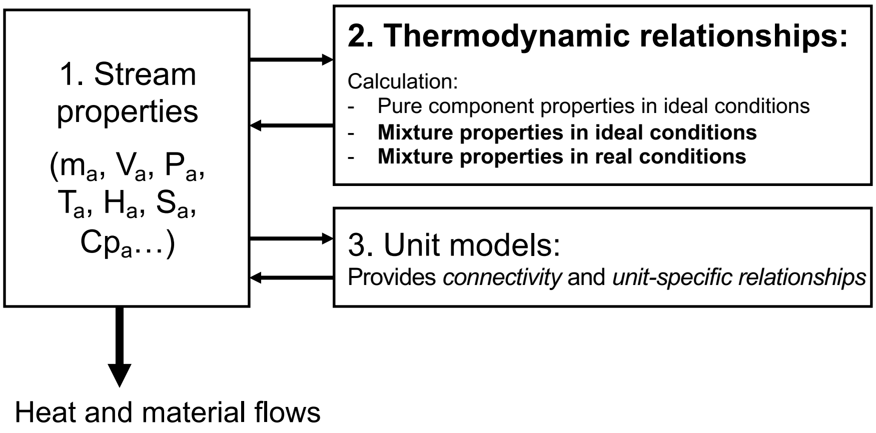
Recap: Part 2

Objective: Cover the basic principles of Systems Modeling for a Renewable Energy Process and be able to model a simple system.

- Importance of Systems Modeling in Renewable Energy
- **Modeling systems**
  - Stream properties
  - **Thermodynamic relationships**
  - Unit models
- Heat integration & Pinch Analysis
  - Basic Principles
  - Composite Curves
  - The Heat Cascade and the Grand Composite Curve
- Life Cycle Assessment
  - Goal & Scope Definition
  - Life Cycle Inventory
  - Life Cycle Impact Assessment
- Uncertainty Analysis & The Monte Carlo Method

Process Modeling

The approach:



1. Stream properties

(m_a, V_a, P_a, T_a, H_a, S_a, Cp_a…)

2. Thermodynamic relationships:

Calculation:
- Pure component properties in ideal conditions
- **Mixture properties in ideal conditions**
- **Mixture properties in real conditions**

3. Unit models:

Provides *connectivity* and *unit-specific relationships*

Heat and material flows

Vapor liquid equilibriums

A key property of mixtures is to calculate their vapor liquid equilibriums (VLLEs).

This is important in:
- Chemical processes: distillation, extraction…etc.
- Environmental processes: atmospheric and ocean modeling

We want to find the state **at equilibrium**. What is the thermodynamic definition of an equilibrium?

$$dG = 0$$

Total free energy change of the system

Change of the quantity of component α in phase *p*

$$dG = -SdT + VdP + \sum_p \sum_\alpha \mu_{p,\alpha} dn_{p,\alpha}$$

Phase Component Chemical potential of component α in phase *p*

Vapor liquid equilibriums

$$dG = -SdT + VdP + \sum_p \sum_\alpha \mu_{p,\alpha} dn_{p,\alpha} = \sum_p \sum_\alpha \mu_{p,\alpha} dn_{p,\alpha} = 0$$

@ an equilibrium @ a given T and P

@ cst T and P, the only variable is n_α → To minimize *G* we have to find the point where:

$$\left(\frac{dG}{dn_\alpha}\right)_{T,P,n_{\alpha\neq\beta}} = 0 \quad = \sum_p \mu_{p,\alpha}$$

For independent components (e.g. no reactions)

$$\rightarrow \mu_{1,\alpha} = \mu_{2,\alpha} = \mu_{3,\alpha} \cdots$$

The chemical potentials of each component **must be equal across phases.**

Vapor liquid equilibriums

For a vapor-liquid equilibrium:

$$\mu_{V,\alpha} = \mu_{L,\alpha}$$

Let's develop this expression:

$$\mu_{V,\alpha} = \mu^0_{V,\alpha} + RT\ln\frac{f_{\alpha,V}}{f^0_{\alpha,V}} = \mu^0_{L,\alpha} + RT\ln\frac{f_{\alpha,L}}{f^0_{\alpha,L}} = \mu_{L,\alpha}$$

Chemical potential of pure α at a reference state in the vapor phase

Fugacity of component of pure α and its corresponding reference fugacity in the vapor phase

The reference state for μ^0_α and f^0_α is **arbitrary** but must be **coherent**.

→ The same state must be chosen for both variables.

Vapor liquid equilibriums

At the reference state, we have:

$$\mu^0_{V,\alpha} - RT\ln f^0_{\alpha,V} = \mu^0_{L,\alpha} - RT\ln f^0_{\alpha,L}$$

Since we are free to choose a reference state, let's choose one where the two phases are at equilibrium (i.e. at $P_{sat,\alpha}$ and $T_{sat,\alpha}$):

$$\mu^0_{V,\alpha} = \mu^0_{L,\alpha} \quad \rightarrow \quad f^0_{V,\alpha} = f^0_{L,\alpha}$$

Substitution into our V-L equilibrium equation:

$$\mu_{V,\alpha} = \mu^0_{V,\alpha} + RT\ln\frac{f_{\alpha,V}}{f^0_{\alpha,V}} = \mu^0_{L,\alpha} + RT\ln\frac{f_{\alpha,L}}{f^0_{\alpha,L}} = \mu_{L,\alpha}$$

Leads to:

$$f_{V,\alpha} = f_{L,\alpha}$$

A fundamental rule of VLEs!

Vapor liquid equilibriums

At the reference state, we have:

$$\mu^0_{V,\alpha} - RT\ln f^0_{\alpha,V} = \mu^0_{L,\alpha} - RT\ln f^0_{\alpha,L}$$

What if we have a random reference state?

$$\mu^0_{V,\alpha} - \mu^0_{L,\alpha} = RT\ln\frac{f^0_{V,\alpha}}{f^0_{L,\alpha}}$$

Substitution into our V-L equilibrium equation:

$$\mu_{V,\alpha} - \mu_{L,\alpha} = \mu^0_{V,\alpha} - \mu^0_{L,\alpha} + RT\ln\frac{f_{\alpha,V}f^0_{\alpha,L}}{f^0_{\alpha,V}f_{\alpha,L}}$$

Leads to:

$$\mu_{V,\alpha} - \mu_{L,\alpha} = 0 = RT\ln\frac{f^0_{\alpha,V}}{f^0_{\alpha,L}} + RT\ln\frac{f_{\alpha,V}f^0_{\alpha,L}}{f^0_{\alpha,V}f_{\alpha,L}}$$

Once again, we get: $f_{V,\alpha} = f_{L,\alpha}$

Note: so far, no simplifications have been made (e.g. ideality, etc.)

