a result, additional measurements have to be made to increase the confidence level of the system. It is then no longer possible to satisfy all the equations of the system, and consequently a technique for analyzing the measurements has to be applied.

The data reconciliation method developed in the BELSIM software, helps to solve this huge problem. To validate the data, the process, the measurements and the standard deviations estimates (errors) affecting each measurement are stored in a database.

Illustration

As an example, the mixing of two stream containing a pure substance is considered (Figure 7.1). The temperature and pressure of the inlet streams are different. The number of specifications necessary to explicitly define the state of the system is DOF=7.

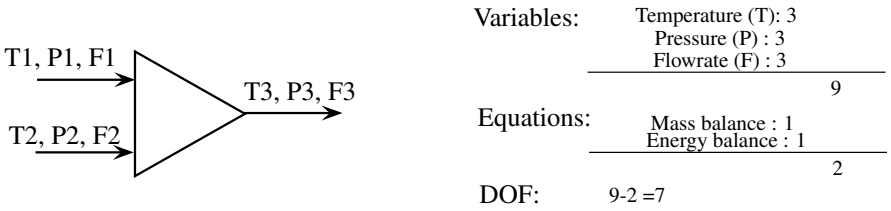


Figure 7.1: Illustrative example

If less than 7 measurements are made, it is not possible to completely determine the state of the system.

- 1st case: 6 variables are measured: P1, P2, P3, T1, T2, F3. In this case, it is not possible to know more about the system.
- 2nd case: 6 variables are measured: P1, P2, P3, T1, F2, F3. The flowrate F1 can be calculated through the mass balance. A subsystem (F1) of non-measured variables is calculable. The temperatures T2 and T3 cannot be assessed.
- 3rd case: 7 variables are measured: P1, P2, P3, T1, T2, T3, F1. The values are T1=300 K, T2=410 K, T3=310 K, P1=P2=P3=1 bar, F1=10 kg/s. Based on the mass and energy balance two non-measured variables: F2 and F3 can be calculated. The system is now completely known, but a systematic error in the measurement of temperature T3 can bias the knowledge of the system. Assuming a constant cp, the flowrates of F2 and F3 are at T3=310 K, F2=1 kg/s and F3=11kg/s and at T3=305 K, F2=0.48 kg/s and F3=10.48 kg/s, respectively. A systematic error of 5 degrees on the measurement of T3 will give a very bad evaluation of F2.

For analyzing the specification and measurement sets, the DOF has to be defined and the following questions have to be addressed:

- Are there enough specifications? If no, where do the missing specifications have to be placed? If yes, what are the extra specifications?
- Are there enough measurements ? Can the model be solved? Are additional measurements needed? What to do if more measurements are available?

7.2 Theory

This chapter gives a brief overview of the theoretical bases of the validation, explaining the techniques and the formalism used (variables, constraints, linking equation, how to analyze the incidence matrices

and the resolution method. More details about the problem statement and resolution are found in the previous Chapters.

7.2.1 Definitions

State variables

The state variables are the variables involved in the equations, mainly mass and energy balances, associated with the physical units of the process. The state variables that are commonly used (also in BELSIM) are:

- T: the temperature of the mixture, if the material stream is involved in a heat balance. NOTE: The temperature variable is advantageously replaced by the molar enthalpy H variable for biphasic flow of a single substance, since the enthalpy uniquely defines the thermodynamic state.
- P: the pressure of the mixture, if it plays a role in heat balance. Very often it is not possible to validate measurements of pressure and these are considered constants.
- Ci (i=1, number of substances): partial molar flowrate of the substance i in the mixture.
- Uj (j=1, number of reactions): extent of the reaction j.
- FRA: split fraction, for example for a splitter, the variable is used when a stream is divided into several other streams with the same composition (0<FRA<1).

All other variables (enthalpy, mole fraction, etc.) can be deduced from the state variables (as far as thermodynamic methods describing the mixture are defined). The state of the system is known once the values of the state variables are known for each stream of the system.

Example: The flowsheet shown in Figure 7.2 is composed of 4 physical units and of 9 streams. The list of state variables is given in Table 7.1; to specify the conversion of CH_4, the state variable of the reactor $U1$ is added.

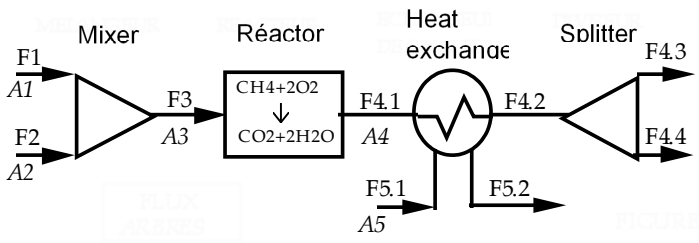


Figure 7.2: Example considered for data reconciliation.

Stream	Variables	Tree	Variables
F1	T, P	A1	O_2, N_2
F2	T, P	A2	CH_4, N_2
F3	T, P	A3	O_2, N_2,CH_4
F4.1	T, P	A4	O_2, N_2,CH_4, CO_2, H_2O
F4.2	T, P		
F4.3	T, P, FRA		
F4.4	T, P, FRA		
F5.1	H, P	A5	H_2O
F5.2	H, P		

Table 7.1: State variables of the example reported in Figure 7.2. The partial molar flowrates associated to a material stream are called tree.

Measured or observed variables

These variables are those that are measured in the plant. To each measurement corresponds an estimate of the standard deviation of the measurement error, and each measurement is considered to be a system variable. Some of these variables are already included in the system state variables; others, called linking variables, are related to the state variables by specific equations: the conversion equations or the linking equations. This is for example the case of the total molar flow $FMOL$, which is connected to the partial molar flow by the equation: $FMOL = \sum_k C_k$ or, the mole fraction FM_k of the substance k given by: $FM_k \cdot \sum_i C_i = C_k$.

Constraint equations

The constraints equations are: the mass and energy balance, the linking equations, but also special equations (liquid-vapor equilibrium equations, equations of equal pressures or temperatures, etc.).

Example: The mixer in Figure 7.2 has two input streams, whose temperatures are T_{F1} and T_{F2}. The variables $O2_{A1}$ and $O2_{A2}$ are the partial molar flowrates of the first input stream (tree A1). The variables $N2_{A2}$ and $CH4_{A2}$ represent the partial molar flowrate of the second input stream (tree A2). The first output stream is characterized by temperature T_{F3} and the partial molar flowrate $O2_{A3}$, $N2_{A3}$ and $CH4_{A3}$. The pressures are constant. Three material balances have to be written:

$$\begin{aligned} O2_{A1} - O2_{A3} &= 0 \quad \text{for the substance O2} \\ N2_{A1} + N2_{A2} - N2_{A3} &= 0 \quad \text{for the substance N2} \\ CH4_{A2} - CH4_{A3} &= 0 \quad \text{for the substance CH4} \end{aligned}$$

The energy balance is expressed by the enthalpy equation:

$$h(T_{F1}, O2_{A1}, N2_{A1}) + h(T_{F2}, N2_{A2}, CH4_{A2}) - h(T_{F3}, O2_{A3}, N2_{A3}, CH4_{A3}) = 0$$

The following linking equation has to be written if the mole fraction of the O2 substance is measured in the output stream.

$$FMO2_{A3} \cdot (O2_{A3} + N2_{A3} + CH4_{A3}) - O2_{A3} = 0$$

Therefore, the state variables of the problem are: $F_1, F_2, T_{F3}, O2_{A1}, N2_{A1}, N2_{A2}, CH4_{A2}, O2_{A3}, N2_{A3}, CH4_{A3}$ while $FMO2_{A3}$ is a linking variable.

7.2.2 Problem statement

The data reconciliation is based on the following assumption. All measurements are affected by errors and corrected or validated values differ from the measured values. On the one hand, the validated values must satisfy the constraint equations, and, on the other hand, they have to minimize the sum of squares of the differences between the validated values and the measured values. These differences are weighted by the corresponding standard deviations. From a mathematical point of view, this is a constrained minimization problem, which is defined as follows.

Are:

y , the vector of measured values (size **MES**);

Y, the vector of the corrected or validated values;

X, the vector of the not measured values which have to be calculated (size **NMES**) ;

F(X,Y), the vectorial function of the balance equations (size **NEQ**) ;

P , weighting matrix which allows to quantify the relative accuracy of the measurements MES. In practice, it is a diagonal matrix whose elements are the inverse of the variance σ_i of the measurement i.

The minimization problem is defined by Eq. 7.1:

$$\sum_{i=1}^{MES} \frac{(Y_i - y_i)^2}{\sigma_i^2} \quad \text{with the constraint} \quad F(X,Y) = 0 \tag{7.1}$$

In matrix notation this becomes Eq. 7.2:

$$M_{X,Y}(Y-y)^T P(Y-y) \quad \text{with} \quad F(X,Y) = 0 \tag{7.2}$$

This constrained minimization problem is solved by the Lagrangian method involving 'Lagrange multipliers' for each equation, expressed by Eq. 7.3 (the factor 2 is introduced for the sake of convenience, as we will see later):

$$M_{X,Y,\lambda} L \quad \text{with} \quad L = (Y-y)^T P(Y-y) + 2\lambda F(X,Y) \tag{7.3}$$

The resolution of the Euler equations gives the solution of the problem. The Euler equations are written:

$$\begin{aligned} \frac{\delta L}{\delta Y_i} &= 0 \qquad i = 1, MES \\ \frac{\delta L}{\delta X_i} &= 0 \qquad i = 1, NMES \\ \frac{\delta L}{\delta \lambda_i} &= 0 \qquad i = 1, NEQ \end{aligned}$$

The Jacobian matrices of the measured variables and non-measured variables are:

$$Aij = \frac{\delta F_i}{\delta Y_j} \text{ and } Bij = \frac{\delta F_i}{\delta X_j}$$

The following equations system is obtained:

$$\begin{aligned} (Y-y)^T P + \lambda^T A = 0 \qquad & \text{MES equations} \\ \lambda^T B \qquad & \text{NMES equations} \\ F(X,Y) = 0 \qquad & \text{NEQ equations} \end{aligned}$$

Which is a system of MES+NMES+NEQ non-linear equations with MES+NMES+NEQ unknowns. A necessary step for all resolution methods is to assess the total Jacobian matrix of this system of equations written as (if one neglects the dependence of A and B with respect to Y and X):

$$\mathrm{J}= \left|\begin{array}{ccc|l} P & 0 & A^T & \text{MES lines} \\ 0 & 0 & B^T & \text{NMES lines} \\ A & B & 0 & \text{NEQ lines} \end{array}\right.$$

Variables		Measurements	Standard deviation
Y1	$O2_{A1}$	1	0.01
Y2	$N2_{A1}$	2	0.01
Y3	$N2_{A2}$	3	0.01
Y4	$CH4_{A2}$	4	0.01
Y5	$FMO2_{A3}$	0.2	0.01
X1	$O2_{A3}$	-	-
X2	$N2_{A3}$	-	-
X3	$CH4_{A3}$	-	-

Table 7.2: Measured values and the corresponding standard deviations for the example reported in Figure 7.2.

Example: Consider the validation of flowrate measurement around the mixer of Figure 7.2. The measured values and the corresponding standard deviations are given in Table 7.2.

The data reconciliation problem becomes:

$$MIN_{X,Y}\left[\frac{(Y1-1)^2}{0.01^2}+\frac{(Y2-2)^2}{0.01^2}+\frac{(Y3-3)^2}{0.01^2}+\frac{(Y4-4)^2}{0.01^2}+\frac{(Y5-0.2)^2}{0.01^2}\right]$$

with the constraints:

$$\begin{aligned} Y1-X1 &= 0 \\ Y2+Y3-X2 &= 0 \\ Y4-X3 &= 0 \\ Y5\cdot(X1+X2+X3)-X1 &= 0 \end{aligned}$$

and

$$A=\begin{pmatrix}1&0&0&0&0\\0&1&1&0&0\\0&0&01&0&\\0&0&0&0&\sum X_i\end{pmatrix} \qquad B=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\\Y5&Y5&Y5\end{pmatrix}$$

7.2.3 Existence of a solution

On the basis of the constraint equations it can be noted that:

1. The system accepts an infinite number of solutions if the number of non-measured variables is greater than the number constraint equations (**NMES>NEQ**). In this particular case the **matrix B is rectangular and horizontal** (more columns than rows) and the Jacobian matrix is singular, since lines MES+1 to MES+NMES are always linearly dependent. The system is **not soluble**.

2. If the number of non-measured variables equals the number of constraint equations (**NMES=NEQ**), the solution of the problem is obtained by considering the measurements as constants and by calculating the non-measured variables using the constraint equations. The system is just computable because there are not enough equations to correct the measurements. The **matrix B is square**.

3. If the number of non-measured variables is smaller than the number of constraint equations (**NMES<NEQ**), the system has a unique solution. The constraint equations are not only used to calculate the non-measured variables, but also to reconcile the measurements. The **matrix B is rectangular vertical** (more rows than columns).

To find a solution, the matrix B should not be rectangular horizontal. In fact, the Jacobian matrix should not be singular, what happens for example,

- If the constraint equations are linearly dependent.
- If the measurements are poorly distributed and certain parts of the process remain undetermined.
- If variables that are put constant are not well-chosen and create an over specification.

In most of the cases, a careful analysis of the systems incidence matrix allows to detect these problems prior to the resolution. The incidence matrix is the matrix whose elements ij are 1 if the variable j occurs in the equation i, otherwise 0.

