EPFL

Solving Process units models

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

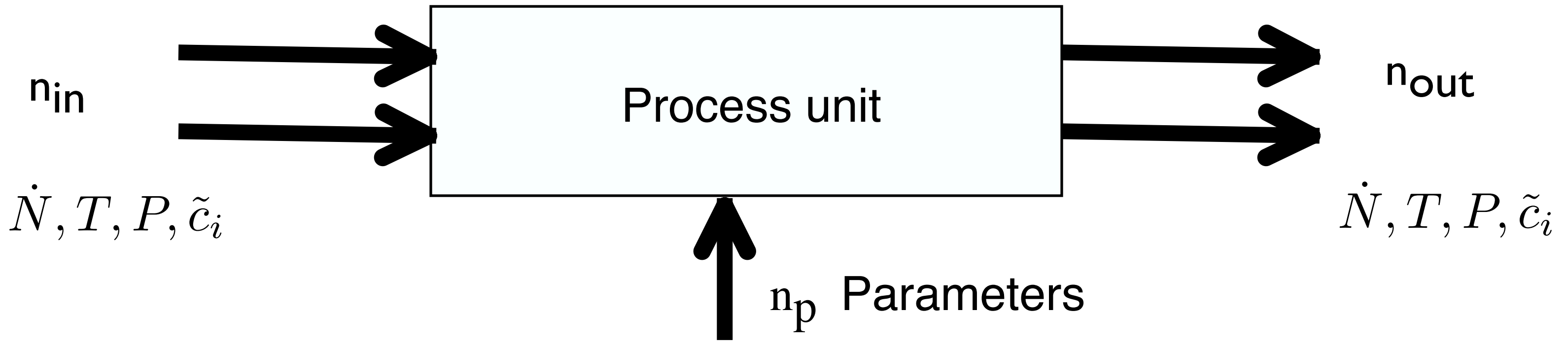
State variable outlet
$\dot{N}, T, P, \tilde{c}_i$

Performances Parameters π_p

Simulation equations

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

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

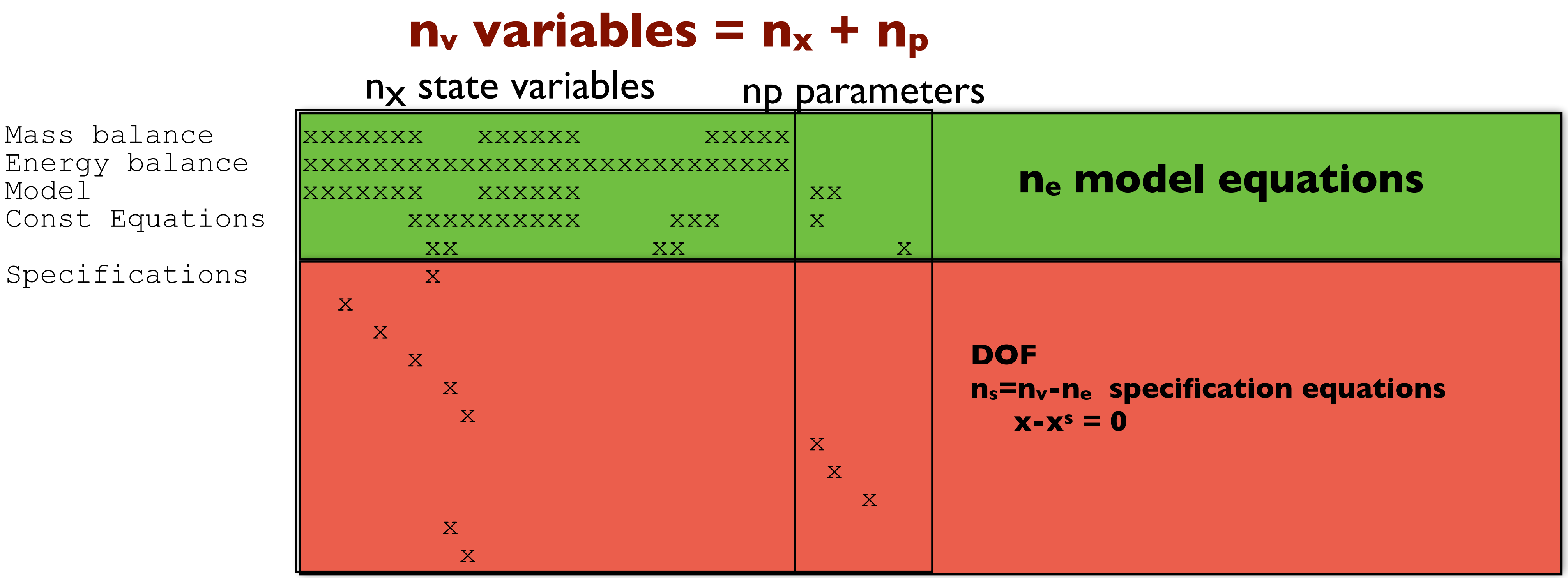
State of the streams	$n_x=(n_{out} + n_{in})*(n_c+2)$
Unit parameters	n_p
Internal variables	n_t