Vapor liquid equilibriums

We know that we can further develop VLE expressions based on:

$$f_{V,\alpha} = f_{L,\alpha}$$

Let's further define fugacities such that:

$$f_{V,\alpha} = \varphi_{\alpha,V}\,y_\alpha P \qquad f_{L,\alpha} = \varphi_{\alpha,L}\,x_\alpha P = \gamma_\alpha x_\alpha f^0_{L,\alpha}$$

Fugacity coefficient for α in the vapor phase

Molar fraction of α in the vapor phase

Pressure

Molar fraction of α in the liquid phase

Activity coefficient for α in the liquid phase

Reference fugacity for α in the liquid phase

Which definition is chosen for $f_{L,\alpha}$ will depend on the property estimation model.

Note: up to this point, we have not solved anything! We have just added terms to make x_α, y_α and P appear.

Vapor liquid equilibriums

Our V-L equilibrium expression becomes:

$$\varphi_{\alpha,V} y_\alpha P = \gamma_\alpha x_\alpha f^0_{L,\alpha}$$

Let's start by defining $f^0_{L,\alpha}$:

$$f^0_{L,\alpha} = f_{L,\alpha}\underbrace{(T,P,x_\alpha = 1)} = \varphi_{\alpha,L} x_\alpha P = \varphi_{\alpha,L} P$$

We just chose a reference state at T, P
(the conditions of interest) and pure α.

Let's add:

$$f^0_{L,\alpha} = \varphi_{\alpha,L} P = \varphi^{sat}_{\alpha,L} P_{sat} \frac{\varphi_{\alpha,L} P}{\varphi^{sat}_{\alpha,L} P_{sat}}$$

Fugacity
coefficient of α
at T and P_{sat}

P_{sat} for pure α at T

Vapor liquid equilibriums

Our V-L equilibrium expression:

$$\varphi_{\alpha,V} y_\alpha P = \gamma_\alpha x_\alpha f^0_{L,\alpha}$$

From Maxwell relations, we have:

Partial molar volume of α

$$\varphi_\alpha = \exp\left[\int_0^P \frac{\overline{v_\alpha}}{RT} - 1/P \;\; dP\right]$$

Therefore:

$$\frac{\varphi_{\alpha,L}}{\varphi^{sat}_{\alpha,L}} = \exp\left[\int_0^P \frac{\overline{v_\alpha}}{RT} - 1/P \;\; dP - \int_0^{P_{sat}} \frac{\overline{v_\alpha}}{RT} - 1/P \;\; dP\right] = \exp\left[\int_{P_{sat}}^P \frac{\overline{v_\alpha}}{RT} - 1/P \;\; dP\right]$$

$$= \exp\left[\int_{P_{sat}}^P \frac{\overline{v_\alpha}}{RT} \;\; dP - \ln\frac{P}{P_{sat}}\right] = \frac{P_{sat}}{P}\exp\left[\int_{P_{sat}}^P \frac{\overline{v_\alpha}}{RT} \;\; dP\right]$$

With this we can rewrite our equation for :

$$f^0_{L,\alpha} = \varphi^{sat}_{\alpha,L} P_{sat} \frac{\varphi_{\alpha,L} P}{\varphi^{sat}_{\alpha,L} P_{sat}} = \varphi^{sat}_{\alpha,L} P_{sat} \exp\left[\int_{P_{sat}}^P \frac{\overline{v_{L,\alpha}}}{RT} \;\; dP\right]$$

Vapor liquid equilibriums

Our V-L equilibrium expression becomes:

$$\varphi_{\alpha,V} y_\alpha P = \gamma_\alpha x_\alpha \varphi_{\alpha,L}^{sat} P_{sat} \exp\left[\int_{P_{sat}}^{P} \frac{\overline{v_{L,\alpha}}}{RT}\, dP\right]$$

At this point, no simplifications have been made. So, why have we done this?

→ To organize our simplifications:

- Simplification 1: ideal solution $\rightarrow \gamma = 1$ **Can rarely be assumed…**
- Simplification 2: ideal gas $\rightarrow \varphi = 1$ **Can usually be assumed…**
- Simplification 3: negligible changes in liquid molar volume (→ incompressible liquids!)

$$\rightarrow \underbrace{\exp\left[\int_{P_{sat}}^{P} \frac{\overline{v_{L,\alpha}}}{RT}\, dP\right]}_{\text{Poynting factor}} = \exp(0) = 1$$

Can almost always be assumed…

Vapor liquid equilibriums

Our equation:

$$\varphi_{\alpha,V} y_\alpha P = \gamma_\alpha x_\alpha \varphi_{\alpha,L}^{sat} P_{sat} \exp\left[\int_{P_{sat}}^{P} \frac{\overline{v_{L,\alpha}}}{RT}\, dP\right]$$

With all these simplifications:

$$\underbrace{\rightarrow \gamma = 1 \qquad \rightarrow \varphi = 1 \qquad \rightarrow \exp\left[\int_{P_{sat}}^{P} \frac{\overline{v_{L,\alpha}}}{RT}\, dP\right] = 1}_{\textbf{Ideal case}}$$

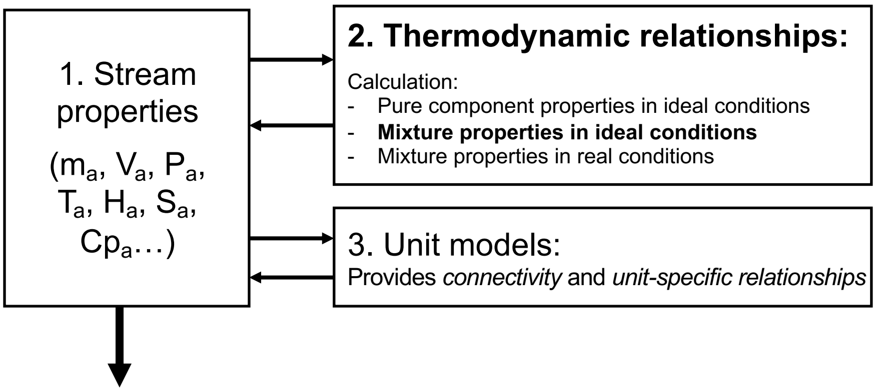
Becomes:

$$y_\alpha P = x_\alpha P_{sat}$$

Raoult’s law can be used to fully calculate VLEs in ideal conditions.

