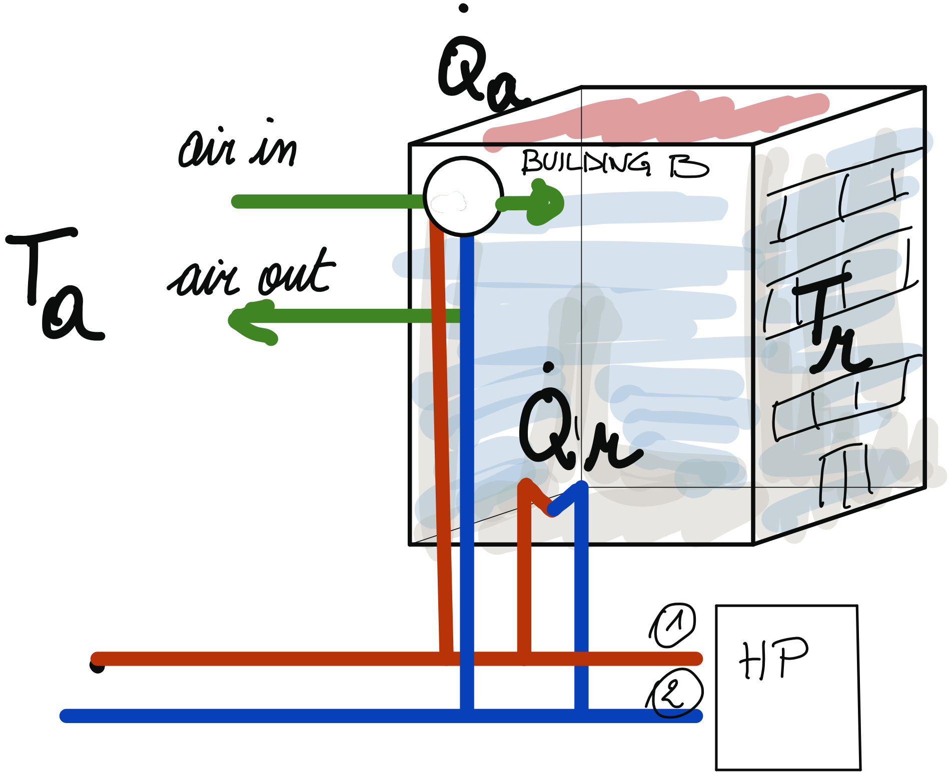
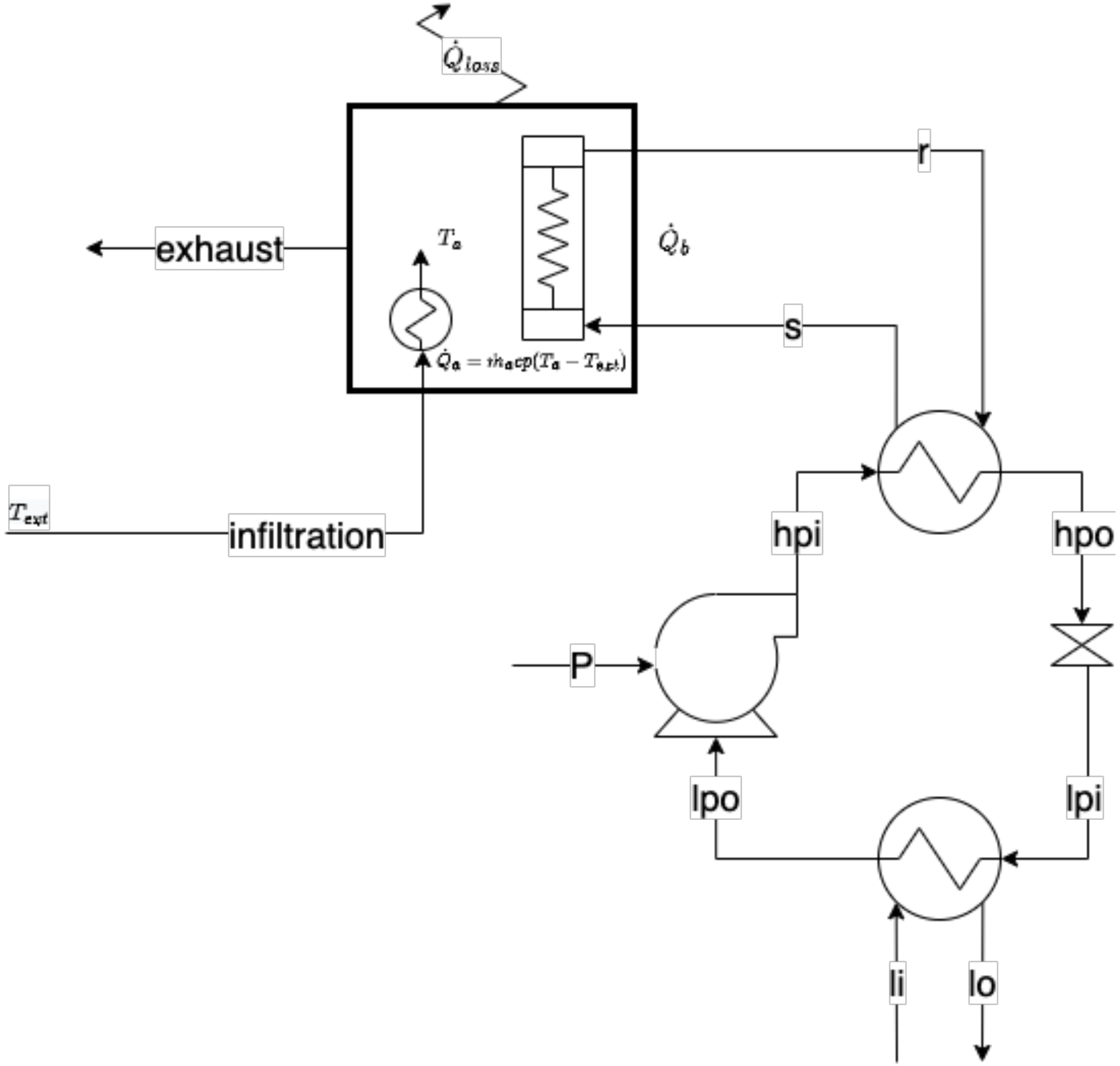
Flowsheets and process unit models

