EPFL

Process units models and DOF

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Process unit model

Unit models represents by a set of equations the thermodynamic phenomena involved in the conversion of the flows in the process unit operation

Thermodynamic state
Constitutive equations

State variables inlet

$\dot{N}, T, P, \tilde{c}_i$

Simulation Equation

$f_m(\dot{N}_n, T_n, P_n, \tilde{c}_n, \pi_p) = 0$

State variable outlet

$\dot{N}, T, P, \tilde{c}_i$

Performances Parameters π_p

Simulation equations

- Mass balances
  - Chemical reactions
- Energy balances
- Performances equations
  - Reaction kinetics
  - Heat and mass transfer
  - Equilibrium
  - Compression

Generic form of balance equations

Accumulation = in - out + Generation - Consumption

Net accumulation in the control volume	=	+ Import in the control volume	- Export from the control volume
		+ Generation in the control volume	- Consumption in the control volume

Steady state model

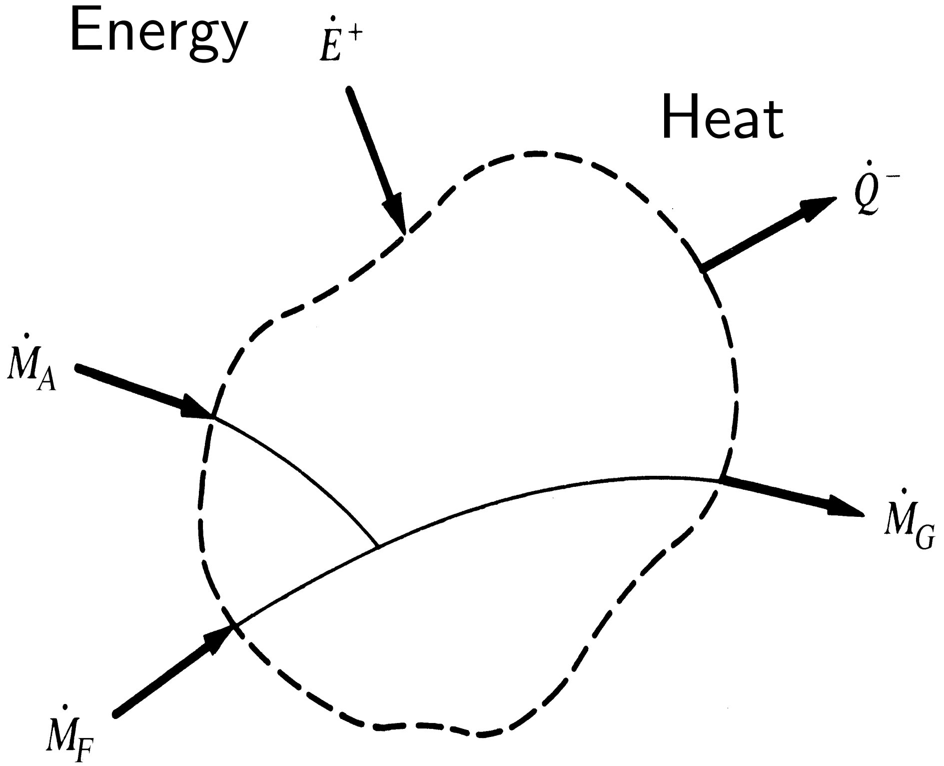
no Accumulation = 0 = in - out + Generation - Consumption

+	Import in the control volume	-	Export from the control volume

=

+	Generation in the control volume	-	Consumption in the control volume

For a given control volume with 1 network with N_c substances without chemical reactions



Materials

Control volume boundary

Mass network

N_c mass balances per network*

1 energy balance

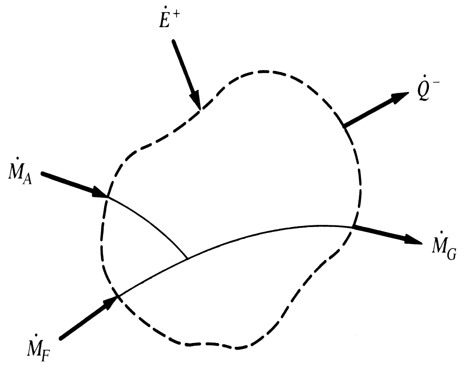
1 impulsion balance (P)

N_c+2 balance equations

*when chemical reactions occur the material balance is the atomic balance

Network : interconnected flows with mass exchange

For a given control volume with 1 network with N_c substances



Material balance

$$\sum_f \dot{m}^+_{c,f} = \underbrace{\frac{dM_c}{dt}}_{\text{Accumulation}} = 0 \qquad \forall c$$

Energy balance

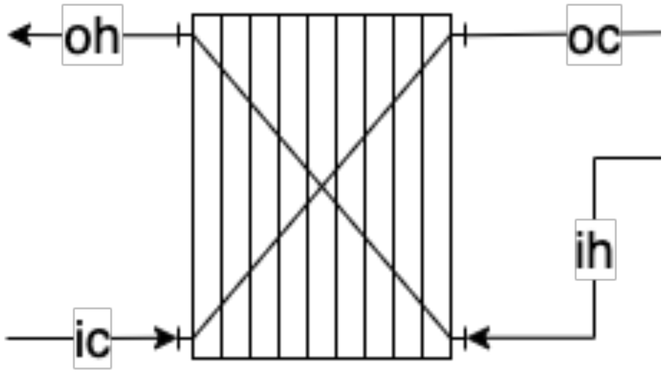
$$\sum_f \dot{m}^+_f \cdot h(T_f, P_f, x_f) + \sum_Q \dot{Q}^+ + \sum_E \dot{E}^+ = \underbrace{\frac{dQ}{dt}}_{\text{Accumulation}} = 0$$