Process Modeling

The approach:



1. Stream properties

(m_a, V_a, P_a, T_a, H_a, S_a, Cp_a…)

2. Thermodynamic relationships:

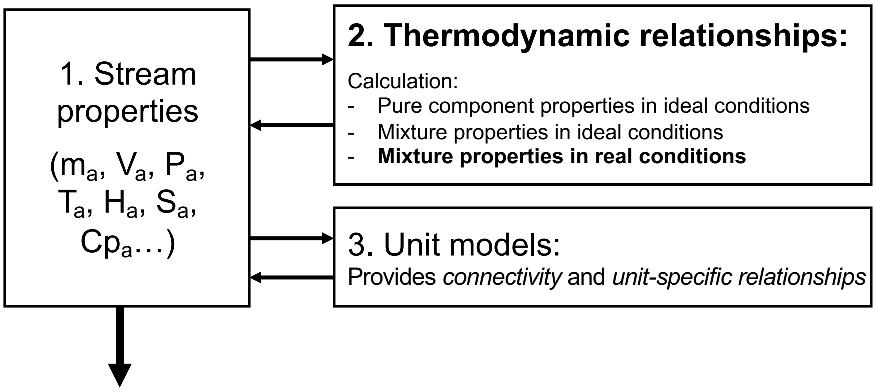
Calculation:
- Pure component properties in ideal conditions
- **Mixture properties in ideal conditions**
- Mixture properties in real conditions

3. Unit models:
Provides *connectivity* and *unit-specific relationships*

Heat and material flows

Process Modeling

The approach:



1. Stream properties

(m_a, V_a, P_a, T_a, H_a, S_a, Cp_a…)

2. Thermodynamic relationships:

Calculation:
- Pure component properties in ideal conditions
- Mixture properties in ideal conditions
- **Mixture properties in real conditions**

3. Unit models:
Provides *connectivity* and *unit-specific relationships*

Heat and material flows

Vapor liquid equilibriums

Starting point for real solution:

$$\varphi_{\alpha,V} y_\alpha P = \gamma_\alpha x_\alpha \varphi^{sat}_{\alpha,L} P_{sat} \exp\left[\int_{P_{sat}}^{P} \frac{\overline{v_{L,\alpha}}}{RT}\, dP\right]$$

This is always true!

The approximation that $\gamma = 1$ is almost never true → We need a model for γ

Strategy 1: Activity coefficient models

The estimation is based on empirical functions that estimate excess Gibbs free energy:

$$\overline{G} = \overline{G}_{Id} + \overline{G}_E$$

Partial molar Gibbs free energy

Partial molar Gibbs free energy in ideal conditions

Excess partial molar Gibbs free energy

$$\overline{G}_E = f(x_\alpha, x_\beta, \ldots, T)$$

Activity coefficient models usually model $\overline{G}_E$ with a function of x_α and T

Vapor liquid equilibriums

Strategy 1: Activity coefficient models

How does $\overline{G}_E$ relate to γ?

The definition of $\overline{G}$:

$$\left(\frac{\partial G}{\partial n_\alpha}\right)_{T,P,n_{\alpha\neq\beta}} = \left(\frac{\partial (n\overline{G})}{\partial n_\alpha}\right)_{T,P,n_{\alpha\neq\beta}} = \overline{G}_\alpha$$

Recall that:

$$dG = -SdT + VdP + \sum_p \sum_\alpha \mu_{p,\alpha} dn_{p,\alpha} \rightarrow \overline{G}_\alpha = \mu_\alpha$$

$$\overline{G}_\alpha = \mu_\alpha = \mu^0_\alpha + RT\ln\frac{f_\alpha}{f^0_\alpha} \underset{\substack{\uparrow \\ f_\alpha = \gamma_\alpha x_\alpha f^0_\alpha}}{=} \mu^0_\alpha + RT\ln\gamma_\alpha x_\alpha = \underbrace{\mu^0_\alpha + RT\ln x_\alpha}_{\overline{G}_{Id,\alpha}} + \underbrace{RT\ln\gamma_\alpha}_{\overline{G}_{E,\alpha}}$$

Therefore:

$$\overline{G}_{E,\alpha} = RT\ln\gamma_\alpha = \frac{\partial}{\partial n_\alpha}\left[\left(\sum_k n_k\right)\left(\overline{G}_E\right)\right] = \frac{\partial}{\partial n_\alpha}\left[\left(\sum_k n_k\right)\left(f(x_\alpha, x_\beta, \ldots, T)\right)\right]$$

Vapor liquid equilibriums

Strategy 1: Activity coefficient models

This formula:

$$RT\ln\gamma_\alpha = \frac{\partial}{\partial n_\alpha}\left[\left(\sum_k n_k\right)\left(f(x_\alpha, x_\beta, ..., T)\right)\right]$$

Allows us to relate γ to our excess Gibbs free energy model *f(*x_α*,* x_β*,…, T)*

See an example of how to use this formula with the Margules model in Problem 1 of Problem Set 6.

Common models include:

- Margules model: binary parameter model: $\overline{G}_E / RT = Ax_1x_2$
- NRTL (non-random two liquid): more complex binary parameter model
- UNIQUAC (Universal Quasi Chemical): parameters model based on functional groups

Vapor liquid equilibriums

Strategy 1: Activity coefficient models

From the excess free energy, we can calculate other thermodynamic properties:

$$\overline{V}_{E,L} = \left(\frac{\partial \overline{G}_{E,L}}{\partial P}\right)_T \qquad \Delta\overline{S}_{E,L} = -\left(\frac{\partial \overline{G}_{E,L}}{\partial T}\right)_P \qquad \Delta\overline{H}_{E,L} = \Delta\overline{G}_{E,L} + T\Delta\overline{S}_{E,L}$$

In summary: we can calculate all excess properties for the liquid phase and the activity coefficients for each component.