Building model



$$\dot{Q}_b = \dot{Q}_r + \dot{Q}_a$$



Building model : air flows

$$k_{th}(T_a - T_{ext}) = \dot{Q}_a + \dot{Q}_{loss}$$

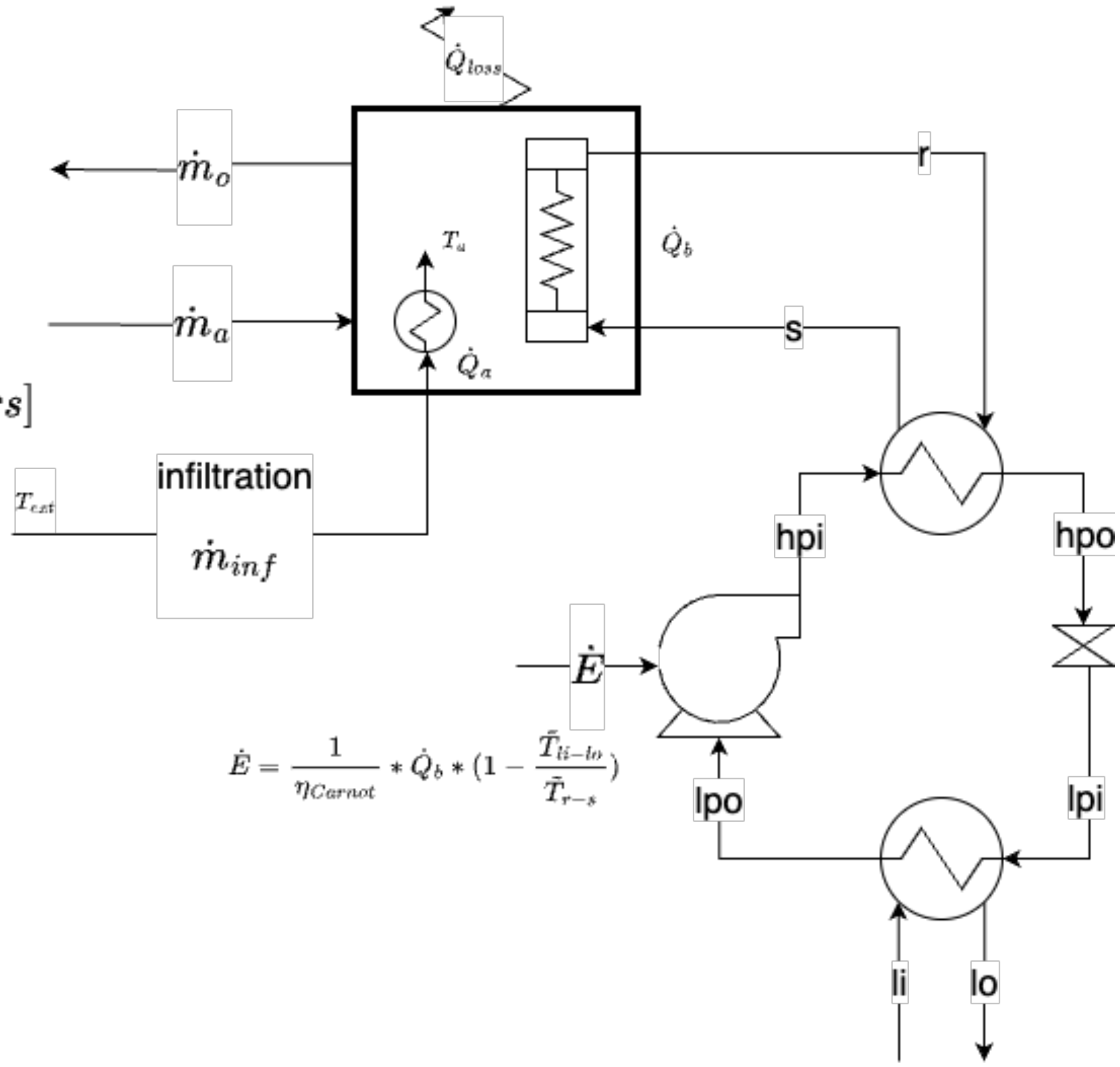
$$\dot{Q}_a = (\dot{m}_a + \dot{m}_{inf})cp(T_a - T_{ext})$$