Example. The incidence matrix of the measured and non-measured variables of the mixer (Figure 7.2 and Table 7.2) is:

$$AB = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$$

Caution: Although this analysis is satisfactory, the equations system, the starting points and the measured values can be such that the program fails to converge to a solution or the solution is located outside the eligible area (defined by physical ranges of variables: temperatures and positive flows,...), or that the system become locally singular during the iteration. This type of problem is explained in more detail in the chapter dealing with the convergence problems.

7.2.4 Incidence matrix analysis

Validity of the constraint equations

The analysis of a system of equations by the means of its incidence matrix is tricky. Indeed, two identical equations will appear as two equations involving the same variables and not as an error. Similarly, a subset of linearly dependent equations cannot be pointed out in an incidence matrix. The chances of encountering such singularities are mostly eliminated if the equations are automatically generated by the software. The verification of certain conditions eliminates the generation of errors in the equations. For example, each stream cannot be connected to more than two physical units; it is necessary to have at least one input stream and one output stream.

Are there enough measurements?

After generation of the measurements and the linking equations, the variables are divided into three categories:

- Variables specified as constants (called also constants)
- Measured variables
- Not measured variables

To determine if the measures allow, at least, to determine the state of the system, the incidence matrix 'equations-not measured variables' corresponding to the matrix B is analyzed. The approach consists in permuting the rows and columns in such a way to get a subsystem $S2$ containing a sub-matrix B2' and a **horizontal sub-matrix B2"** (Figure 7.3). The sub-matrix B2" being horizontal, there are not enough equations containing the non-measured variables (unknowns) with respect to the matrix B2". Therefore, the non measured variables of B" cannot be determined (they occur in too few equations).

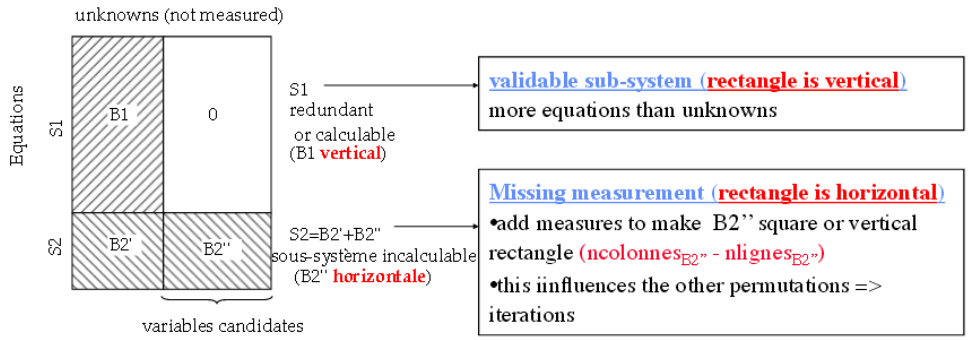


Figure 7.3: Incidence matrix of non-measured variables: Non-calculable system

To make the system calculable, an additional measurement has to be chosen from the variables of the sub-matrix B2". This variable will be added to the measured variables and the corresponding column in the sub-matrix B2" will be eliminated. When a measure is selected, one repeats again the procedure of searching for a non-calculable subsystem.

Can the measurements be validated?

Consider now that sufficient additional measurements have been made to ensure that the system can be solved (positive or zero redundancy). Let's again analyze the incidence matrix and permute lines and columns or vice and versa to try to isolate a sub-system of equations S2 containing a sub-matrix B2' and a **square sub-matrix B2"** (Figure 7.4). The non-measured variables associated with the matrix B2" are just computable because there are just enough equations to calculate them.

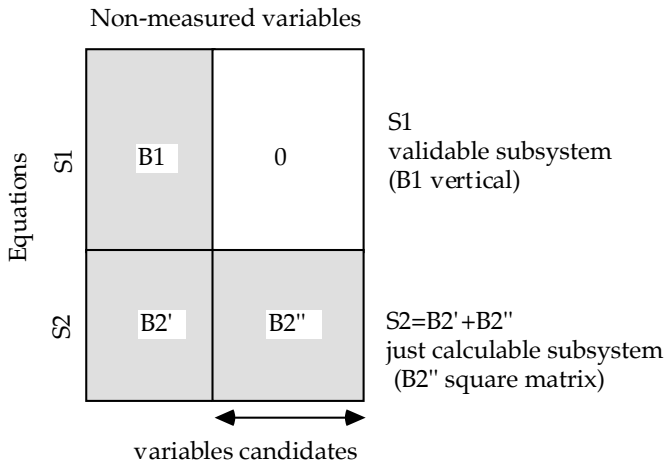


Figure 7.4: Incidence matrix of non-measured variables: Calculable system.

In the global incidence matrix corresponding to "equations-variables measured and not measured" the columns of the measured variables involved in the equations of the subsystem S1 are added at the left side (Figure 7.5). The remaining measured variables cannot be validated because their values can be arbitrarily fixed to their measured values: no equation allows to correct them.

Example: Figure 7.6 shows a process containing three units. The three substances are separated in the unit A before entering the reactor B. The unit C separates the reaction products. In this case, we consider that there is not enough measurements around the units A and C. The energy balance is only generated for the reactor B while the mass balances are generated for all the units. Figure 7.7 shows the

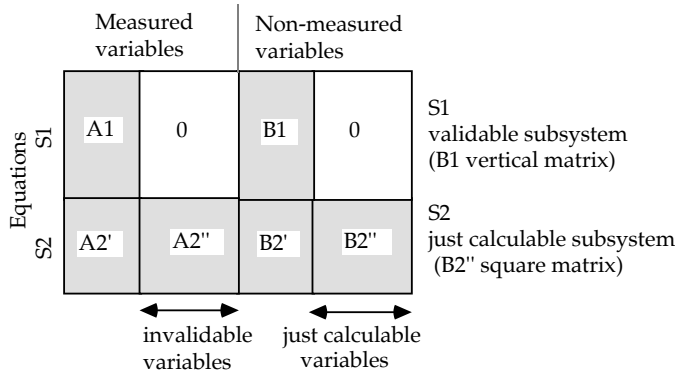


Figure 7.5: Global Incidence matrix: Calculable system.

corresponding incidence matrix.

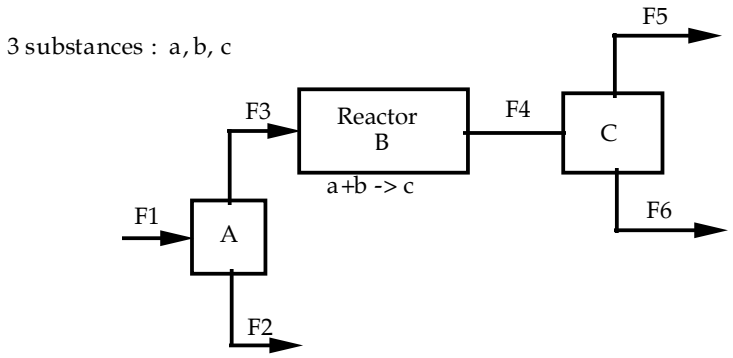


Figure 7.6: Flowsheet.

Mass balance	A a	X		X		X					
	A b		X		X		X				
	A c		X		X		X				
Mass balance	B a					X		X			
	B b						X		X		
	B c						X		X		
Energy balance	B					X	X	X	X	X	X	X	X
Mass balance	C a							X			
	C b								X		
	C c								X		

Figure 7.7: Incidence matrix.

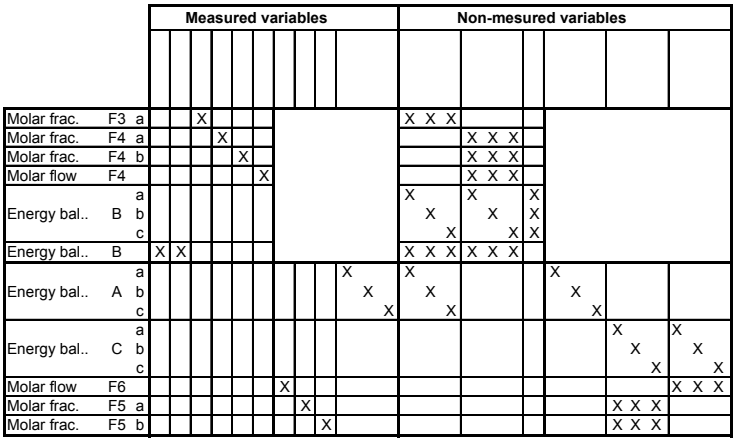


Figure 7.8: Incidence matrix.

Figure 7.8 shows the measurements that can not be validated when the measured variables are:

- Temperature of the streams F4 and F5
- Total molar flowrate of the streams F4 and F6
- Mole fraction of the substance a in streams F3, F4 and F5
- Mole fraction of the substance b in the streams F4 and F5
- Molar partial flowrate of substances a, b and c in the stream F1

Are there over-specifications?

Consider a system whose resolution seems possible (positive or zero redundancy) and in which constants have been introduced for certain measurements with a very small standard deviation. During the resolution, the variables corresponding to these measurements will be ignored and considered as real constants. However, these constants might not be well chosen and the problem will be overspecified. The analysis of the incidence matrix "equations-variables" and the permutation of lines and columns allows to isolate a subsystem of equations S1 whose matrix is vertical (Figure 7.9). Variables associated with this matrix are overspecified because there are too many equations to solve.

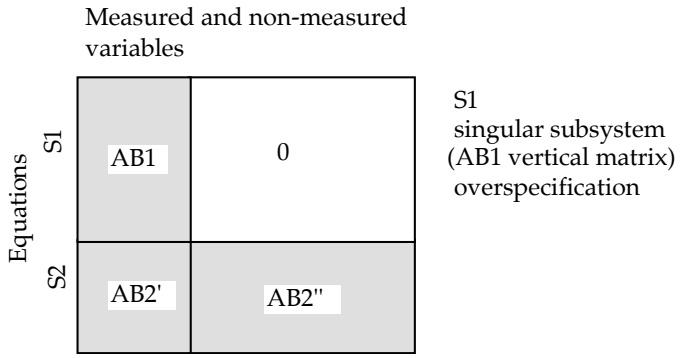


Figure 7.9: Incidence matrix: Overspecification.

In the global incidence matrix corresponding to "equations-variable+constants" the columns of the constants involved in the equations of the S1 subsystem are added to the right (Figure 7.10). The constants to make variable must be selected from these columns.

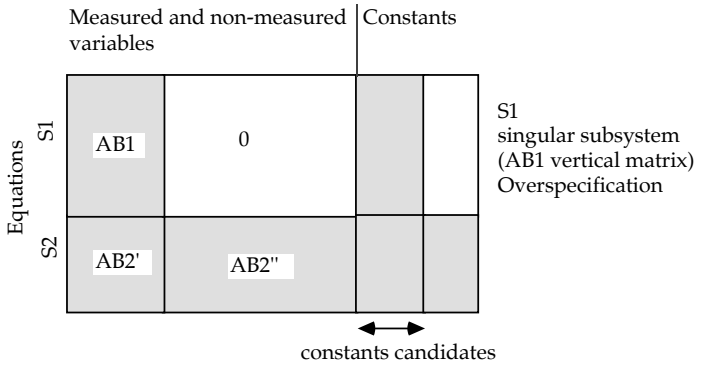


Figure 7.10: Global incidence matrix: Overspecification.

Search for trivial redundancy

The incidence matrix corresponding to "equations-variables" is analyzed and by permutation of the lines and columns a subsystem of equations S1 whose matrix is squared is isolated (Figure 7.11). The variables associated with this matrix are just calculable because there are just enough equations to calculate them. If among these variables there are measured variables, their computed values are independent of the measured values and these measures are worthless, they generate trivial redundancy.

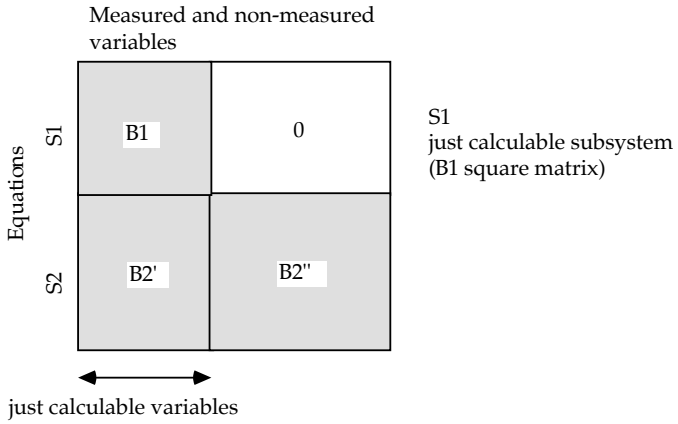


Figure 7.11: Incidence matrix: Trivial redundancy.

Linear dependence in a subsystem

When a part of the flow-sheet generates a just computable subsystem (square sub-matrix), the non-measured variables, apparently just calculable, may be indeterminable. This is the case of loops in which no action is given but for which it is necessary to measure a mass flowrate or thermal load to assess what 'turns' in the loop. A loop is identified when a series of non-oriented streams forms a loop. It is the case of recycling but also when a mixture is done on previously separate streams. Mathematically, the square matrix is numerically singular, which can be detected by analysis of the incidence matrices. This singularity can be highlighted by transforming the balance equation of one of the units of the loop in a global balance around all units of the loop.