This takes care of all cases where liquids do not behave ideally: $\rightarrow \gamma \neq 1$

→ **Very often**

What about when the gases are acting non-ideally? $\rightarrow \varphi \neq 1$

Vapor liquid equilibriums

Strategy 2: Equation of state (EOS) models

With activity coefficient models, we started by modeling a thermodynamic property (G_E) and derived a volumetric property (V_E). With EOS models, we start with volumetric properties and will arrive at thermodynamic properties.

An EOS: $P = f(R, T, V, z_\alpha, z_\beta, \ldots)$ → Allows you to calculate $V_{L\ or\ V}$

Molar fraction of α in the
total mixture

From Maxwell relations:

$$\varphi_{\alpha,L} = \exp\left[\int_0^P \frac{\overline{v_{\alpha,L}}}{RT} - 1/P \;\; dP\right] \qquad \varphi_{\alpha,V} = \exp\left[\int_0^P \frac{\overline{v_{\alpha,V}}}{RT} - 1/P \;\; dP\right]$$

Where: $\bar{v}_{\alpha,\,\mathrm{L\ or\ V}} = \left(\dfrac{\partial V_{\mathrm{L\ or\ V}}}{\partial n_\alpha}\right)_{T,P,n_{\beta\neq\alpha}}$

Vapor liquid equilibriums

Strategy 2: Equation of state (EOS) models

With activity coefficient models, we started by modeling a thermodynamic property (G_E) and derived a volumetric property (V_E). With EOS models, we start with volumetric properties and will arrive at thermodynamic properties.

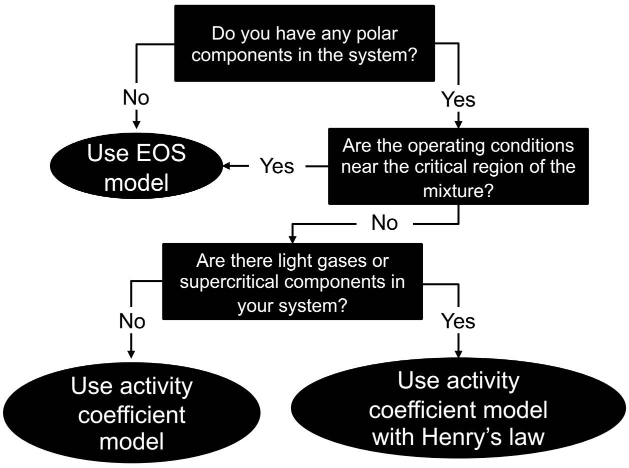
An EOS: $P = f(R, T, V, z_\alpha, z_\beta, \ldots)$ → Allows you to calculate $V_{L\ or\ V}$

Molar fraction of α in the
total mixture

Note: Most EOS are *P = f(V,T…)* not *V = f(P,T…)*, but we can use another Maxwell relation:

$$RT\ln\varphi_{\alpha,\mathrm{L\ or\ V}} = \int_{V_{\mathrm{L\ or\ V}}}^{\infty}\left[\left(\frac{\partial P}{\partial n_\alpha}\right)_{T,P,n_{\beta\neq\alpha}} - RT/V_{\mathrm{L\ or\ V}}\right] dV - RT\ln\frac{PV_{\mathrm{L\ or\ V}}}{nRT}$$

Choosing your thermodynamic property estimation method



Source: Aspentech

Thermodynamic relationships

Now we have:

- Pure component properties in ideal conditions
- Mixture properties in ideal conditions
- Mixture properties in real conditions

We have all the necessary thermodynamic relationships. We can use these relations to construct the matrix ***Th$_a$*** (for stream a):

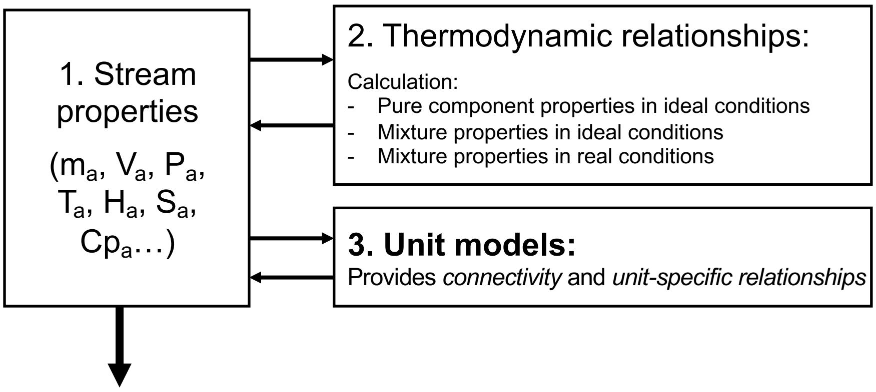
$$\mathbf{Th}_a(T_a, P_a, Cp_{a,}, h_a, z_{\alpha,a}, z_{\beta,a}, \ldots) = 0$$

Temperature
Pressure
Heat capacity of stream a
Enthalpy of stream a
Molar (or mass) fractions of components α or β in the total mixture of stream a

An overall specification matrix ***Th*** is constructed by putting together all of these stream matrices.

Process Modeling

The approach:



1. Stream properties

(m_a, V_a, P_a, T_a, H_a, S_a, Cp_a…)

2. Thermodynamic relationships:

Calculation:

- Pure component properties in ideal conditions
- Mixture properties in ideal conditions
- Mixture properties in real conditions

3. Unit models:
Provides *connectivity* and *unit-specific relationships*

Heat and material flows

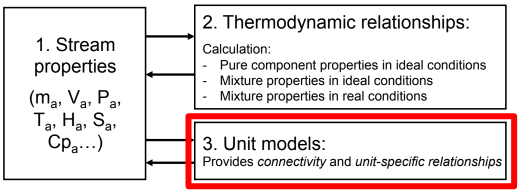
Unit models

Recall the total number of specifications needed for streams:

$$N_{Specifications} = N_{streams,Q} + N_{streams,W_{el}} + 2N_{streams,W_{mech.}} + N_{streams,material}(2+N_c)$$

This number of specifications can be reduced through unit models:

- Mass balances
- Energy balances
- Momentum balances
- Unit-specific relations



1. Stream properties

(m_a, V_a, P_a, T_a, H_a, S_a, Cp_a…)

2. Thermodynamic relationships:

Calculation:

- Pure component properties in ideal conditions
- Mixture properties in ideal conditions
- Mixture properties in real conditions

3. Unit models:
Provides *connectivity* and *unit-specific relationships*

Unit models

1. Balances:

Basic balance structure (mass, energy or momentum):

$$In - Out = Accumulation + Source$$

For continuous processes, there is no accumulation. For total mass, energy or momentum balances, there is no source:

$$In - Out = 0$$

Momentum balances are used in specialized systems (including prominently in atmospheric models).