$$DOF = n_v - n_e$$

DOF = number of set points to make the unit calculable

Equations (n_e+n_s) = Variables (n_v)

Incidence Matrix of a Unit model

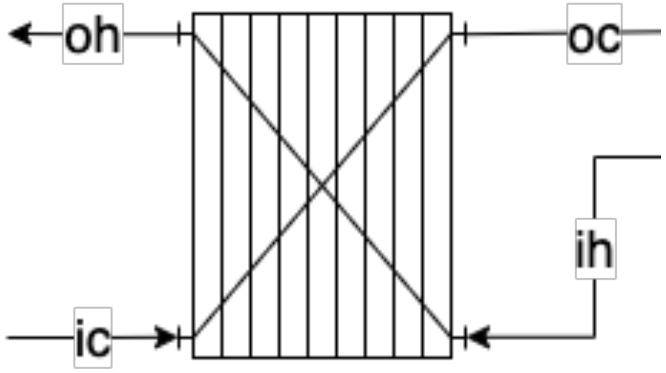


To solve the problem :

1) square matrix
2) independent equations

In the incidence matrix, the element (i,j) is equal to 1 if variable i is in equation j
It indicates the presence (incidence) of a variable (i) in the equation (j)

EPFL Unit model : heat exchanger



Nb.	Equation	1.$\dot{m}_{ci}$	2.T_{ci}	3.P_{ci}	4.$\dot{m}_{co}$	5.T_{co}	6.P_{co}	7.$\dot{m}_{hi}$	8.T_{hi}	9.P_{hi}	10.$\dot{m}_{ho}$	11.T_{ho}	12.P_{ho}	13.A	14.$\dot{Q}$	15.U
1(EB)	$\dot{Q} = \dot{m}_{ci} cp_c (T_{co} - T_{ci})$	x	x			x									x	
2(EB)	$\dot{Q} = \dot{m}_{hi} cp_h (T_{hi} - T_{ho})$							x	x			x			x	
3(MB)	$\dot{m}_{hi} = \dot{m}_{ho}$							x			x					
4(MB)	$\dot{m}_{ci} = \dot{m}_{co}$	x				x										
5(P)	$P_{hi} = P_{ho}$								x			x				
6(P)	$P_{ci} = P_{co}$			x			x									
7(M)	$\dot{Q} = UA\frac{(T_{hi}-T_{co})-(T_{ho}-T_{ci})}{ln(\frac{(T_{hi}-T_{co})}{(T_{ho}-T_{ci})})}$		x			x			x			x		x	x	x

Unit model : Incidence matrix

F(X) : Equations

Ne=Ns + Nb + Nm

X : Variables

- Nv state
- Ni intermediate
- Np parameters

Nx=Nv+Ni+Np

		X01	X02	X03	X04	X05	X06	X07	X08	X09	X10	X11	X12	X13	X14
Ns Specifications X-Xs=0	Eq1	x													
	Eq2		x												
	Eq3			x											
	Eq4				x										
	Eq5					x									
	Eq6						x								
Nb Balances B(Xin)-B(Xout)=0	Eq8		x						x						
	Eq9		x	x						x					
	Eq7	x						x							
	Eq10		x	x							x				
Nm Models M(X,P)=0	Eq11					x					x	x			
	Eq13					x							x	x	
Nc Constitutive equations C(X)=0	Eq14	x				x								x	x
	Eq12					x		x					x		

DOF analysis

Ne=Nx

Types of modelling equations

- Form of the equations
  - **Implicit form**
    - $f(x,y)=0$
  - **Explicit* form**
    - $y=f(x)$
- Types of equations
  - Balance equations
  - Constitutive equations (thermodynamic state) : non linear
  - Model equation
  - Specification equations (constants)
    - $x=x^s$
    - $x-x^s=0$

*Explicit could be also in the form of $y=f(x,y)$, in this case there is the need to solve a non linear equation (iterations) to calculate the value of y.