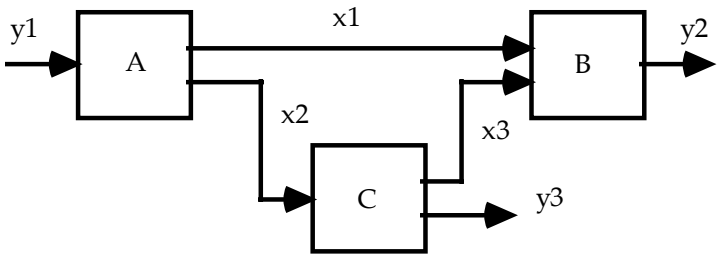


Figure 7.12: Example: Flowsheet with loops.

Example For the example illustrated in Figure 7.12:

Measured flowrates	Y1, y2, y3	
Non-measured flowrates	x1, x2, x3	
Mass balance equations		Jacobian matrices:
unit A	y1-x1-x2=0	
unit B	x1+x3-y2=0	
unit C	x2-x3-y3=0	

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad B = \begin{pmatrix} -1 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix}$$

The indencidence matrix 'equations-non measured variables' (matrix B) is obviously not singular but it is numerically singular. Indeed, a singular incidence matrix is obtained by replacing the mass balance equation of unit C by the overall mass balance equation:$y1 - y2 - y3 = 0$. The corresponding Jacobian matrices are:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & -1 & -1 \end{pmatrix} \qquad B = \begin{pmatrix} -1 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

Another method would be to separate the square matrix in triangular blocks and check, for each of them, that all variables and equations of a given block are not involved in a 'loop': this problem has been solved for a recycling of material. However, it should be noted that detecting such singularities becomes a very difficult task when one is faced with recycling of heat and matter.

The flow-sheet of Figure 7.13 highlights a case of material and heat indeterminacy. The singularity is located in the square block in the right corner of Figure 7.14. The analysis of such a system requires some experience in validation of flowsheets.

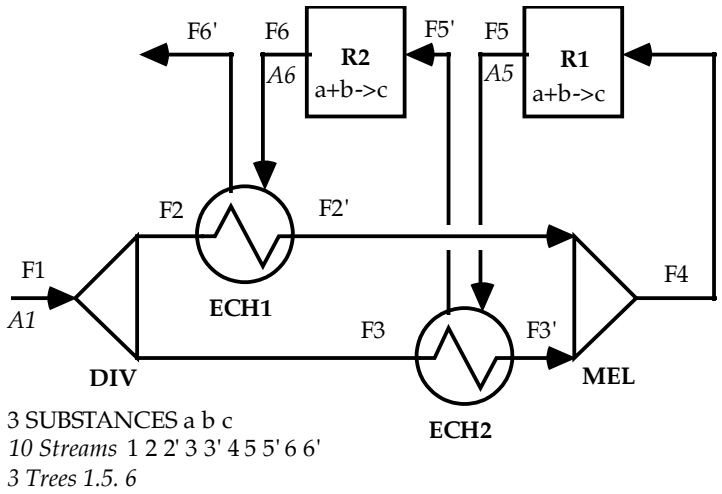


Figure 7.13: Example: Flowsheet with loops (heat and matter).

			Measured variables							Non-measured variables								
R1	Mass balance	a	X							X	X							
		b		X							X		X					
		c			X							X	X					
R1	Energy bal..		X	X	X		X	X			X	X	X						
R2	Mass balance	a								X				X		X		
		b									X				X	X		
		c										X				X		
R2	Energy bal.							X	X		X	X	X		X	X	X		
DIV	Energy bal.	1			X												X		
	Energy bal.	2			X													X	
	Mass balance																	X	X
ECH1	Energy bal.		X	X	X				X	X				X	X	X		X	
ECH2	Energy bal.		X	X	X			X	X		X	X	X				X		X	
MEL	Energy bal.		X	X	X		X											X	X	X

Figure 7.14: Incidence matrix of example with heat and matter loops.

7.2.5 Numerical method

The system is solved by a DOGLEG method. This implies that the correction made in the assessment of the currentsolution is a combination of the correction of Newton and the direction of steepest descent for the squared sum of the residuals of the equation system. Without going into the details, we can say that the passage towards the direction of the greatest slope is even more important that the reduction of the squared sum of the residuals in the direction of Newton is small, when it is not completely zero.

The calculation of the Jacobian matrix required to determine these directions is partly analytical and partly numerical. To save the calculation time, this matrix is not calculated at each iteration but according to a chosen frequency. Its calculation also depends on the speed at which the solution is approached. The matrix is stored using a technique of storage for sparse matrices; only non-zero matrix elements are stored.

It is reminded here that the second derivatives of the constraints over the measured and non-measured variables is neglected. If the new point proposed by the method is outside the validity domain, the software brings the point back within the area of validity by relaxing the proposed step. Depending on the case, all variables are subject to relaxation, or only those who violate the physical constraints.

In almost all cases, the non convergence is to be attributed to the poor quality of the measurements, or

to a lack of measurements which has not been detected by the analysis of the incidence matrix.

7.3 Sensitivity analysis

Previously, it has been shown that the validation problem (data reconciliation problem) can be expressed as a constrained minimization problem. The subsequent developments imply that the constraints are linear or that they have been linearized:

$$\begin{aligned} & min_{X,Y}(Y-y)^T P(Y-y) \\ \text{subject to the constraint: } & AY + BX + C = 0 \end{aligned}$$

The problem with constraints can also be transformed into a non-constrained problem by using the Lagrange formulation:

$$min_{X,Y\lambda}(Y-y)^T P(Y-y) + 2\lambda^T(AY + BX + C)$$

Thus, the following system of equations is obtained:

$$\begin{aligned} PY + A^T\lambda &= Py \\ B^T\lambda &= 0 \\ AY + BX &= -C \end{aligned}$$

A square matrix M and vectors V and D can be defined such that:

$$M = \begin{pmatrix} P & 0 & A^T \\ 0 & 0 & B^T \\ A & B & 0 \end{pmatrix} \quad V = \begin{pmatrix} Y \\ X \\ \lambda \end{pmatrix} \quad D = \begin{pmatrix} Py \\ 0 \\ -C \end{pmatrix}$$

In this way, the solution of the validation problem is written:

$$V = M^{-1}D$$

7.3.1 Sensitivity matrix

The matrix M^{-1} is the sensitivity matrix of the system. The vectors X and Y are linear combinations of the measured values y. The sensitivity matrix allows to evaluate how the validated value of a variable depends on all the measured variables and their standard deviations. In particular:

$$\begin{aligned} Y_i &= \sum_{j=1}^{m+n+p} (M^{-1})_{ij} D_j \\ &= \sum_{j=1}^{m} (M^{-1})_{ij} P_{jj} y_j - \sum_{k=1}^{p} (M^{-1})_{i,n+m+k} C_k \\ X_i &= \sum_{j=1}^{m+n+p} (M^{-1})_{n+i,j} D_j \\ &= \sum_{j=1}^{m} (M^{-1})_{n+i,j} P_{jj} y_j - \sum_{k=1}^{p} (M^{-1})_{n+i,n+m+k} C_k \end{aligned}$$

The variance of a linear combination Z of multiple variables X_j is calculated as follows:

$$\begin{aligned} Z &= \sum_{j=1}^{m} a_j \cdot X_j \\ var(Z) &= \sum_{j=1}^{m} a_j^2 var(X_j) \end{aligned} \tag{7.4}$$

The estimation of the variance of the validated measured variables is given by:

$$var(Y_i) = \sum_{j=1}^{m} \left\{ (M_{ij}^{-1} P_{jj} \right\}^2 var(y_j)$$

and for the estimation of the variance of the non-measured variables:

$$var(X_i) = \sum_{j=1}^{m} \left\{ (M_{n+i,j}^{-1} P_{jj} \right\}^2 var(y_j)$$

These expressions can be simplified by knowing that:

$$var(y_i) = \frac{1}{P_{jj}}$$

and therefore:

$$\begin{aligned} var(Y_i) &= \sum_{j=1}^{m} \frac{(M^{-1})_{ij}^2}{var(y_j)} \\ var(X_i) &= \sum_{j=1}^{m} \frac{(M^{-1})_{n+i,j}^2}{var(y_j)} \end{aligned} \tag{7.5}$$

7.3.2 Conclusions

The purpose of data reconciliation and validation is to improve the knowledge of the state variables of the system. Providing values is of course a great help, but evaluating their reliability is equally important. With this in mind that standard deviations for the validated variables and those not measured have been developed.

Three types of questions can be analyzed by using sensitivity analysis:

- Check how the accuracy of a given state variable is influenced by the set of measurements: What are the measurements that significantly contribute to the variance of the validated result for a set of state variables?
- Determine the state variables whose precision is the most influenced by a given measurement: What are the state variables whose variance is influenced significantly by the precision of a given measurement?
- Study how the value of a state variable is influenced by the value and the standard deviation of the set of measurements.

From this information, decisions can be taken either for the analysis of the measurements of an existing process, or during the design of a measuring system. Unnecessary analysis may be eliminated or made less frequently, thus reducing the operating cost. One can also identify the key measurements for which an accuracy improvement would allow better monitoring of the process. One can also determine the location of the sensors to get a good estimate of all the key variables of the process at the lowest investment cost.

7.4 Summary

The key points of data reconciliation are summarized here and illustrated in Figure 7.15.

- Corrects the measurement values (most probable consistent values)
- Consistent with heat and mass balances and thermodynamic laws
- Considers balances as additional measures
- A posteriori precision of each value (measured and non-measured)
- Precision of performance indicators
- Sensitivity of measurements on performance indicators
- Quality of sensors

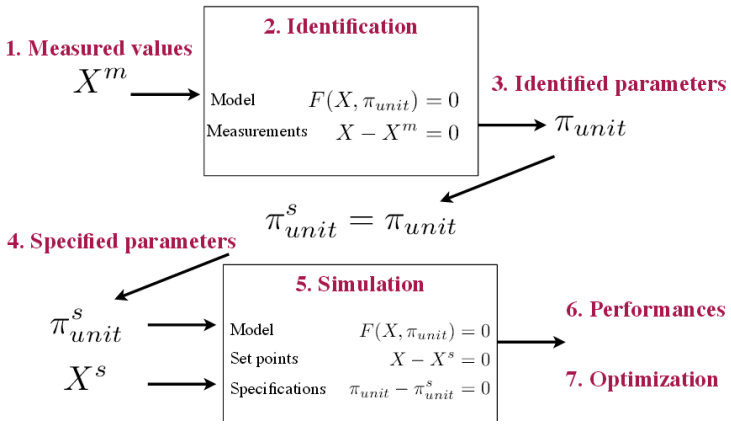


Figure 7.15: Measurement and parameter identification.

The analogy between measurements and DOF analysis is compared in Table 7.3.

DOF analysis	Measurements system analysis
-specifications	-measurements
-over-specifications	-redundancy
(spec to be suppressed)	(more information)
-under-specifications	-missing measurements
(add specs)	(add measures)

Table 7.3: Analogy between measurements and DOF analysis.

More information about data reconciliation are found in the lecture notes of Prof. Georges Heyen at University of Liège `http://www.lassc.ulg.ac.be/webCheng00/meca0468-1/Validation_intro.pdf` and `http://www.lassc.ulg.ac.be/webCheng00/meca0468-1/Validation_review.pdf` or in [19]

Chapter 8

Model resolution: Mathematical methods

This chapter recalls the main methods for solving nonlinear equations systems in the context of solving energy system models or unit models. These methods have been presented in detail in the numerical analysis course. This chapter is divided into two parts: a) the resolution of an equation with an unknown (1 dimensional) and b) the resolution of an equation system (n dimensions). The most important methods such as Newton-Raphson, Wegstein, Rubin and Runge-Kutta are described.

8.1 Resolution of 1 dimensional problems

The resolution of two types of equations is considered: explicit equations (f(x)=0) and the implicit equations (x=f(x)). For the first type, the Newton-Raphson method and the Chord method are described, while for the second type, the Wegstein method is described.

8.1.1 Newton-Raphson method

Description

The equation f(x)=0 has to be solved, knowing an approximate value x^0 of the solution x^*. A Taylor development gives:

$$f(x) = f(x^0) + (x - x^0)f'(x^0) + \frac{(x - x^0)^2}{2!}f''(x^0) + ...$$

where $f', f'', ...$ are the first, second,... derivative of the function f.

The Newton's approximation consists in neglecting the terms of order higher than one assuming that x^0 is sufficiently close to the solution x^* and replacing the initial equation by the following approximate linear equation:

$$f(x^0) + (x - x^0)f'(x^0) \cong f(x^*) = 0$$

A value close to the root is given by:

$$x^1 = x^0 - \frac{f(x^0)}{f'(x^0)}$$

This value must be a better estimation of the solution (this is not always the case!). To find the solution, the recursion formula is used:

$$x^{n+1} = x^n - \frac{f(x^n)}{f'(x^n)}$$

Geometrical interpretation

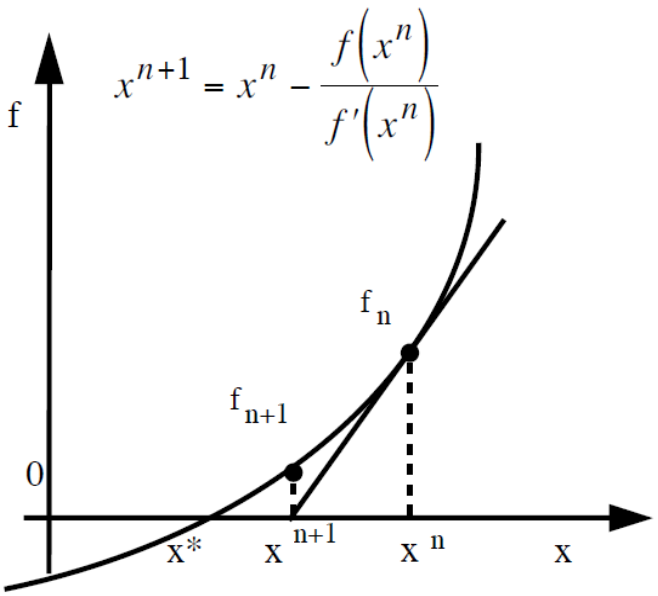


Figure 8.1: Geometrical interpretation: Newton's method (1 dimension).