Subscript + means positive when entering

$h(T_f, P_f, x_f)$ enthalpy of flow f with temperature T_f, Pressure P_f and composition x_f

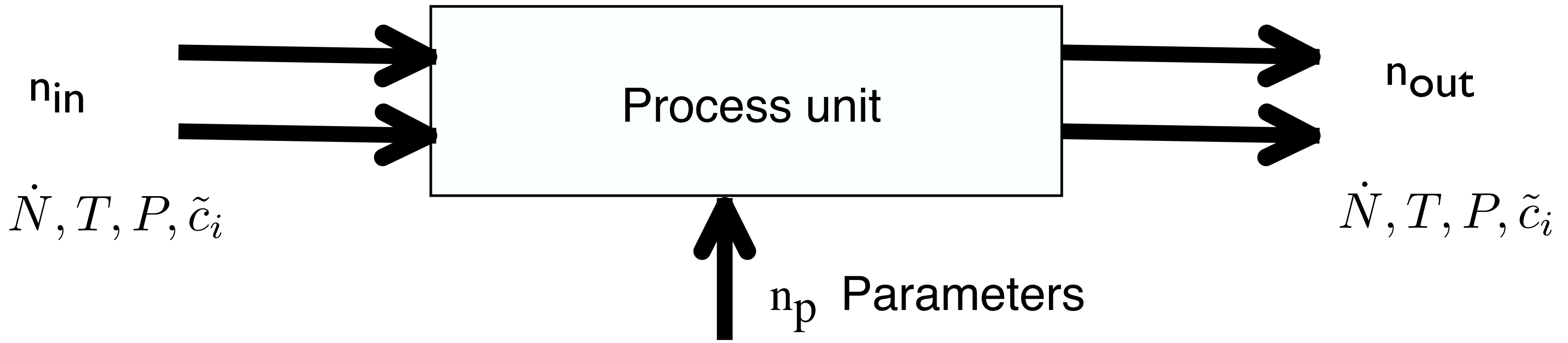
Non linear equations !

Unit model : heat exchanger



Nb.	Equation
1(EB)	$\dot{Q} = \dot{m}_{ci} cp_c (T_{co} - T_{ci})$
2(EB)	$\dot{Q} = \dot{m}_{hi} cp_h (T_{hi} - T_{ho})$
3(MB)	$\dot{m}_{hi} = \dot{m}_{ho}$
4(MB)	$\dot{m}_{ci} = \dot{m}_{co}$
5(P)	$P_{hi} = P_{ho}$
6(P)	$P_{ci} = P_{co}$
7(M)	$\dot{Q} = UA \frac{(T_{hi}-T_{co})-(T_{ho}-T_{ci})}{ln(\frac{(T_{hi}-T_{co})}{(T_{ho}-T_{ci})})}$

Degrees of freedom (DOF) of a unit model



Equations : n_e	
mass balances/network	n_c
Energy	1
Impulsion	n_i
models	n_m
specification	n_s

Variables : n_v	
State of the streams	$n_x=(n_{out} + n_{in})*(n_c+2)$
Unit parameters	n_p
Internal variables	n_t

$$DOF = n_v - n_e$$

DOF = number of set points to make the unit calculable

Equations (n_e+n_s) = Variables (n_v)

Fixing the degree of freedom : $n_s = n_v - n_e$

- Parameters : π_p are needed by the calculation mode of the unit
  - values from the literature -> references
- Specifications : $n_s = n_v - n_e$
  - Input flows X_u^+ : $\{\dot{N}_i, T, P\}$
  - Decision variables

    A decision variable is a variable for which you do not have a good reason to specify it to a given value

    - Operating conditions
    - Value is an assumption to a typical value (literature)
    - Will be defined by min and max bounds
    - Values to be tested by sensitivity analysis or to be obtained by optimisation

Different use of a process unit model: example heat exchanger

- Sizing to obtain the cost
  - Calculating the size of the unit

$$A = \frac{Q}{U \Delta T_{lm}}$$

U estimated

- Simulation
  - Outlet as a function of inlet $Q = U A \Delta T_{lm}$ U calculated by correlations

- Identification
  - Identify the heat transfer coefficient from measurement

$$U = \frac{Q}{A \Delta T_{lm}}$$

T measured

Unit models for process design : decision variables

- Type : defined by the model type
  - Temperature, pressure conditions
  - Purity for a separation
  - Reactor conversion
  - Reactor temperature and pression
  - Recycling rate
  - Purge fraction
- Expected values (prefer relative values)
  - Literature
  - Typical range

Conclusions

1. Draw the flowsheet
2. Identify the states to calculate the state of the system
    - list of flows with
        - a **name**
        - List of compounds
        - **Equation of state**
3. Calculate the degrees of freedom for the system
    - number of specifications
    - identify the variables to specify
    - define the values for the specification