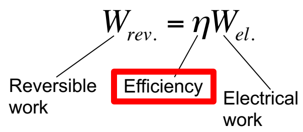
Balances are the basis of **connectivity** in systems models!

Unit models

2. Unit models:

Unit models are the second category of equations within Units. They define a relation that is specific to the unit in question and usually introduce model parameters which must be specified.

Example 1:



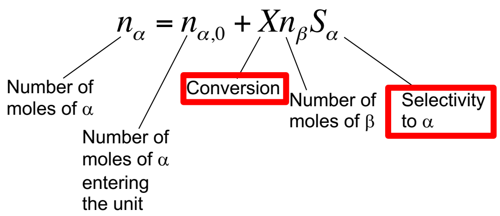
$$W_{rev.} = \eta W_{el.}$$

Reversible work

Efficiency

Electrical work

Example 2:



$$n_{\alpha} = n_{\alpha,0} + X n_{\beta} S_{\alpha}$$

Number of moles of α

Number of moles of α entering the unit

Conversion

Number of moles of β

Selectivity to α

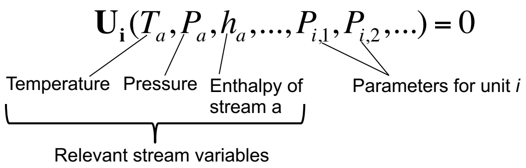
Parameters are added to the total number of system variables.

Unit models

Overall we have:

- Balance equations (mass, energy, momentum)
- Unit equations

These equations will form their own matrix ***Ui*** (for unit i):

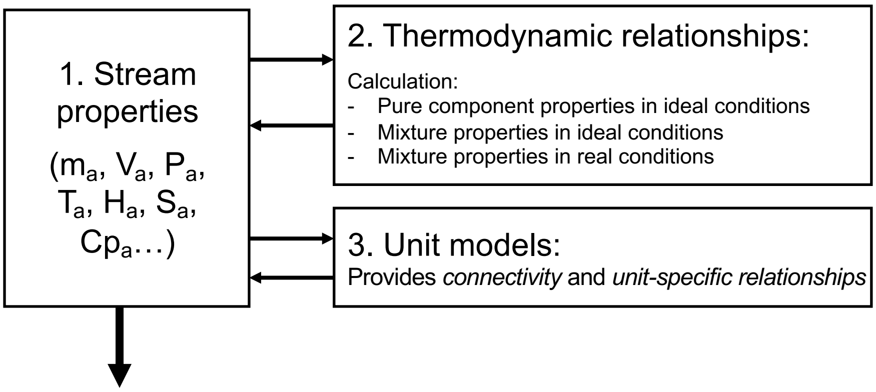


$$\mathbf{U_i}(T_a, P_a, h_a, \ldots, P_{i,1}, P_{i,2}, \ldots) = 0$$

An overall specification matrix ***U*** is constructed by putting together all of these unit matrices.

Process Modeling

The approach:



1. Stream properties

(m_a, V_a, P_a, T_a, H_a, S_a, Cp_a…)

2. Thermodynamic relationships:

Calculation:
- Pure component properties in ideal conditions
- Mixture properties in ideal conditions
- Mixture properties in real conditions

3. Unit models:

Provides *connectivity* and *unit-specific relationships*

Heat and material flows

Process modeling

Now we have everything:

- Stream properties
- Thermodynamic relationships
- Unit models

We can now build an overall set of equations represented by the matrix ***F***:

$$\mathbf{F} = \begin{bmatrix} \mathbf{S}_a(T_a, P_a, h_{\alpha,a}, x_{\alpha,a}, x_{\beta,a}, ...) \\ \mathbf{S}_b(T_b, P_b, h_{\alpha,b}, x_{\alpha,b}, x_{\beta,b}, ...) \\ ... \\ \mathbf{Th}_a(T_a, P_a, h_a, Cp_a, z_{\alpha,a}, z_{\beta,a}, ...) \\ \mathbf{Th}_b(T_b, P_b, h_b, Cp_b, z_{\alpha,b}, z_{\beta,b}, ...) \\ ... \\ \mathbf{U}_\mathbf{i}(T_a, P_a, h_a, ..., P_{i,1}, P_{i,2}, ...) \\ \mathbf{U}_j(T_b, P_b, h_b, ..., P_{j,1}, P_{j,2}, ...) \\ ... \end{bmatrix} = 0$$

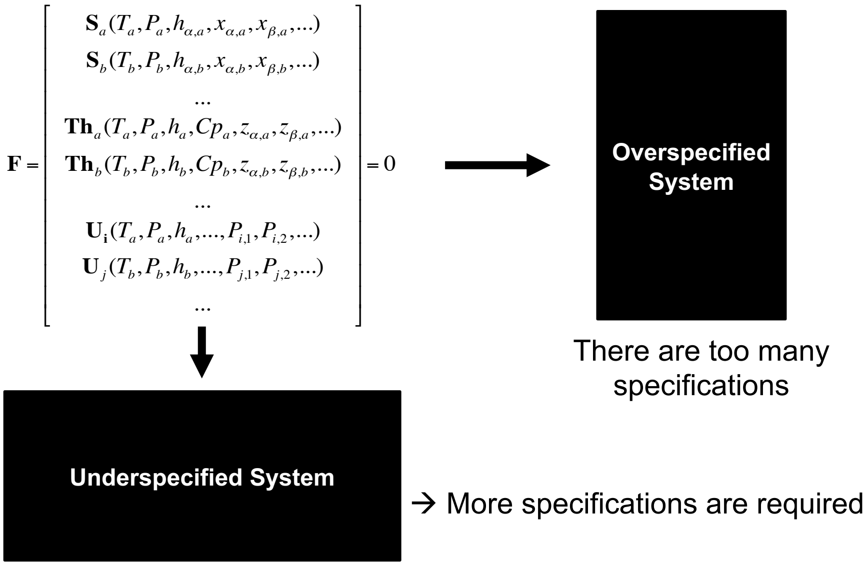
Process modeling

Requirements for solving ***F***:

- The matrix must be square
  → Number of variables must equal the number of equations
- The equations must be independent
  → Line and column permutations must lead to the placement of a nonzero element on each diagonal position

$$\mathbf{F} = \begin{bmatrix} \mathbf{S}_a(T_a, P_a, h_{\alpha,a}, x_{\alpha,a}, x_{\beta,a}, ...) \\ \mathbf{S}_b(T_b, P_b, h_{\alpha,b}, x_{\alpha,b}, x_{\beta,b}, ...) \\ ... \\ \mathbf{Th}_a(T_a, P_a, h_a, Cp_a, z_{\alpha,a}, z_{\beta,a}, ...) \\ \mathbf{Th}_b(T_b, P_b, h_b, Cp_b, z_{\alpha,b}, z_{\beta,b}, ...) \\ ... \\ \mathbf{U}_\mathbf{i}(T_a, P_a, h_a, ..., P_{i,1}, P_{i,2}, ...) \\ \mathbf{U}_j(T_b, P_b, h_b, ..., P_{j,1}, P_{j,2}, ...) \\ ... \end{bmatrix} = 0$$

Process modeling



$$\mathbf{F} = \begin{bmatrix} \mathbf{S}_a(T_a,P_a,h_{\alpha,a},x_{\alpha,a},x_{\beta,a},\ldots) \\ \mathbf{S}_b(T_b,P_b,h_{\alpha,b},x_{\alpha,b},x_{\beta,b},\ldots) \\ \ldots \\ \mathbf{Th}_a(T_a,P_a,h_a,Cp_a,z_{\alpha,a},z_{\beta,a},\ldots) \\ \mathbf{Th}_b(T_b,P_b,h_b,Cp_b,z_{\alpha,b},z_{\beta,b},\ldots) \\ \ldots \\ \mathbf{U}_\mathbf{i}(T_a,P_a,h_a,\ldots,P_{i,1},P_{i,2},\ldots) \\ \mathbf{U}_j(T_b,P_b,h_b,\ldots,P_{j,1},P_{j,2},\ldots) \\ \ldots \end{bmatrix} = 0$$

Overspecified System

There are too many specifications

Underspecified System

→ More specifications are required

Outline of Part 3

Objective: Cover the basic principles of Systems Modeling for a Renewable Energy Process and be able to model a simple system.

- Importance of Systems Modeling in Renewable Energy
- Modeling systems
  - Stream properties
  - Thermodynamic relationships
  - Unit models
- **Heat integration & Pinch Analysis**
  - Basic Principles
  - Composite Curves
  - The Heat Cascade and the Grand Composite Curve
- Life Cycle Assessment
  - Goal & Scope Definition
  - Life Cycle Inventory
  - Life Cycle Impact Assessment
- Uncertainty Analysis & The Monte Carlo Method

Energy integration

Energy integration is the concept of recovering and valorizing heat within a process.

Energy integration shapes our current energy landscape

Without energy integration, several common products would be significantly more expensive, including:

- Gasoline
- Petrochemicals
- Electricity
- Heating in certain cities or complexes

Energy integration

Source: *Wikimedia commons*

Energy integration

For energy production the important question is: **How much energy do I need after a cost effective heat recovery was performed?**

Heat integration answers that question.

Pinch analysis

Definition: *Pinch analysis* is a systematic method for performing heat integration (it can be performed by a computer!).

Pinch analysis calculates:

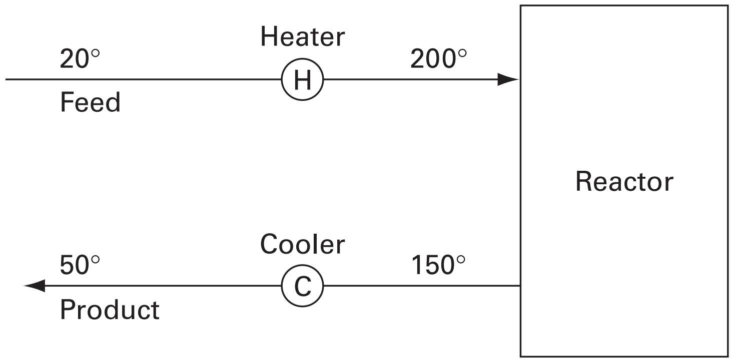
- The minimum heating requirement
- The minimum cooling requirement

} These define the minimum external requirements of the process. Reaching these minima depends on economic factors…

Let's begin with an example…

Pinch analysis

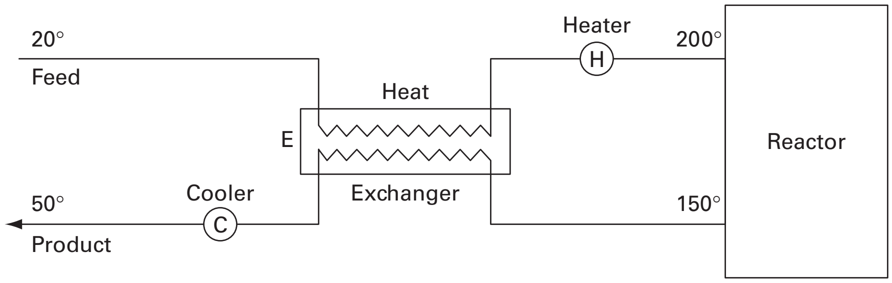
An example:



This could be more efficient...

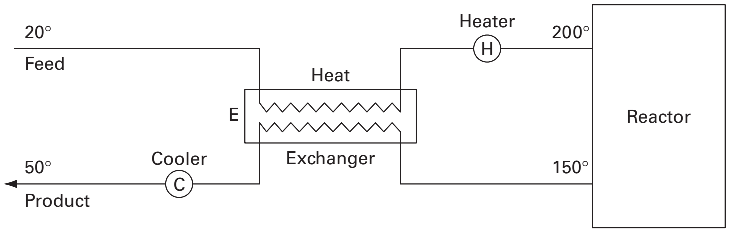
Pinch analysis

A slightly more efficient example:



By introducing a heat exchanger, we can recover some of the heat, but how much?