Representing the curve $y = f(x)$ in the coordinates system Oxy, the equation of the tangent to the curve at the point f_n with the x-coordinate x^n is:

$$y - f(x^n) = (x - x^n)f'(x^n)$$

The intersection of the tangent with the x-axis (y=0) is (assuming that $f'(x^n) \neq 0$) :

$$x^n - \frac{f(x^n)}{f'(x^n) = x^{n+1}}$$

In the same way x^{n+2}, x^{n+3} are obtained by drawing the tangents to the points f_{n+1} , f_{n+2}, ... and in seeking the intersection with the x-axis (Ox). That's why the Newton's method is also called the tangent method.

Remarks

- Note that the successive values of x are found taking into account the signs of f(x) and f'(x). In this case, to avoid divergence, a second form of recurrence inspired by Wegstein (see below) can be used: $\tilde{x}^{n+1} = q \cdot \tilde{x}^n + (1 - q)x^{n+1}$ (relaxation). This means in the example given before, that, on the tangent through f_0, one stops at a point defined by the value of q. q is known as relaxation factor, if q=*0* full step, if q» small steps and more iterations, if q« Newton step (direct convergence if linear problem).
- The disadvantage of the Newton-Raphson method is that it requires the calculation of derivatives and a good initial point.

- If the function f(x) presents an extrema, it may happen that the method is divergent (Figure 8.2).

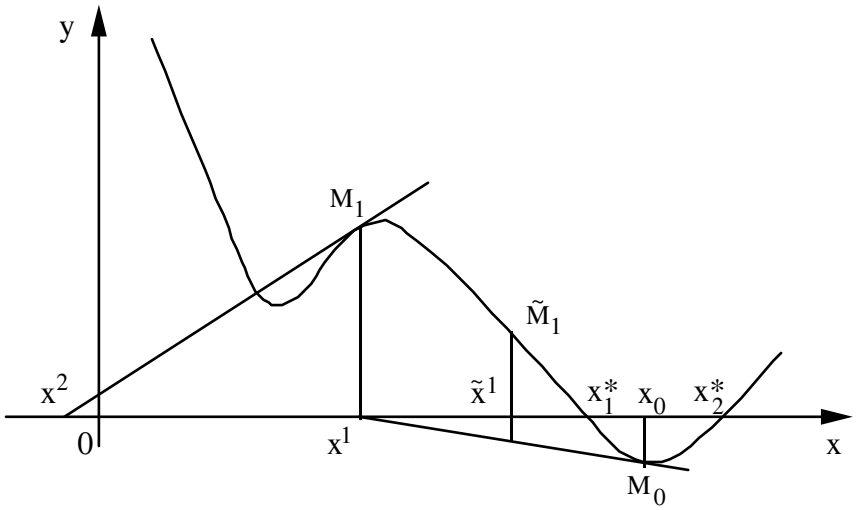


Figure 8.2: Newton-Raphson method: divergence problem (multiple solution, wrong starting point).

To accelerate the convergence, one can take an ausculatrice of the quadratic curve instead of assimilating the curve at a point to its tangent, this is the Richmond method.

8.1.2 Chord method or Regula-Falsi method

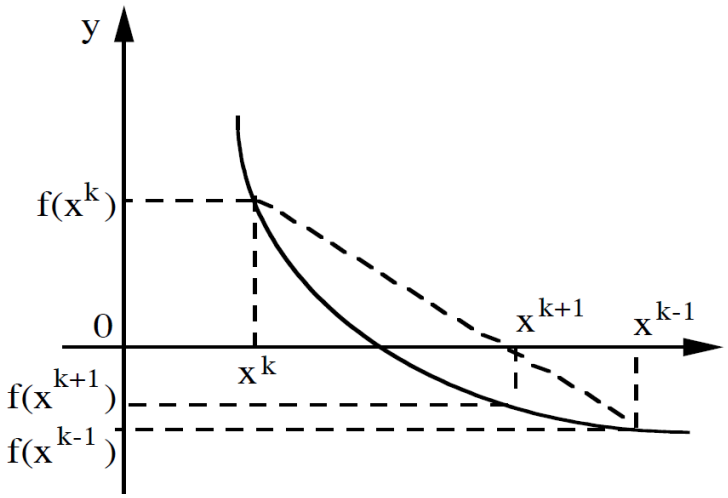


Figure 8.3: Geometrical interpretation: Chord method.

If there is no analytical expression of f(x), the Chord method which is similar to the one of Newton can be applied. The tangent is replaced by the chord given by:

$$f(x) - f(x^k) = \frac{f(x^k) - f(x^{k-1})}{x^k - x^{k-1}}(x - x^k)$$

the point x^{k+1} is obtained by setting $f(x^{k+1}) = 0$, yielding the equation:

$$\begin{aligned} x^{k+1} &= x^k - \psi^{-1} f(x^k) \\ with \quad \psi &= \frac{f(x^k) - f(x^{k-1})}{x^k - x^{k-1}} \end{aligned}$$

This equation differs from that of Newton by the value ψ that is only an approximation of the inverse of the derivative of f at the point x^k.

- Advantages:
  - No calculation of derivatives
  - Robustness and speed identical to Newton-Raphson
- Disadvantages:
  - Slow near the solution
  - Initial point requirement as for Newton-Raphson

8.1.3 Wegstein method

This method is very interesting in the common case in chemistry, where one is led to solve implicit equations (x=f(x)), leading to solve $\phi(x) = x - f(x) = 0$. Graphically, the solution is given by the intersection of the bisector y=x with the curve y=f(x). The method is also based on an iterative process. Admit that one has obtained a value of x after i iterations; the method illustrated in Figure 8.4) can be used to get the next value:

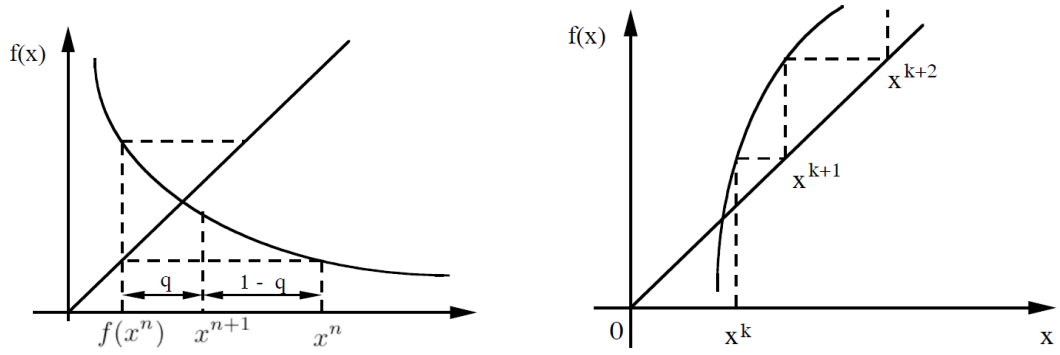


Figure 8.4: Geometrical interpretation: Wegstein method.

1. Intersection of the linear slope $x = x^k$ with the curve $y = f(x) \longrightarrow (x^k, y^k)$
2. Intersection of the linear slope $y = y^k$ with the bisector $y = x \longrightarrow (x^{k+1}, y^k)$
3. Intersection of the linear slope $x = x^{k+1}$ with the curve $y = f(x) \longrightarrow (x^{k+1}, y^{k+1})$

By proceeding in this way, the implicit method is used which can diverge. Furthermore, the convergence is very slow.

Wegstein proposes another procedure to avoid certain inconveniences of the implicit method and to accelerate the convergence. To this end, he proposes to correct the value of x^{k+1} by drawing the chord between the points k and $k+1$ and seeking its intersection with the linear slope $y = x$. To get this new value of x^{k+1}, the following system has to be solved (ψ angle coefficient of the chord (chord slope)):

$$\begin{aligned} y - y^k &= \frac{y^{k+1} - y^k}{x^{k+1} - \tilde{x}^k}(x^k - \tilde{x}^k) = \psi(x^k - \tilde{x}^k) \\ y &= x \end{aligned}$$

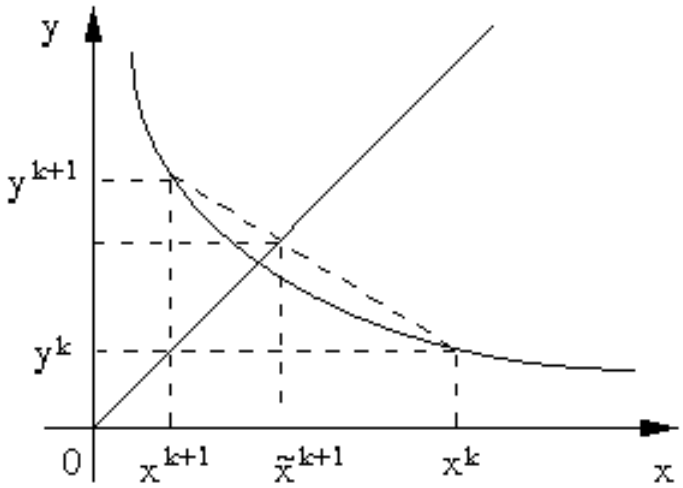


Figure 8.5: Geometrical interpretation: Wegstein method.

This corresponds to search for q so that:

$$\tilde{x}^{k+1} = q\tilde{x}^k + (1-q)x^{k+1}$$

The chord will pass through the point $(\tilde{x}^{k+1}, \tilde{x}^{k+1})$ and as $y = x^{k+1}$ this gives:

$$\begin{aligned} \tilde{x}^{k+1} - x^{k+1} &= \psi(\tilde{x}^{k+1} - \tilde{x}^k) \\ \tilde{x}^{k+1} &= \frac{1}{1-\psi}(x^{k+1} - \psi\tilde{x}^k) \end{aligned}$$

Therefore:

$$q = \frac{-\psi}{1-\psi} \quad and \quad 1 - q = \frac{1}{1-\psi}$$

In the case of the implicit method, it may converge in different ways or even diverge, depending on the value of ψ (the curve tangent) (Figure 8.6).
If ψ varies from $-\infty$ to $+\infty$, we will be able to observe, for the implicit method, the following phenomena (see sec. 8.4.1):

- $[-\infty, -1]$: oscillatory divergence
- $[-1, 0]$: oscillatory convergence
- $[0, 1]$: monotonic convergence
- $[1, +\infty]$: monotonic divergence

The Wegstein method converges on the other hand, even in cases where the implicit method diverges. However, according to Figure 8.7, we can see that q can take very large absolute values for $0.75 < \psi < 1.25$.

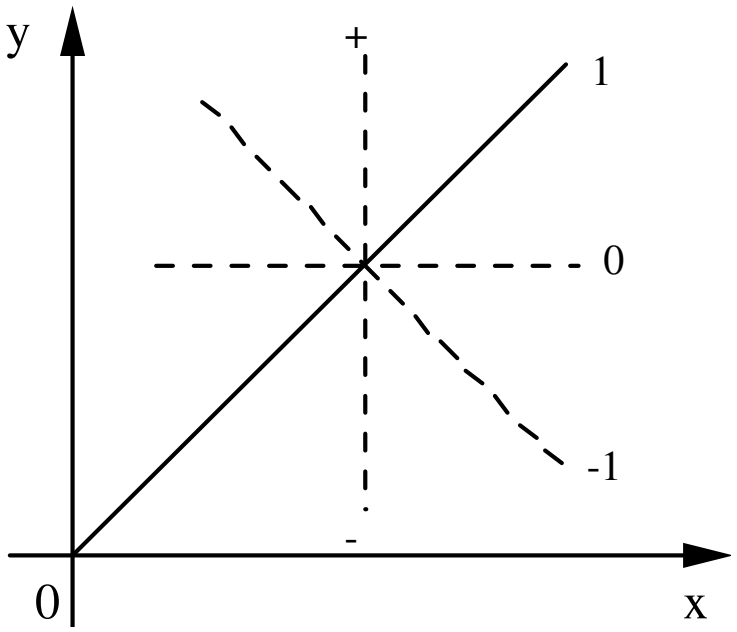


Figure 8.6: Implicit method variation of ψ.