$$\dot{m}_o[kg/hours] = \delta_a[kg/m^3] \cdot V_b[m^3] \cdot n_r[1/hours]$$

$$\dot{m}_{inf} = k_{inf} \cdot \dot{m}_o$$

$$\dot{m}_a = (1 - k_{inf}) \cdot \dot{m}_o$$

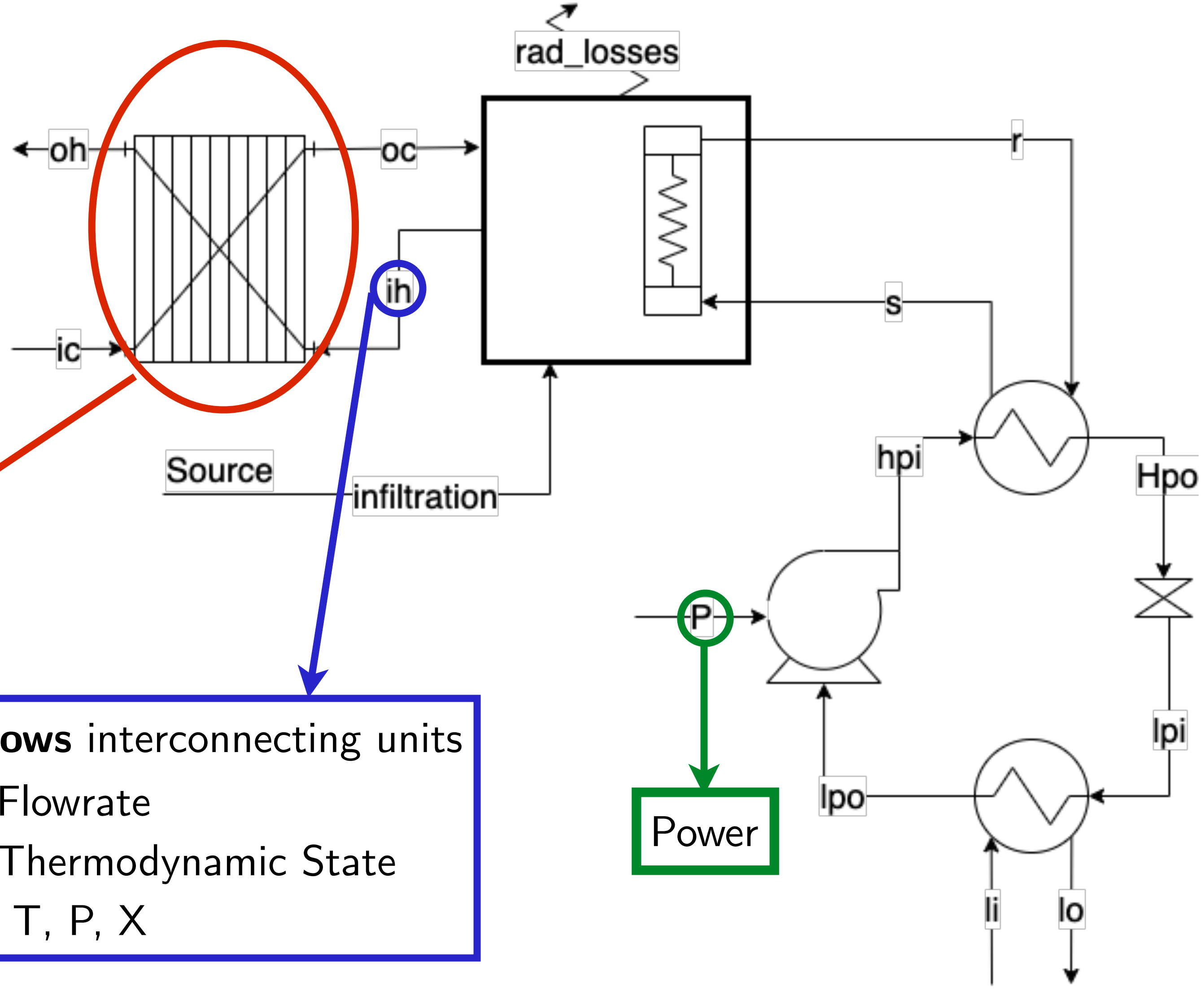
$$\dot{m}_o = \dot{m}_a + \dot{m}_{inf}$$