Solving a model : simultaneous approach

		X01	X02	X03	X04	X05	X06	X07	X08	X09	X10	X11	X12	X13	X14
Ns X-Xs=0	Eq1	x													
	Eq2		x												
	Eq3			x											
	Eq4				x										
	Eq5					x									
	Eq6						x								
Nb B(Xin)-B(Xout)=0	Eq8		x						x						
	Eq9		x	x						x					
	Eq7	x						x							
	Eq10		x	x							x				
Nm M(X,P)=0	Eq11					x					x	x			
	Eq13					x							x	x	
Nc C(X)=0	Eq14	x				x								x	x
	Eq12					x		x					x		

Find X such that

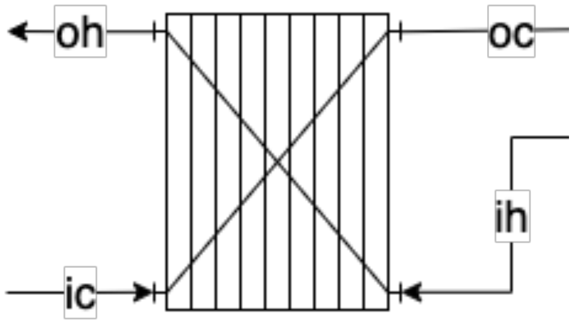
$F(X)=0$

For a given X, F(X) is evaluated

NxN

set of N non linear equations

Unit model : heat exchanger simultaneous resolution



Find X such that

F(X)=0

15x15

set of 15 non linear equations

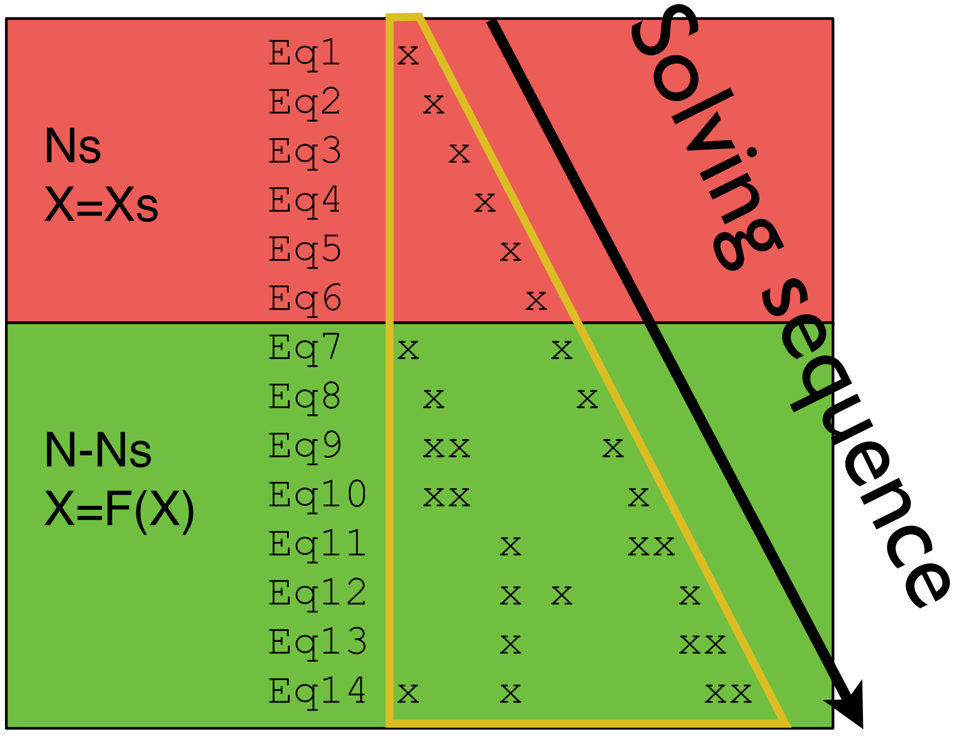
Nb.	Equation	$1.\dot{m}_{ci}$	$2.T_{ci}$	$3.P_{ci}$	$4.\dot{m}_{co}$	$5.T_{co}$	$6.P_{co}$	$7.\dot{m}_{hi}$	$8.T_{hi}$	$9.P_{hi}$	$10.\dot{m}_{ho}$	$11.T_{ho}$	$12.P_{ho}$	$13.A$	$14.\dot{Q}$	$15.U$
1(EB)	$\dot{Q} = \dot{m}_{ci} cp_c (T_{co} - T_{ci})$	x	x			x									x	
2(EB)	$\dot{Q} = \dot{m}_{hi} cp_h (T_{hi} - T_{ho})$							x	x			x			x	
3(MB)	$\dot{m}_{hi} = \dot{m}_{ho}$							x			x					
4(MB)	$\dot{m}_{ci} = \dot{m}_{co}$	x				x										
5(P)	$P_{hi} = P_{ho}$								x			x				
6(P)	$P_{ci} = P_{co}$			x			x									
7(M)	$\dot{Q} = UA \frac{(T_{hi} - T_{co}) - (T_{ho} - T_{ci})}{ln(\frac{(T_{hi} - T_{co})}{(T_{ho} - T_{ci})})}$		x			x			x			x		x	x	x
8(S)	$\dot{m}_{ci} = \dot{m}_{ci}^s$	x														
9(S)	$T_{ci} = T_{ci}^s$		x													
10(S)	$P_{ci} = P_{ci}^s$			x												
11(S)	$T_{hi} = T_{hi}^s$								x							
12(S)	$P_{hi} = P_{hi}^s$									x						
13(S)	$\dot{m}_{hi} = \dot{m}_{hi}^s$							x								
14(S)	$A = A^s$													x		
15(S)	$U = U^s$															x