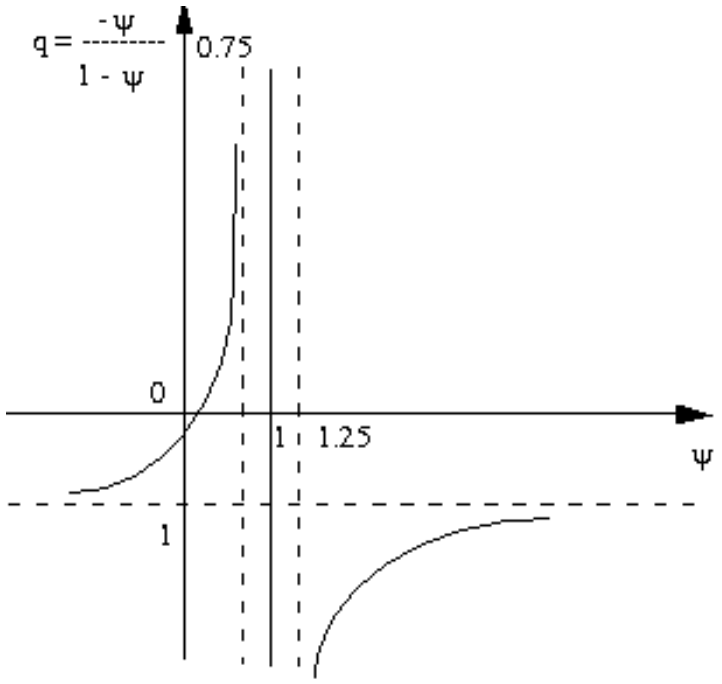


Figure 8.7: Wegstein method variation of ψ.

To restrict the advancement and to not deviate too much from the solution the absolute value of q has to be limited.
The general procedure of calculation is:

Estimate the solution x^0, and then compute the first two points: $x^1 = f(x^0)$ and $x^2 = f(x^1)$.

Calculate q to correct x^2

$$\psi = \frac{x^2 - x^1}{x^1 - x^0}$$

Successively calculate:

$$\begin{aligned}
\tilde{x}^2 &= qx^1 + (1-q)x^2 \\
x^3 &= f(\tilde{x}^2) \\
\psi &= \frac{x^3 - x^2}{\tilde{x}^2 - x^1} \\
x^4 &= f(\tilde{x}^3) \\
&\dots \\
\psi &= \frac{x^{k+1} - x^k}{\tilde{x}^k - \tilde{x}^{k-1}} \\
x^{k+2} &= f(\tilde{x}^{k+1})
\end{aligned}$$

and so on until the solution is reached. It is clear that in each iteration a test is done to see if the solution is reached.

8.2 Resolution of n-dimensional problems

The resolution of n-dimensional problems is discussed here. For explicit equations, the Newton-Raphson method, the method of the generalized secant method, and the Broyden method are considered. For the implicit equations, the Rubin method is described.

8.2.1 Newton-Raphson method generalization to n-dimensions

The resolution of $\underline{F}(\underline{x} = 0)$, where $\underline{F}$ is a vector function, corresponds, according to the mathematical conventions, to:

$$\begin{aligned}
f_1(\underline{x}) = f_1(x_1, x_2, ..., x_n) = 0 \\
f_2(\underline{x}) = f_2(x_1, x_2, ..., x_n) = 0 \\
f_n(\underline{x}) = f_n(x_1, x_2, ..., x_n) = 0
\end{aligned}$$

A starting vector $\underline{x}^0 =^t \left[x_1^0 ... x_n^0\right]$ is chosen and by analogy with the one-dimensional case, the n-dimensional Taylor development is limited to the terms of the first derivatives, which gives:

$f_i(\underline{x}) = f_i(\underline{x}^0) + \sum_{j=1}^{n} \left(\frac{\delta f_i}{\delta x_j}\right)_{\underline{x}^0} \cdot \Delta x_j = 0$; i=1,...,n
with $\Delta x_j = x_j - x_j^0$

In matrix form, this system of equations is written:

$$\begin{bmatrix}
\frac{\delta f_1}{\delta x_1} & \dots & \frac{\delta f_1}{\delta x_j} & \dots & \frac{\delta f_1}{\delta x_n} \\
\vdots & \ddots & \vdots & & \vdots \\
\frac{\delta f_i}{\delta x_1} & \dots & \frac{\delta f_i}{\delta x_j} & \dots & \frac{\delta f_i}{\delta x_n} \\
\vdots & & \vdots & \ddots & \vdots \\
\frac{\delta f_n}{\delta x_1} & \dots & \frac{\delta f_n}{\delta x_j} & \dots & \frac{\delta f_n}{\delta x_n}
\end{bmatrix} \cdot \begin{bmatrix} \delta x_1 \\ \dots \\ \delta x_i \\ \dots \\ \delta x_n \end{bmatrix} + \begin{bmatrix} f_1(\underline{x}^0) \\ \dots \\ f_i(\underline{x}^0) \\ \dots \\ f_n(\underline{x}^0) \end{bmatrix} = \begin{bmatrix} f_1(\underline{x}) \\ \dots \\ f_i(\underline{x}) \\ \dots \\ f_n(\underline{x}) \end{bmatrix}$$

where the partial derivatives are calculated at the point $\underline{x}^0$. This is written in the condensed (and conventional) form:

$$ {}^t\underline{\underline{J}} \cdot \underline{\Delta x} + \underline{F}(\underline{x}^0) = \underline{F}(\underline{x}) $$

This leads to:

$$ \underline{x}^1 = \underline{x}^0 - {}^t\underline{\underline{J}}^{-1}_{\underline{x}^0} \underline{F}(\underline{x}^0) $$

and for the (n+1)$^t h$ term:

$$ \underline{x}^{n+1} = \underline{x}^n - {}^t\underline{\underline{J}}^{-1}_{\underline{x}^n} \underline{F}(\underline{x}^n) $$

the transposed Jacobian matrix being calculated in x^n.

Remarks :

- The method requires a matrix inversion, it is therefore necessary that the Jacobian matrix $\underline{\underline{J}}$ is non-singular.
- At each iteration, the matrix $\underline{\underline{J}}$ must be recalculated, which corresponds each time to nxn derivatives, n functions and the inverse of a matrix (nxn).
- A convergence process based on Wegstein can be applied: $\tilde{\underline{x}}^{n+1} = \tilde{\underline{x}}^n - {}^t\underline{\underline{J}}^{-1}_{\underline{x}^n} \underline{F}(\tilde{\underline{x}}^n)(1-q)$ At the beginning, it is advantageous to choose a large q and decrease it thereafter. In fact, far from the solution, one should advance in small steps, while near the solution, one can progress faster.

8.2.2 Generalized secant method

Newton's method described previously presents the disadvantage of having to recalculate the Jacobian at each iteration. However, it is possible to develop an algorithm that renews the Jacobian in a slightly different way. The generalized secant method is described first and than the Broyden method which is similar.

The n-dimensional system to be solved is $\underline{F}(\underline{x} = 0)$. This system can contain implicit equations, since these can always be reduced in an explicit form. The vector $\underline{x}$ has to found such that $\underline{e} = \underline{F}(\underline{x}) = 0$.

One can try to solve this system by finding the linear functions that approximate the non-linear functions. Then one can find the zeros of these linear functions and hope that they are close to the zeros (solution) of the non-linear system.
Suppose that:

$$ \begin{array}{ll} \underline{x}^0 & \underline{e}^0 = \underline{F}(\underline{x}^0) \\ \underline{x}^1 & \underline{e}^1 = \underline{F}(\underline{x}^1) \\ \underline{x}^2 & \underline{e}^0 = \underline{F}(\underline{x}^2) \\ \vdots & \vdots \\ \underline{x}^n & \underline{e}^n = \underline{F}(\underline{x}^n) \end{array} $$

A linear model $\underline{e}^* = \underline{\underline{A}} \cdot \underline{x} + \underline{b}$ can be written to reproduce these data and accordingly:

$$ \begin{array}{l} \underline{e}^0 = \underline{\underline{A}} \cdot \underline{x}^0 + \underline{b} \\ \underline{e}^1 = \underline{\underline{A}} \cdot \underline{x}^1 + \underline{b} \\ \vdots \\ \underline{e}^n = \underline{\underline{A}} \cdot \underline{x}^n + \underline{b} \end{array} $$

The matrix $\underline{\underline{A}}$ has nxn unknowns and the vector $\underline{b}$ n unknowns. To solve this system, there are $(n+1)xn$ linear equations, and consequently the solution can be found. First the vector b can be eliminated by writing:

$$\underline{\Delta e^1} = \underline{e}^1 - \underline{e}^0 = \underline{\underline{A}}(\underline{x}^1 - \underline{x}^0) = \underline{\underline{A}} \cdot \underline{\Delta x^1}$$
$$\vdots$$
$$\underline{\Delta e^n} = \underline{e}^n - \underline{e}^{n-1} = \underline{\underline{A}}(\underline{x}^n - \underline{x}^{n-1}) = \underline{\underline{A}} \cdot \underline{\Delta x^n}$$

Which leads to the system:

$$\underline{\underline{\Delta E}} = \underline{\underline{A}} \cdot \underline{\underline{\Delta X}}$$

And therefore $\underline{\underline{A}}$ is given by the following expression if the matrix $\underline{\underline{\Delta X}}$ has an inverse. Since $\underline{\underline{\Delta X}}$ is completely under our control (we choose $\underline{x}$), an inverse can be guaranteed.

$$\underline{\underline{A}} = \underline{\underline{\Delta E}} \cdot \underline{\underline{\Delta X}}^{-1}$$

The values for $\underline{b}$ can be found with $\underline{b} = \underline{e} - \underline{\underline{\Delta A}} \cdot \underline{x}^n$. The following value of $\underline{x}$ can be estimated by the one that makes $\underline{e}^* = 0$. This step induces the resolution of a system of linear equations $\underline{e}^* = 0 = \underline{\underline{\Delta A}} \cdot \underline{x}^{n+1} + \underline{b}$. Which gives
$\underline{x}^{n+1} = -\underline{\underline{\Delta A}}^{-1}\underline{b} = -\underline{\underline{\Delta A}}^{-1}(\underline{e}^n - \underline{\underline{\Delta A}} \cdot \underline{x}^n) = \underline{x}^n - \underline{\underline{\Delta A}}^{-1}\underline{e}^n$

Improvement of the generalized secant method

The approach presented above implies that at each step the matrix $\underline{\underline{A}}$ has to be recalculated from the original data. It is however possible to develop algorithms that modify $\underline{\underline{A}}$ in another way. Suppose that $\underline{\underline{A}}$ can be estimated by a matrix called $\underline{\underline{A^1}}$. Suppose that $\underline{\Delta e^1}$ has been evaluated for a given $\underline{\Delta x^1}$. One would like to obtain a matrix $\underline{\underline{A^2}}$ such that:

$$\underline{\Delta e^1} = \underline{\underline{A^2}} \cdot \underline{\Delta x^1}$$

To get $\underline{\underline{A^2}}$, $\underline{\underline{A^1}}$ can be changed in the following way:

$$\underline{\underline{A^2}} = \underline{\underline{A^1}} + \underline{u^1} \cdot^t \underline{v^1}$$

This results in

$$\underline{\Delta e^1} = \left[\underline{\underline{A^1}} + \underline{u^1} \cdot^t \underline{v^1}\right] \underline{\Delta x^1}$$

$\underline{v^1}$ can be chosen arbitrarily and $\underline{u^1}$ is given by:

$$\underline{u^1} = \frac{\underline{\Delta e^1} - \underline{\underline{A^1}} \cdot \underline{\Delta x^1}}{{}^t\underline{v^1} \cdot \underline{\Delta x^1}}$$

As long as $\underline{v^1}$ is not orthogonal to $\underline{x^1}$, the vector $\underline{u^1}$ is well defined and therefore the matrix $\underline{\underline{A^2}}$ can be obtained from the matrix $\underline{\underline{A^1}}$.

To get a second point $\underline{\Delta e^2}$, for the stage $\underline{x^2}$, where $\underline{x^2}$ can for example be the result of: $\underline{x^2} = \underline{x^1} - (\underline{\underline{A^2}})^{-1}\underline{e^1}$. With $\underline{\Delta x^2} = \underline{x^2} - \underline{x^1}$, one may then try to have:

$$\underline{\Delta e^2} = \underline{\underline{A^3}} \cdot \underline{\Delta x^2} = \left[\underline{\underline{A^2}} + \underline{u^2} \cdot^t \underline{v^2}\right] \underline{\Delta x^2}$$

$\underline{u^2}$ and $\underline{v^2}$ can easily be found as before, but $\underline{\underline{A^3}}$ has also to satisfy:

$$\underline{\Delta e^1} = \underline{\underline{A^3}} \cdot \underline{\Delta x^1} = \left[\underline{\underline{A^2}} + \underline{u^2} \cdot^t \underline{v^2}\right] \underline{\Delta x^1}$$

If $\underline{u^2} \cdot^t \underline{v^2} \cdot \underline{\Delta x^1}$ is equal to the zero vector, then the equation above is reduced to the definition equation of $\underline{\underline{A^2}}$ and would therefore be satisfied. $\underline{v^2}$ has therefore to be chosen orthogonal to $\underline{x^1}$. One solution is to choose the vector $\underline{v^2}$ equal to the vector $\underline{x^2}$ orthogonalized with respect to $\underline{x^1}$. In this case, the equation to get $\underline{v^2}$ is:

$$\underline{v^2} = \underline{\Delta x^2} - \frac{\left[{}^t\underline{\Delta x^1} \cdot \underline{\Delta x^2}\right] \underline{\Delta x^1}}{{}^t\underline{v^1} \cdot \underline{\Delta x^1}}$$

One then gets another point $\underline{\Delta e^3}$ for the stage $\underline{\Delta x^3}$ and can impose that:

$$\underline{\Delta e^3} = \underline{\underline{A^4}} \cdot \underline{\Delta x^3}$$

with

$$\underline{\Delta e^1} = \underline{\underline{A^4}} \cdot \underline{\Delta x^1}$$
$$\underline{\Delta e^2} = \underline{\underline{A^4}} \cdot \underline{\Delta x^2}$$

For $\underline{\underline{A^4}} = \underline{\underline{A^3}} + \underline{u^3} \cdot^t \underline{v^3}$, $\underline{v^3}$ should be orthogonal to $\underline{\Delta x^1}$ and $\underline{\Delta x^2}$ .This result can be generalized by:

$$\underline{\underline{A^{i+1}}} = \underline{\underline{A^i}} + \frac{\underline{\Delta e^i} - \underline{\underline{A^i}} \cdot \underline{\Delta x^i}^{\,t}}{{}^t\underline{v^i} \cdot \underline{\Delta x^i}} \, \underline{v^i}$$

where $\underline{v^i}$ is orthogonalized with regard to (i-1) predecessors $\underline{\Delta x^i}$.