$$\dot{E} = \frac{1}{\eta_{Carnot}} * \dot{Q}_b * (1 - \frac{\bar{T}_{li-lo}}{\bar{T}_{r-s}})$$

Heat recovery by a double flux heat exchanger

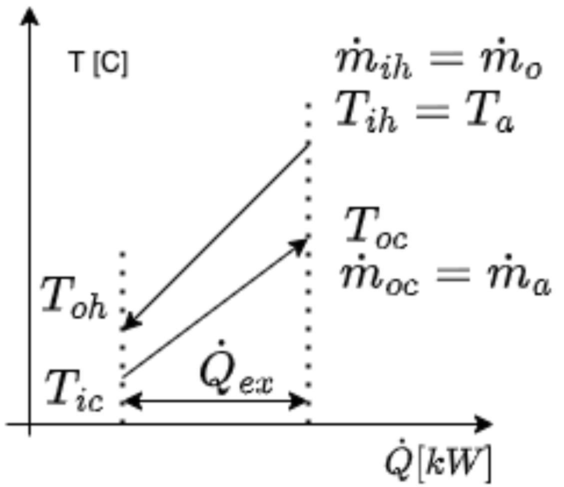
- Flowsheet
  - Flows
  - Units
- State of the system
  - Flows characterisation
  - Units size