Sequential resolution : case 1 (happy case)

1. Process mathematical equations to have an explicit form $X_i= f(X_{k \neq i})$
2. Rearrange the matrix to have a diagonal matrix

if $$diag_i = f(diag_k, k = 1, \ldots, i-1)$$

3. Define the order of resolution
   Solve the sequence



Sequential resolution : case 2 (non happy case)

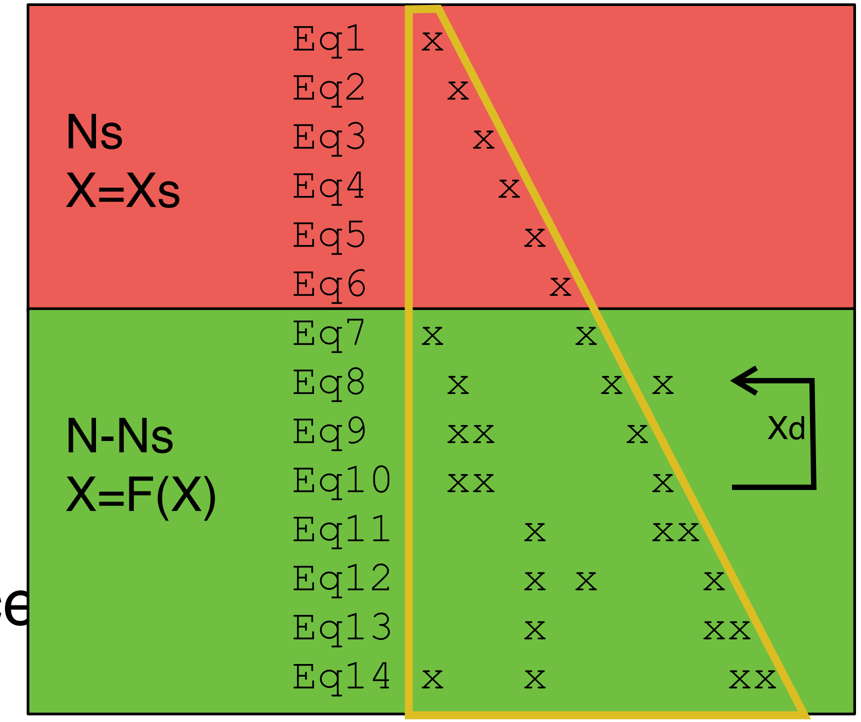
1. Process mathematical equations to have an explicit form $X_i = f(X)$
2. Rearrange the matrix to have a diagonal matrix