8.2.3 Broyden method

There is a great similarity between the Broyden method and the generalized secant method. Only one step of the algorithm distinguishes them. However the Broyden method performs better in terms of time usage and computation memory. Instead of selecting a new matrix in a way that the previous steps are satisfied, the Broyden algorithm requires that (the vectors $\underline{z}$ being orthogonal to $\underline{\Delta x^i}$):

$$\underline{\underline{A}}^{i+1}\underline{z} = \underline{\underline{A}}^{i}\underline{z}$$

The advantage is that the different $\underline{\Delta x^i}$ have no longer to be stored since all the information will be retained in the matrix $\underline{\underline{A}}$. As previously:

$$\underline{\Delta e^i} = \underline{\underline{A^{i+1}}} \cdot \underline{\Delta x^i} = \left[\underline{\underline{A^i}} + \underline{u^i}^{\,t} \underline{v^i}\right] \underline{\Delta x^i}$$

And for each vector $\underline{z} \neq 0$ orthogonal to $\underline{\Delta x^i}$

$$\left[\underline{\underline{A^i}} + \underline{u^i}^t \underline{v^i}\right] \underline{\Delta z} = \underline{\underline{A^i}} \cdot \underline{\Delta z}$$

If $\underline{v^i} = \underline{\Delta x^i}$, ${}^t\underline{v^i} \cdot \underline{z} = {}^t \underline{\Delta x^i} \cdot \underline{z} = 0$, if and only if $\underline{z} \neq 0$ orthogonal to $\underline{\Delta x^i}$. With this choice, one gets:

$$\underline{\underline{u^i}} = \frac{\underline{\Delta e^i} - \underline{\underline{A^i}} \cdot \underline{\Delta x^i}}{{}^t\underline{\Delta x^i} \cdot \underline{\Delta x^i}}$$

$$\underline{\underline{A^{i+1}}} = \underline{\underline{A^i}} + \frac{\underline{\Delta e^i} - \underline{\underline{A^i}} \cdot \underline{\Delta x^i}^t}{{}^t\underline{\Delta x^i} \cdot \underline{\Delta x^i}} \underline{\Delta x^i}$$

The advantage of the Broyden method compared to the generalized secant method is, as said earlier, that it is not necessary to preserve the vectors $\underline{\Delta x^i}$. However the disadvantage is that the convergence is linear, while the secant method converges quadratically.

Rubin method (quasi Newton)

In various mathematical models discussed previously, it was shown that some of them took the form: $\underline{x}^{k+1} = \psi(\underline{x}^k)$. Where ψ is an operator and not necessarily an analytic vector function (here the case where it is a vector $\underline{\psi}$ is considered).

Example. As this situation occurs frequently in the calculations of a flowsheet, let's consider a simplified example (Figure 8.8):

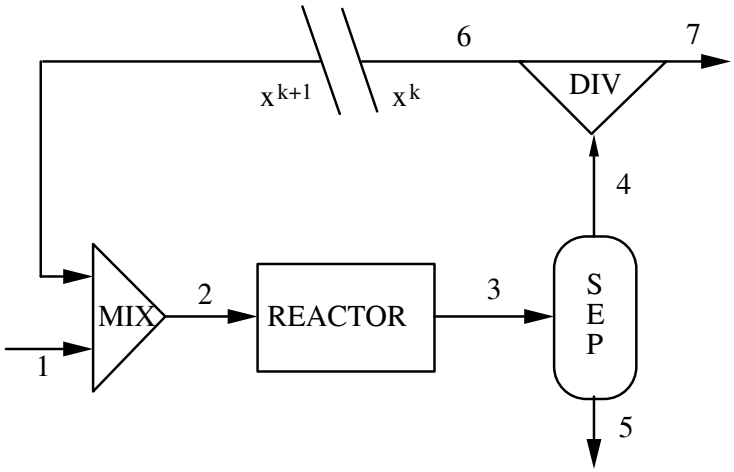


Figure 8.8: Process flowsheet.

The process involves a reactor R, a separator S, a splitter D and a mixer J. The input stream 1 is known, as well as the equipment models. The output streams 5 and 7 have to be calculated, which requires also to calculate all flows internal to the loop (2,3,4 and 6). It is therefore necessary to iterate over the values of the parameters of the stream 6 contained in the vector $\underline{x}$. During the iteration, the problem of how to improve the convergence is faced (like in the Wegstein method getting faster or arrive to the solution).

The method is the one of the generalized chord, but applied to the particular shape of the vector function to solve: $\underline{x} - \underline{\psi}(\underline{x}) = 0$ where $\underline{x}$ and $\underline{\psi}$ are a vector and a vector function, respectively. One can expect to estimate a Jacobian of this function.

If $\underline{\psi}(\underline{x})$ is analytical:

$$\underline{f}(\underline{x}) = \underline{x} - \underline{\psi}(\underline{x}) = 0$$

By applying the Newton's method, this gives:

$$\underline{x}^{k+1} = \underline{x}^k - \left\{ {}^t\underline{\underline{J}} \left[\underline{f}(\underline{x}^k) \right] \right\}^{-1} \underline{f}(\underline{x}^k)$$
$$\underline{x}^{k+1} = \underline{x}^k - \left\{ \underline{\underline{E}} - {}^t\underline{\underline{J}} \left[\underline{\psi}(\underline{x}^k) \right] \right\}^{-1} \left[\underline{x}^k - \underline{\psi}(\underline{x}^k) \right]$$

Therefore, looking for an approximation of the Jacobian of $\underline{\psi}$ becomes the objectif. The Taylor development of these recurrence functions (limited to the first term) becomes:

$$\begin{aligned}
\psi_1(\underline{x}) &= \psi_1(\underline{x}^k) + \left(\frac{\delta\psi_1}{\delta x_1}\right)^k \cdot \left(x_1 - x_1^k\right) + \ldots + \left(\frac{\delta\psi_1}{\delta x_n}\right)^k \cdot \left(x_n - x_n^k\right) \\
&\ldots \\
\psi_j(\underline{x}) &= \psi_j(\underline{x}^k) + \left(\frac{\delta\psi_j}{\delta x_1}\right)^k \cdot \left(x_1 - x_1^k\right) + \ldots + \left(\frac{\delta\psi_j}{\delta x_n}\right)^k \cdot \left(x_n - x_n^k\right) \\
&\ldots \\
\psi_n(\underline{x}) &= \psi_n(\underline{x}^k) + \left(\frac{\delta\psi_n}{\delta x_1}\right)^k \cdot \left(x_1 - x_1^k\right) + \ldots + \left(\frac{\delta\psi_n}{\delta x_n}\right)^k \cdot \left(x_n - x_n^k\right)
\end{aligned}$$

where k is the number of iterations, j indicates the element and n the dimension of the problem (number of variables). This is written in vector form:

$$\underline{\psi}(\underline{x}) = \underline{\psi}(\underline{x}^k) + \left\{ {}^t\underline{\underline{J}} \left[\underline{\psi}(\underline{x}^k) \right] \right\} \underline{\Delta x}^k$$

With respect to the resolution perspective, the vectors $\underline{x}^1, \underline{x}^2, \underline{x}^3, ..., \underline{x}^k$ can be known after k iterations, as well as $\underline{\psi}(\underline{x}^{k+1}) - \underline{\psi}(\underline{x}^k)$. Indeed, the implicit method gives (assume that it has started at a point $\underline{x}^0$): $x_j^k = \psi_j(\underline{x}^{k-1})$ (element j, iteration k). However, for a system of n equations, there are n^2 unknowns which are the derivatives of ψ with regard to x (for each x and ψ). After an iteration, there are n equations, and after n iterations, there are n^2 equations and the expression of the Jacobian can therefore be obtained. To obtain this, two matrices C and D are used to store the information given by each iteration. In matrix form, the system to be solved is:

$$\underline{\psi}(\underline{x}) - \underline{\psi}(\underline{x}^k) = \left\{ {}^t\underline{\underline{J}} \left[\underline{\psi}(\underline{x}^k) \right] \right\} \underline{\Delta x}^k$$

And in the condensed form ${}^t\underline{\underline{B}} = {}^t\underline{\underline{J}}\,{}^t\underline{\underline{A}}$ or ${}^t\underline{\underline{B}}\,{}^t\underline{\underline{A}}^{-1} = {}^t\underline{\underline{J}}$ and $\underline{\underline{J}} = \underline{\underline{A}}^{-1}\underline{\underline{B}}$
with

$$\underline{\underline{A}} = \begin{bmatrix}
x_1^1 - x_1^0 & \cdots & x_j^1 - x_j^0 & \cdots & x_n^1 - x_n^0 \\
\vdots & \ddots & \vdots & & \vdots \\
x_1^k - x_1^0 & \cdots & x_j^k - x_j^0 & \cdots & x_n^k - x_n^0 \\
\vdots & & \vdots & \ddots & \vdots \\
x_1^n - x_1^0 & \cdots & x_j^n - x_j^0 & \cdots & x_n^n - x_n^0
\end{bmatrix}$$

$$\underline{\underline{B}} = \begin{bmatrix}
\psi_1(\underline{x}^1) - \psi_1(\underline{x}^0) & \cdots & \psi_j(\underline{x}^1) - \psi_j(\underline{x}^0) & \cdots & \psi_n(\underline{x}^1) - \psi_n(\underline{x}^0) \\
\vdots & \ddots & \vdots & & \vdots \\
\psi_1(\underline{x}^k) - \psi_1(\underline{x}^0) & \cdots & \psi_j(\underline{x}^k) - \psi_j(\underline{x}^0) & \cdots & \psi_n(\underline{x}^k) - \psi_n(\underline{x}^0) \\
\vdots & & \vdots & \ddots & \vdots \\
\psi_1(\underline{x}^n) - \psi_1(\underline{x}^0) & \cdots & \psi_j(\underline{x}^n) - \psi_j(\underline{x}^0) & \cdots & \psi_n(\underline{x}^n) - \psi_n(\underline{x}^0)
\end{bmatrix}$$

The Jacobian $\underline{\underline{J}}$ is obtained by inverting $\underline{\underline{A}}$ and multiplying by $\underline{\underline{B}}$. From a numerical point of view, to obtain the transposed Jacobian matrix, n iterations are performed by simple substitution, and the information is stored in 2 matrices $\underline{\underline{C}}$ and $\underline{\underline{D}}$:

$$\underline{\underline{C}} = \begin{bmatrix} x_1^0 & \cdots & x_j^0 & \cdots & x_n^0 \\ x_1^1 & \cdots & x_j^1 & \cdots & x_n^1 \\ \vdots & \ddots & \vdots & & \vdots \\ x_1^k & \cdots & x_j^k & \cdots & x_n^k \\ \vdots & & \vdots & \ddots & \vdots \\ x_1^n & \cdots & x_j^n & \cdots & x_n^n \end{bmatrix}$$

$$\underline{\underline{D}} = \begin{bmatrix} \psi_1(\underline{x}^0) & \cdots & \psi_j(\underline{x}^0) & \cdots & \psi_n(\underline{x}^0) \\ \psi_1(\underline{x}^1) & \cdots & \psi_j(\underline{x}^1) & \cdots & \psi_n(\underline{x}^1) \\ \vdots & \ddots & \vdots & & \vdots \\ \psi_1(\underline{x}^k) & \cdots & \psi_j(\underline{x}^k) & \cdots & \psi_n(\underline{x}^k) \\ \vdots & & \vdots & \ddots & \vdots \\ \psi_1(\underline{x}^n) & \cdots & \psi_j(\underline{x}^n) & \cdots & \psi_n(\underline{x}^n) \end{bmatrix}$$

These two matrices have each (n+1) rows and n columns. $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are obtained by subtracting in each matrix the first line to all the others. However, the Jacobian calculated in this way is the one at the point $\underline{x}^0$. It is preferable to calculate it after n iterations. For this reason, the first obtained information will be stored by starting with the last line (it is as if the matrices $\underline{\underline{C}}$ and $\underline{\underline{D}}$ were returned with regard to the horizontal).

At the point $\underline{x}^n$ one has $\underline{\underline{J}}(\underline{\psi}) = \underline{\underline{A}}^{-1}\underline{\underline{B}}$. The $(n+1)^{th}$ iteration gives $\underline{x^{n+1}}$ by $\underline{x^{n+1}} = \underline{\psi}(\underline{x}^n)$. This value is then corrected in the following way:

$$\tilde{\underline{x}}^{n+1} = \underline{x}^n - \left\{\underline{\underline{E}} - {}^t\left(\underline{\underline{A}}^{-1}\underline{\underline{B}}\right)\right\}^{-1}\left[\underline{x}^n - \underline{\psi}(\underline{x}^n)\right]$$

The Rubin method is therefore a Newton-Raphson method which has been modified to allow the estimation of the Jacobian, because in the case of the flowsheet, the function $\underline{\psi}(\underline{x})$ is not known analytically. This method is also called the generalized chord method. In fact, the calculation of the Jacobian based on the matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ corresponds to estimating the slope of the chord between two points $\frac{\psi_j(\underline{x}^k) - \psi_j(\underline{x}^n)}{x_j^k - x_j^n} = p_j$.