Pinch analysis



How much heat can we recover? We are limited by:

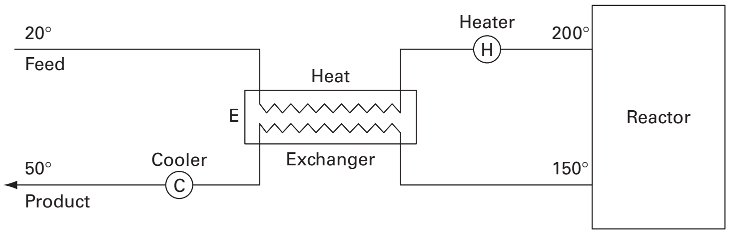
- Temperature difference = the driving force of heat exchange

  You cannot heat water from 90 to 100°C with water that needs to be cooled from 80°C to 60°C

- 1st law of thermodynamics: heat loads are conserved

  You cannot heat 1kg of water from 90 to 100°C with 1 g of water that needs to be cooled from 200°C to 190°C

Pinch analysis



Heat load calculation:

$$Q = \Delta H \;=\int_{T_1}^{T_2} Cp\,dT \;= Cp\;(T_2 - T_1)$$

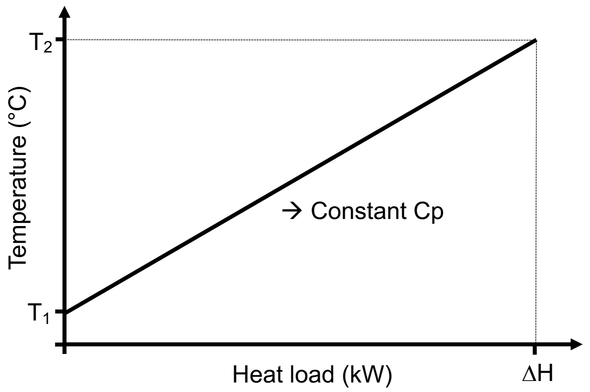
For a continuous process, we use enthalpy

Heat capacity

Assuming a constant Cp (or taking an average Cp)

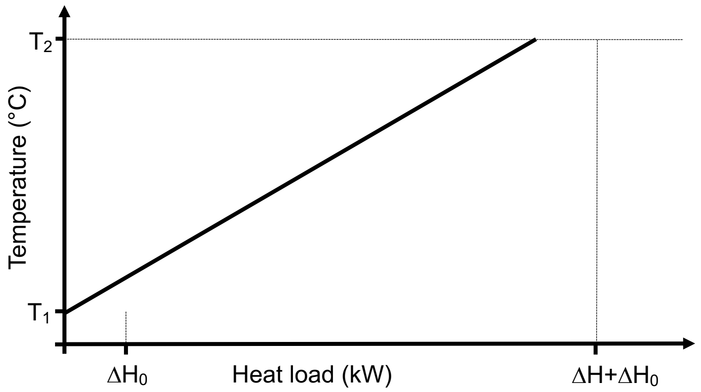
Pinch analysis

$$Q = \Delta H = Cp\ (T_2 - T_1) \quad \text{or} \quad T_2 = T_1 + \frac{1}{Cp}\Delta H$$