if not $$diag_i = f(diag_k, k = 1, \ldots, i-1)$$

3. Guess off-diagonal terms Xd

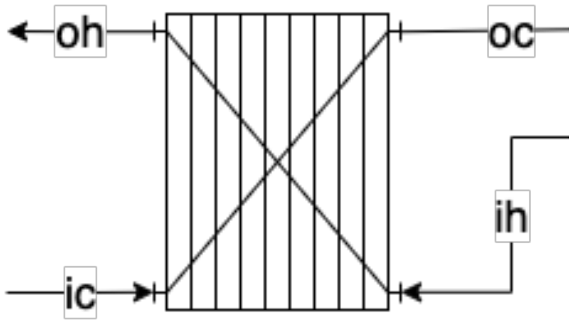
4. Define the order of resolution
5. Solve the sequence until Xd
   6.1 test convergence
   $Xd^k \;?\!= Xd^{k-1}$
   6.2 if No : update $Xd^{k+1} = Xd^k$
   -> back to 5
   6.3 if Yes continue with the sequence

Xd needed by Eq8 but calculated by Eq10



6.2 can also be solved by iterating to solve $Xd^k - Xd^{k-1} = 0$

Unit model : heat exchanger



Explicit form

$$diag_i = f(diag_k, k = 1, \ldots, i-1)$$

Nb.	Equation	$1.\dot{m}_{ci}$	$2.T_{ci}$	$3.P_{ci}$	$9.P_{hi}$	$8.T_{hi}$	$7.\dot{m}_{hi}$	$13.A$	$15.U$	$10.\dot{m}_{ho}$	$4.\dot{m}_{co}$	$6.P_{co}$	$12.P_{ho}$	$5.T_{co}$	$11.T_{ho}$	$14.\dot{Q}$
8(S)	$\dot{m}_{ci} = \dot{m}^s_{ci}$	x														
9(S)	$T_{ci} = T^s_{ci}$		x													
10(S)	$P_{ci} = P^s_{ci}$			x												
11(S)	$T_{hi} = T^s_{hi}$				x											
12(S)	$P_{hi} = P^s_{hi}$					x										
13(S)	$\dot{m}_{hi} = \dot{m}^s_{hi}$						x									
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3(MB)	$\dot{m}_{hi} = \dot{m}_{ho}$						x			x						
4(MB)	$\dot{m}_{ci} = \dot{m}_{co}$	x									x					
5(P)	$P_{hi} = P_{ho}$				x							x				
6(P)	$P_{ci} = P_{co}$			x									x			
1(EB)	$\dot{Q} = \dot{m}_{ci} cp_c (T_{co} - T_{ci})$	x	x											x		x
2(EB)	$\dot{Q} = \dot{m}_{hi} cp_h (T_{hi} - T_{ho})$					x	x								x	x
7(M)	$\dot{Q} = UA \frac{(T_{hi}-T_{co})-(T_{ho}-T_{ci})}{ln(\frac{(T_{hi}-T_{co})}{(T_{ho}-T_{ci})})}$		x			x		x	x					x	x	x

Sequential resolution

$$x_i = f(x_{j<i})$$

Solve $x_i - f(x_{j\leq i}) = 0$

Unit models : conclusions

- A flowsheet is a set of interconnected units
- System State Variables : what we need to know to characterize the system
  - State variables for each flow
  - Unit parameters
- Model (simulation) equations
  - Constitutive equations define the thermodynamic state of the flows
  - Unit models model the thermo-chemical transformations in units
    - Balance equations : mass + energy + impulsion
    - Thermo-chemical and mechanical transformations/transfer
- Specifications
  - Variables that needs to be fixed to fix the degrees of freedom
- Define the resolution strategy
  - simultaneous or sequential

Pros and cons

	Simultaneous	Sequential
Problem statement	Incidence matrix implicit	DOF analysis required
Robustness	unique solving scheme	specific solving procedure bounds; if-then-else
calculation modes	specifications	solving scheme
Derivatives	Required	numerical noise at flowsheet level if iterative scheme