In order to further accelerate the convergence, the Wegstein method can be applied on the most sensitive variable (that which has been the most modified).

8.3 Solving differential equations: the Runge-Kutta method

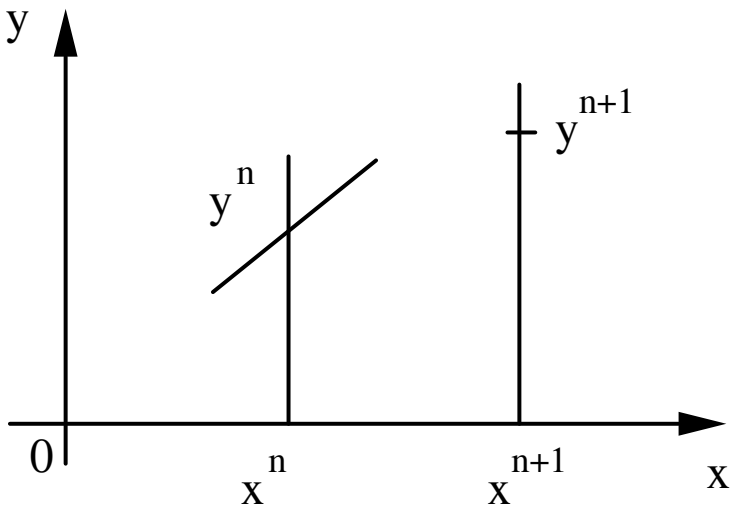
The purpose of the Runge-Kutta method is to obtain an approximate numerical solution from a non-linear ordinary differential equation or a system of nonlinear ordinary differential equations.
Consider first the case of one equation, given by:

$$\frac{dy}{dx} = y' = f[x, y(x)]$$

with the initial conditions:$y(x^0) = y^0$ where x^0 is the initial point.

The slope of the function y, allows to estimate the value of y at a point $x^0 + h$ where h is the integration interval.

If $y^n = y(x^0 + nh)$ is the estimation of the function y the Taylor development (centered at x^n) gives after n steps of integration:



$$\begin{aligned} y(x^{n+1}) &= y(x^n + h) \\ &= y(x^n) + h \cdot y'(x^n) + \frac{h^2}{2!} y''(x^n) + \frac{h^3}{3!} y'''(x^n) + ... \end{aligned} \tag{8.1}$$

Knowing $y' = f(x, y)$, one tries to obtain an approximation of $y'', y''', ...$ All these derivatives taken at the same point, one has:

$$\begin{aligned} y'' &= \frac{dy'}{dx} = \frac{df}{dx} = \frac{\delta f}{\delta y} \cdot \frac{\delta y}{\delta x} + \frac{\delta f}{\delta x} = f_y \cdot f + f_x \\ y''' &= \frac{dy''}{dx} = \frac{d}{dx}(f_y \cdot f + f_x) = \frac{\delta}{\delta y}(f_y \cdot f + f_x)\frac{\delta y}{\delta x} + \frac{\delta}{\delta x}(f_y \cdot f + f_x) \\ &= f_{xx} + 2 \cdot f \cdot f_{xy} + f^2 f_{yy} + f_y(f_y \cdot f + f_x) \end{aligned}$$

where $f_x = \frac{\delta}{\delta x}$, $f_x y = \frac{\delta^2}{\delta x \delta y}$ and noting that in this case $\frac{dy}{dx} = \frac{\delta y}{\delta x}$.

Introducing the values of y'' in Eq. 8.1 and one gets Eq. 8.2:

$$\Delta y^{n+1} = y^{n+1} - y^n = h \cdot f + \frac{h^2}{2!}(f_x + f_y \cdot f) \tag{8.2}$$

Then one searches an expression of y^{n+1} involving only estimates of the function f at a specific point:

$$\begin{aligned} y^{n+1} &= y^n + N_0 \cdot k_0 + N_1 \cdot k_1 + N_2 \cdot k_2 + ... \\ k_0 &= h \cdot f(x^n, y^n) \\ k_1 &= h \cdot f(x^n + \alpha_1 \cdot h, y^n + \beta_{10} \cdot k_0) \\ k_2 &= h \cdot f(x^n + \alpha_2 \cdot h, y^n + \beta_{20} \cdot k_0 + \beta_{21} \cdot k_1) \\ k_3 &= h \cdot f(x^n + \alpha_3 \cdot h, y^n + \beta_{30} \cdot k_0 + \beta_{31} \cdot k_1 + \beta_{32} \cdot k_2) \end{aligned}$$

If one develops k_1 by dropping the second order term, one gets:

$$k_1 = h \cdot (f + \alpha_1 \cdot h \cdot f_x + \beta_{10} \cdot k_0 \cdot f_y)$$

Consequently:

$$\Delta y^{n+1} = N_0 \cdot h \cdot f + N_1 \cdot h \cdot (f + \alpha_1 \cdot h \cdot f_x + \beta_{10} \cdot k_0 \cdot f_y) \tag{8.3}$$

The comparison of the h terms of Eq. 8.2 and Eq. 8.3 gives:

$$\begin{aligned} h \cdot f &\longmapsto N_0 + N_1 = 1 \\ h^2 \cdot f_x &\longmapsto N_1 \cdot \alpha_1 = 1/2 \\ h^2 \cdot f_y \cdot f &\longmapsto N_1 \cdot \beta_{12} = 1/2 \end{aligned}$$

There are three relations for four parameters; consequently there is an infinite number of solutions that can be written in the form:

$$\begin{aligned} N_0 &= 1 - \frac{1}{2 \cdot \alpha_1} \\ N_1 &= \frac{1}{2 \cdot \alpha_1} \\ \beta_{12} &= \alpha_1 \end{aligned}$$

Taking $\alpha_1 = 1$, on has that $N_0 = 1/2$, $N_1 = 1/2$ and $\beta_{10} = 1$ and

$$\begin{aligned} k_0 &= h \cdot f(x^n, y^n) \\ k_1 &= h \cdot f(x^n + h, y^n + k_0) \\ y^{n+1} &= y^n + \frac{1}{2}(k_0 + k_1) \end{aligned}$$

In the third order, there are 8 parameters for 6 equations, in the fourth order, 13 parameters for 10 equations, etc. The method that is used here is the one that has been developed by Runge which is a method of the 4th order. With Table 8.1 one gets:

	N_0	N_1	N_2	N_3	α_1	α_2	α_3	β_{10}	β_{20}	β_{21}	β_{30}	β_{31}	
RUNGE	1/6	2/6	2/6	1/6	1/2	1/2	1	1/2	0	1/2	0	0	1
KUTTA	1/8	3/8	3/8	1/8	1/3	2/3	1	1/3	1/3	1	1	-1	1

Table 8.1: Runge and Kutta values

$$\begin{aligned} k_0 &= h \cdot f(x^n, y^n) \\ k_1 &= h \cdot f(x^n + h/2, y^n + k_0/2) \\ k_2 &= h \cdot f(x^n + h/2, y^n + k_1/2) \\ k_3 &= h \cdot f(x^n + h, y^n + k_2) \\ \Delta y^{n+1} &= \frac{1}{6} \cdot (k_0 + 2 \cdot k_1 + 2 \cdot k_2 + k_3) \end{aligned}$$

If there are several differential equations, the development will be the same but it will apply to the vector functions. In this case however, there will be interest to weight the equations so that the variations of each are of the same order of magnitude. The system to be solved is then (with α, β, γ weighting coefficients):

$$\begin{aligned} \alpha \cdot f_1(x) &= \frac{dy_1}{dx} \\ \beta \cdot f_2(x) &= \frac{dy_2}{dx} \\ \gamma \cdot f_3(x) &= \frac{dy_3}{dx} \end{aligned}$$

8.4 Numerical applications

Through some numerical examples the use of some of the models that have been described are illustrated.

8.4.1 Comparison between simple substitution and Wegstein method

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First case: monotonic convergence

$x=a+bx+cx^2$		a	1,4			
		b	0,0417			
Substitution		c	0,1583			
iter	x	f(x)				
1	0	1,4				
	1,4	1,4				
2	1,4	1,7687				
	1,7687	1,7687				
3	1,7687	1,969				
	1,969	1,969				
4	1,969	2,0959				
	2,0959	2,0959				
5	2,0959	2,1828				
	2,1828	2,1828				
6	2,1828	2,2454				
	2,2454	2,2454				
7	2,2454	2,2918				
	2,2918	2,2918				
8	2,2918	2,3271				
	2,3271	2,3271				
9	2,3271	2,3544				
	2,3544	2,3544				
10	2,3544	2,3758				
Wegstein						
iter	x	f(x)	psi	q	x amʼlior˜	
1	0	1,4				
	1,4	1,4				
2	1,4	1,7687	0,2633	-0,357	1,9005	
	1,9005	1,9005				
3	1,9005	2,051	0,5642	-1,295	2,246	
	2,246	2,246				
4	2,246	2,2923	0,6982	-2,313	2,3994	
	2,3994	2,3994				
5	2,3994	2,4115	0,7772	-3,488	2,4538	
	2,4538	2,4538				
6	2,4538	2,4556	0,8101	-4,266	2,4632	
	2,4632	2,4632				

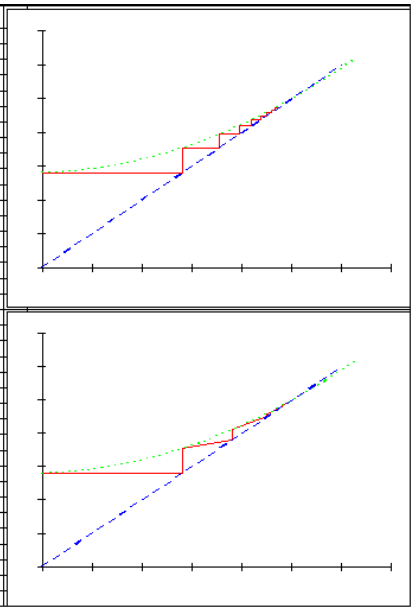


Figure 8.9: Monotonic convergence.

Second case: oscillatory convergence (only for simple substitution)

$x=a+bx+cx^2$		a	3			
		b	-1,3			
Substitution		c	0,2			
iter	x	f(x)				
1	0	3				
	3	3				
2	3	0,9				
	0,9	0,9				
3	0,9	1,992				
	1,992	1,992				
4	1,992	1,204				
	1,204	1,204				
5	1,204	1,7247				
	1,7247	1,7247				
6	1,7247	1,3528				
	1,3528	1,3528				
7	1,3528	1,6074				
	1,6074	1,6074				
8	1,6074	1,4271				
	1,4271	1,4271				
9	1,4271	1,5521				
	1,5521	1,5521				
10	1,5521	1,4641				
Wegstein						
iter	x	f(x)	psi	q	x am'lior'	
1	0	3				
	3	3				
2	3	0,9	-0,7	0,4118	1,7647	
	1,7647	1,7647				
3	1,7647	1,3287	-0,3471	0,2576	1,441	
	1,441	1,441				
4	1,441	1,542	-0,6588	0,3972	1,5019	
	1,5019	1,5019				
5	1,5019	1,4987	-0,7114	0,4157	1,5	
	1,5	1,5				
6	1,5	1,5	-0,6996	0,4116	1,5	
	1,5	1,5				

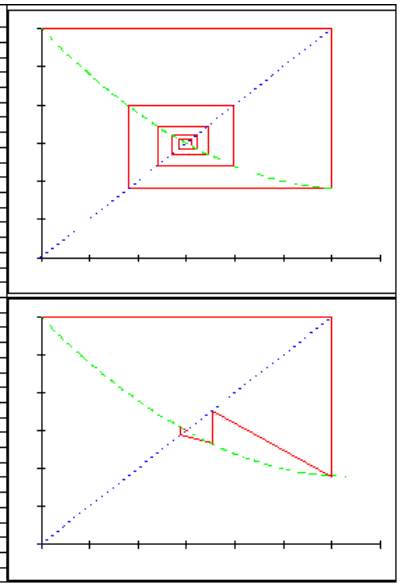


Figure 8.10: Oscillatory convergence.