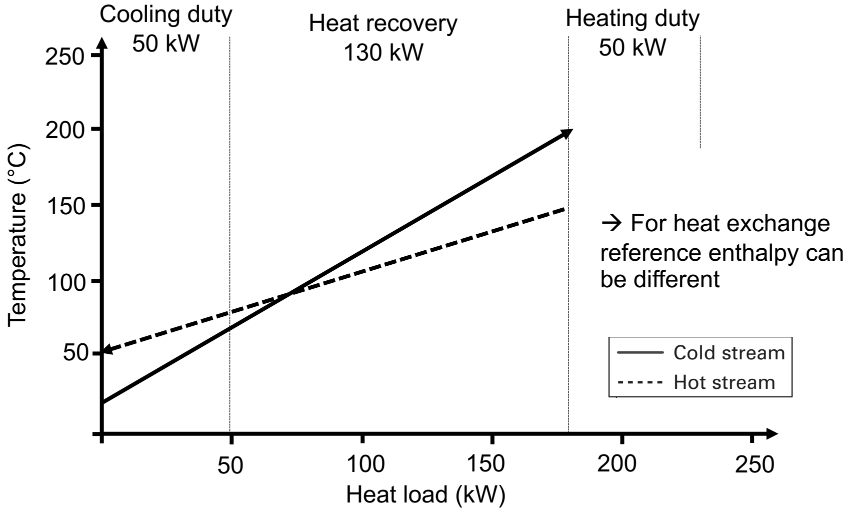


Pinch analysis

$$T_2 = T_1 + \frac{1}{Cp}(\Delta H_0 + \Delta H)$$

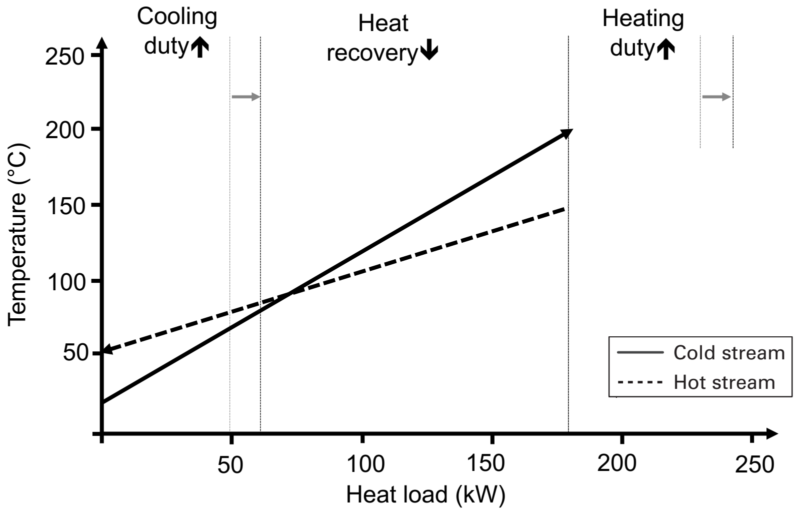


Pinch analysis

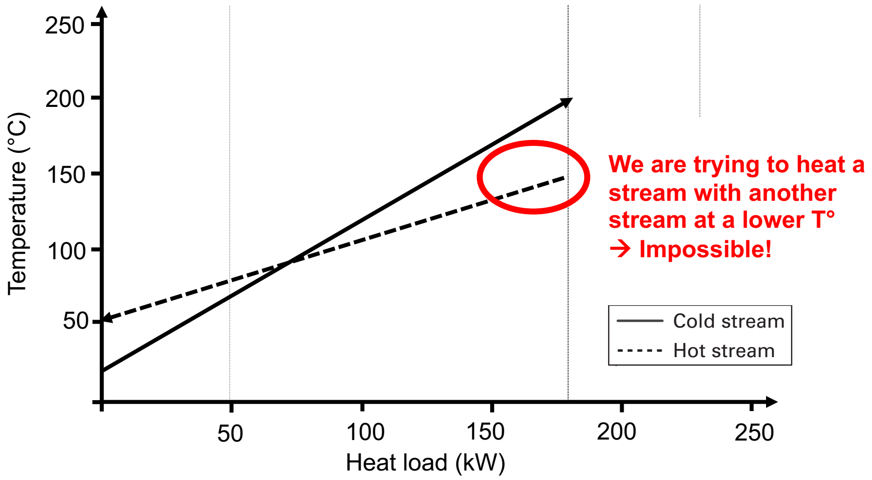


→ For heat exchange reference enthalpy can be different

Pinch analysis

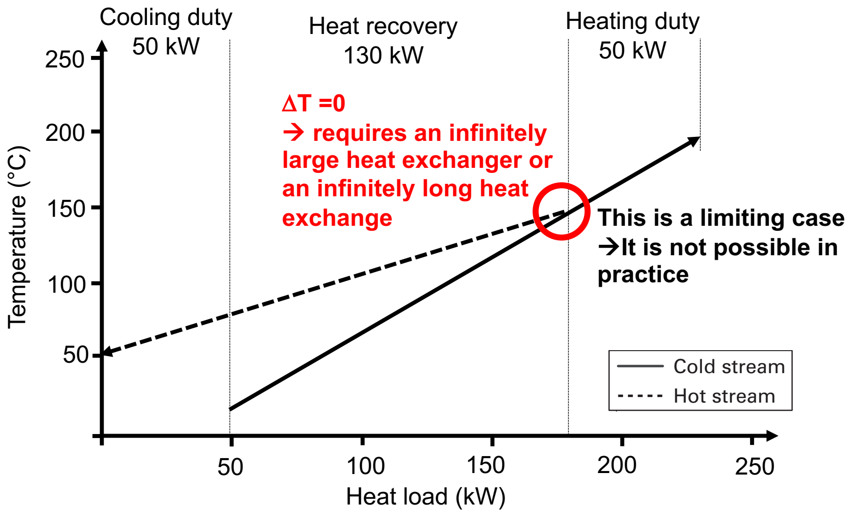


Pinch analysis



We are trying to heat a stream with another stream at a lower T°
→ Impossible!

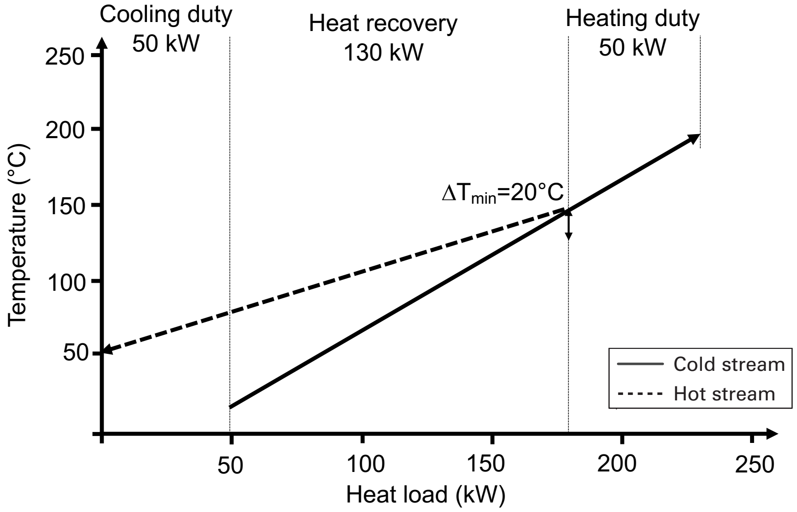
Pinch analysis



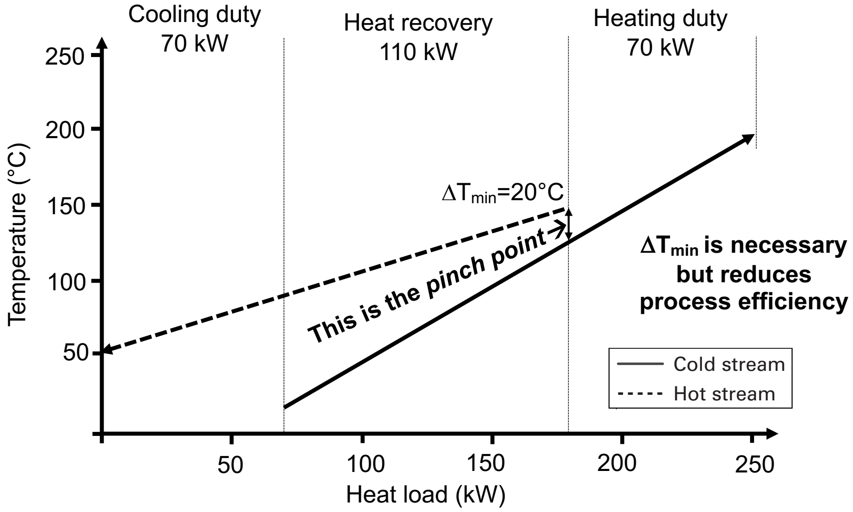
ΔT =0
→ requires an infinitely large heat exchanger or an infinitely long heat exchange

This is a limiting case
→It is not possible in practice

Pinch analysis



Pinch analysis



ΔT_{min} is necessary but reduces process efficiency