Third case: monotonic divergence (only for simple substitution)

$x=a+bx+cx^2$		a	-0,3			
		b	1,15			
Substitution		c	0,05			
iter	x	f(x)				
1	1	0,9				
	0,9	0,9				
2	0,9	0,7755				
	0,7755	0,7755				
3	0,7755	0,6219				
	0,6219	0,6219				
4	0,6219	0,4345				
	0,4345	0,4345				
5	0,4345	0,2091				
	0,2091	0,2091				
6	0,2091	-0,057				
	-0,057	-0,057				
7	-0,057	-0,366				
	-0,366	-0,366				
8	-0,366	-0,714				
	-0,714	-0,714				
9	-0,714	-1,096				
	-1,096	-1,096				
10	-1,096	-1,5				
Wegstein						
iter	x	f(x)	psi	q	x am'lior'	
1	1	0,9				
	0,9	0,9				
2	0,9	0,7755	1,245	5,0816	1,40816	
	1,4082	1,4082				
3	1,4082	1,4185	1,2654	4,7678	1,36909	
	1,3691	1,3691				
4	1,3691	1,3682	1,2889	4,4619	1,37226	
	1,3723	1,3723				
5	1,3723	1,3723	1,2871	4,4835	1,37228	
	1,3723	1,3723				
6	1,3723	1,3723	1,2872	4,4816	1,37228	
	1,3723	1,3723				

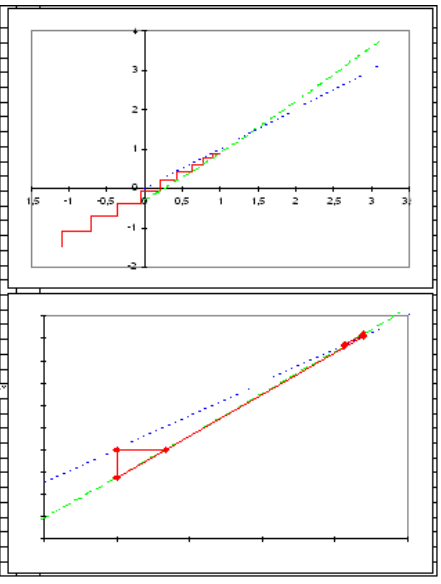
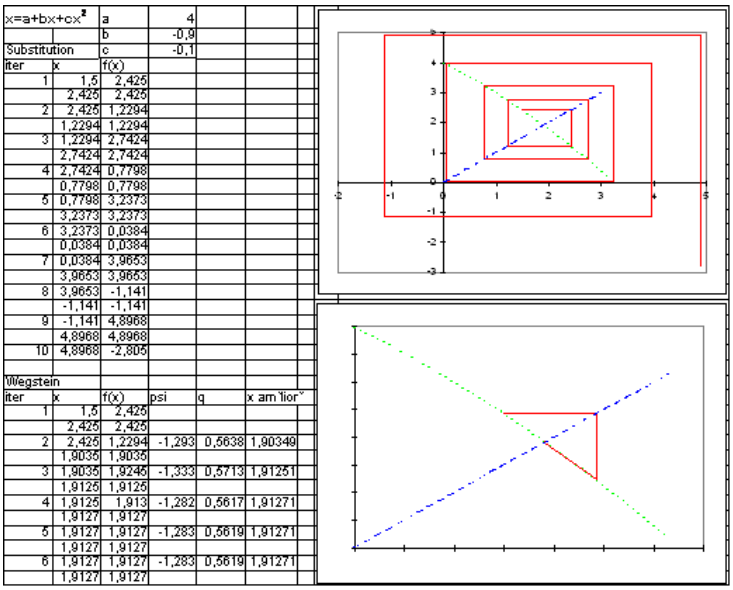


Figure 8.11: Monotonic divergence.



$x=a+bx+cx^2$		a	4			
		b	-0,9			
Substitution		c	-0,1			
iter	x	f(x)				
1	1,5	2,425				
	2,425	2,425				
2	2,425	1,2294				
	1,2294	1,2294				
3	1,2294	2,7424				
	2,7424	2,7424				
4	2,7424	0,7798				
	0,7798	0,7798				
5	0,7798	3,2373				
	3,2373	3,2373				
6	3,2373	0,0384				
	0,0384	0,0384				
7	0,0384	3,9653				
	3,9653	3,9653				
8	3,9653	-1,141				
	-1,141	-1,141				
9	-1,141	4,8968				
	4,8968	4,8968				
10	4,8968	-2,805				
Wegstein						
iter	x	f(x)	psi	q	x amʻlior˜	
1	1,5	2,425				
	2,425	2,425				
2	2,425	1,2294	-1,293	0,5638	1,90349	
	1,9035	1,9035				
3	1,9035	1,9245	-1,333	0,5713	1,91251	
	1,9125	1,9125				
4	1,9125	1,913	-1,282	0,5617	1,91271	
	1,9127	1,9127				
5	1,9127	1,9127	-1,283	0,5619	1,91271	
	1,9127	1,9127				
6	1,9127	1,9127	-1,283	0,5619	1,91271	
	1,9127	1,9127				

Figure 8.12: Oscillatory divergence.

Fourth case: oscillatory divergence (only for simple substitution)

8.4.2 Comparison between simple substitution and Rubin method

	x1=1.4 racine(1+x2)-0.4 x1			
	x2=1.5 racine(x1) -0.5 x2 +1.5			
Substitution simple				
It	x1	x2	f1	f2
1	3,000	2,000	1,225	3,098
2	1,225	3,098	2,344	1,611
3	2,344	1,611	1,325	2,991
4	1,325	2,991	2,267	1,731
5	2,267	1,731	1,407	2,893
6	1,407	2,893	2,200	1,833
7	2,200	1,833	1,476	2,808
8	1,476	2,808	2,142	1,918
9	2,142	1,918	1,535	2,736
10	1,535	2,736	2,092	1,990
11	2,092	1,990	1,584	2,674
12	1,584	2,674	2,050	2,051
13	2,050	2,051	1,625	2,622
14	1,625	2,622	2,014	2,101
15	2,014	2,101	1,660	2,578
16	1,660	2,578	1,984	2,143
17	1,984	2,143	1,688	2,541
18	1,688	2,541	1,959	2,178
19	1,959	2,178	1,712	2,510
20	1,712	2,510	1,938	2,208
21	1,938	2,208	1,732	2,485
22	1,732	2,485	1,921	2,232
23	1,921	2,232	1,749	2,463
24	1,749	2,463	1,906	2,252
25	1,906	2,252	1,762	2,445
26	1,762	2,445	1,893	2,269
27	1,893	2,269	1,774	2,430
28	1,774	2,430	1,883	2,283
29	1,883	2,283	1,783	2,417
30	1,783	2,417	1,874	2,295
31	1,874	2,295	1,791	2,406
32	1,791	2,406	1,867	2,305
33	1,867	2,305	1,798	2,397
34	1,798	2,397	1,861	2,313
35	1,861	2,313	1,804	2,390
36	1,804	2,390	1,856	2,319
37	1,856	2,319	1,808	2,384
38	1,808	2,384	1,852	2,325
39	1,852	2,325	1,812	2,379
40	1,812	2,379	1,849	2,330
41	1,849	2,330	1,815	2,375
42	1,815	2,375	1,846	2,334
43	1,846	2,334	1,818	2,371
44	1,818	2,371	1,843	2,337
45	1,843	2,337	1,820	2,368
46	1,820	2,368	1,841	2,340
47	1,841	2,340	1,822	2,366
48	1,822	2,366	1,840	2,342
49	1,840	2,342	1,823	2,364
50	1,823	2,364	1,838	2,344
51	1,838	2,344	1,825	2,362
52	1,825	2,362	1,837	2,345
53	1,837	2,345	1,826	2,360
54	1,826	2,360	1,836	2,347
55	1,836	2,347	1,827	2,359

Rubin						
	x1=1.4 racine(1+x2)-0.4 x1					
	x2=1.5 racine(x1) -0.5 x2 +1.5					
Iter	x1	x2	f1	f2		
1	4,0000	5,0000	1,8293	2,0000		
2	1,8293	2,0000	1,6932	2,5288		
3	1,6932	2,5288	1,9526	2,1874		
Iter	x1	x2	f1	f2	x1-f1	x2-f2
4	1,8071	2,3325	1,8329	2,3501	-0,0258	-0,0176
C	1,8071	2,3325		D	1,8329	2,3501
	1,8293	2,0000			1,6932	2,5288
	1,6932	2,5288			1,9526	2,1874
A	0,0222	-0,3325		B	-0,1397	0,1786
	-0,1139	0,1962			0,1197	-0,1627
A-1	-5,8552	-9,9218	(A-1).B=	J	-0,3697	0,5684
	-3,3986	-0,6631			0,3956	-0,4992
E-J	1,3697	-0,5684	(E-J)-1		0,8199	0,3108
	-0,3956	1,4992			0,2163	0,7490
Iter	x1	x2	f1	f2	x1-f1	x2-f2
5	1,8337	2,3513	1,8294	2,3556	0,0043	-0,0043
ligne	modifier	2				
lodif C	1,8071	2,3325		modif D	1,8329	2,3501
	1,8337	2,3513			1,8294	2,3556
	1,6932	2,5288			1,9526	2,1874

8.4.3 n-dimensional Newton-Raphson method

	f1=x1^2-x2-1									
	f2=x1-(x2-1)^2									
	Newton-Raphson									
Iter	x1	x2	f1	f2		J			J-1	
1	5,000	5,000	19,000	-11,000		10	-1		0,1013	-0,0127
						1	-8		0,0127	-0,1266
2	2,937	3,367	4,257	-2,666		5,87342	-1		0,1766	-0,0373
						1	-4,7342		0,0373	-0,2191
3	2,085	2,624	0,725	-0,552		4,17076	-1		0,2589	-0,0797
						1	-3,2481		0,0797	-0,3324
4	1,854	2,383	0,054	-0,058		3,7075	-1		0,2989	-0,1081
						1	-2,7655		0,1081	-0,4007
5	1,831	2,354	0,000	-0,001		3,66285	-1		0,3036	-0,1122
						1	-2,7072		0,1122	-0,4108
6	1,831	2,353	0,000	0,000		3,66235	-1		0,3037	-0,1122
						1	-2,7064		0,1122	-0,4110
7	1,831	2,353	0,000	0,000		3,66235	-1		0,3037	-0,1122
						1	-2,7064		0,1122	-0,4110
8	1,831	2,353	0,000	0,000		3,66235	-1		0,3037	-0,1122
						1	-2,7064		0,1122	-0,4110
9	1,831	2,353	0,000	0,000		3,66235	-1		0,3037	-0,1122
						1	-2,7064		0,1122	-0,4110
10	1,831	2,353	0,000	0,000		3,66235	-1		0,3037	-0,1122
						1	-2,7064		0,1122	-0,4110
11	1,831	2,353	0,000	0,000		3,66235	-1		0,3037	-0,1122
						1	-2,7064		0,1122	-0,4110

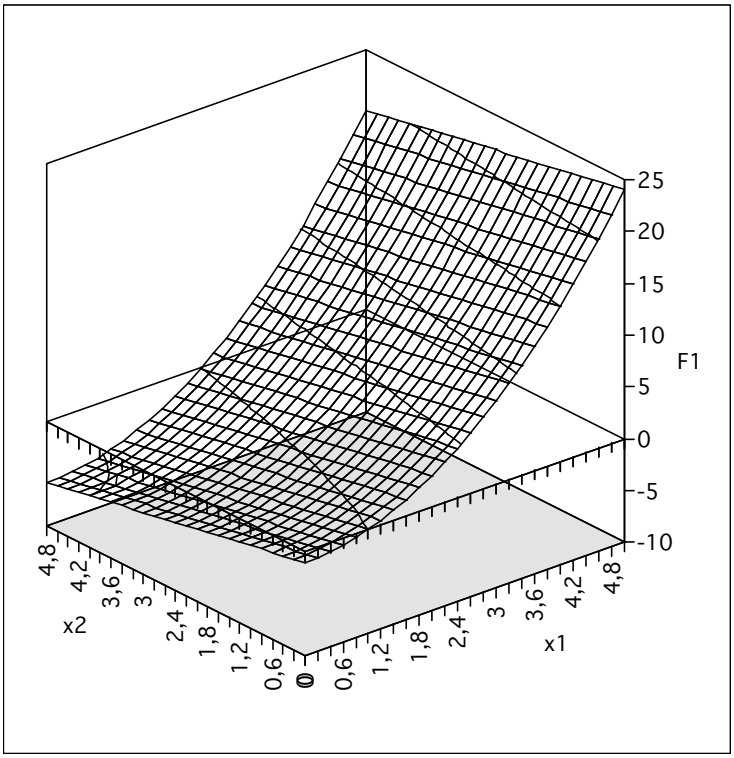


Figure 8.13: F1 according to x1 and x2.

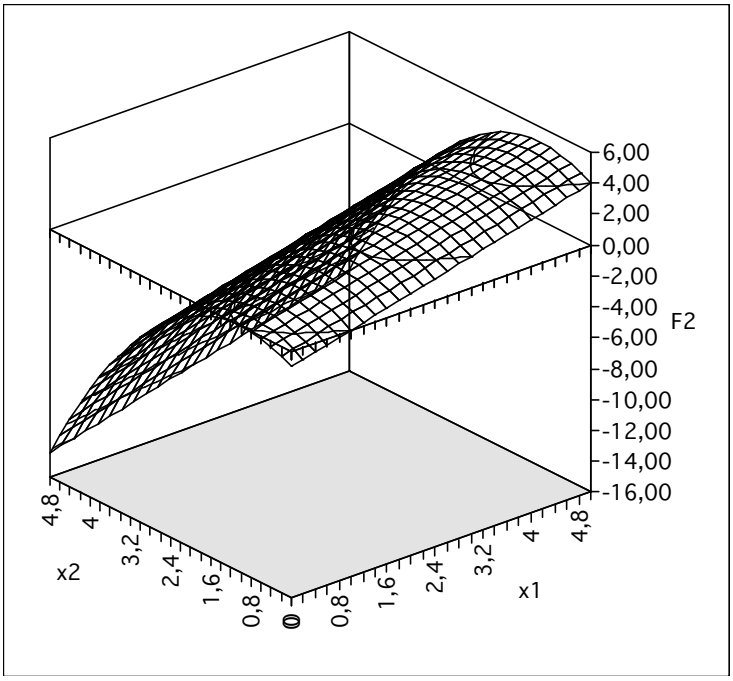


Figure 8.14: F2 according to x1 and x2.

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