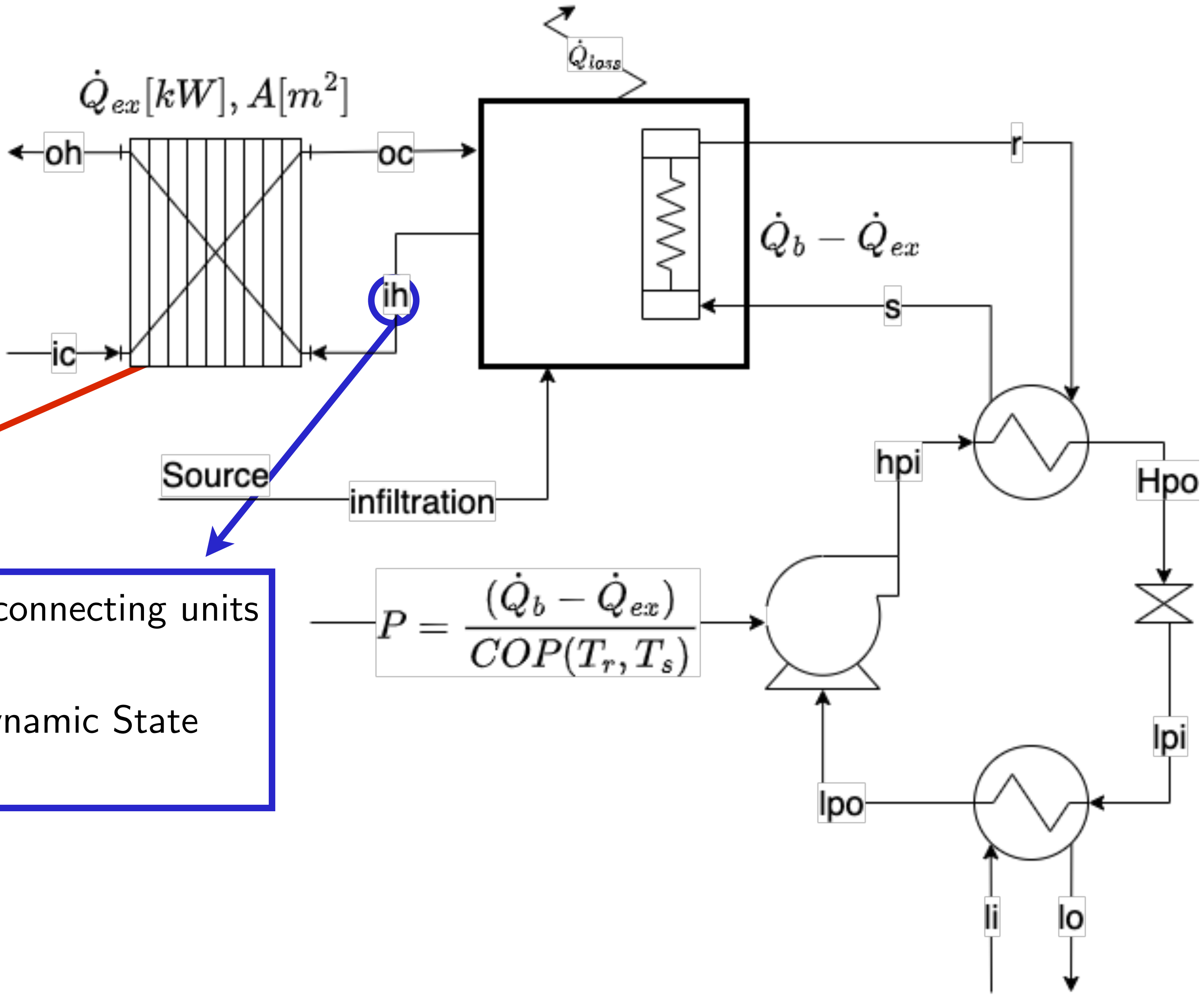


Process unit : converting flows
- Size
- Type
- Conversion of mass and energy

Flows interconnecting units
- Flowrate
- Thermodynamic State
  T, P, X

Heat recovery by a double flux heat exchanger





Process unit : converting flows

- Size
- Type
- Conversion of mass and energy

Flows interconnecting units

- Flowrate
- Thermodynamic State
  T, P, X

Streams : Degrees of freedom

- To characterize the state of a stream with N compounds
  - only **N+2** variables are required
    (Gibbs phase rule, Degree of freedom of a flow)
  - in which at least one will characterise a flow
    - i.e. **1 extensive variable**
- Examples :

$$T, P, \dot{m}_i$$

$$P, h, \dot{m}, c_i \quad for \quad i = 1, \ldots, N-1$$

$$P, \dot{V}, \dot{m}_i \quad for \quad i = 1, \ldots, N$$

Constitutive equations

- Calculating the other properties when the degrees of freedom are fixed
  - Enthalpy for T and P
  - Entropy for T and P
  - Density for T and P
  - Temperature for P and S

Constitutive equations : Enthalpy calculations

T0 : reference temperature
Perfect gas : 25 C 1 atm

Gas ideal

$$H_{id}^{g}(T,P,x_i) = \sum_i x_i * \Delta H^{0f}{}_i + \int_{T^\circ}^{T} \left(\sum_i x_i * Cp_i\,(T) \right) .dT$$

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

a_i,b_i,c_i,d_i from data bases

Liquid ideal

$$H_{id}^{l}(T,P,x_i) = \sum_i x_i * \Delta H^{0f}{}_i + \int_{T^\circ}^{T} \left(\sum_i x_i * Cp_i\,(T) \right) dT - \sum_i x_i * \Delta Hvap_i(T)$$

$$\Delta Hvap_i(T) = \Delta Hvap_i(T_i^b) * \left(\frac{T_i^{crit} - T}{T_i^{crit} - T_i^b} \right)^{0.38}$$

Mixture liquid - vapor $T = T^{sat}(P, x_i)$

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

Constitutive equation : Entropy calculation

- For a gas state

$$ds = cp\frac{dT}{T} - \left(\frac{\delta v}{\delta T}\right)_P dP$$

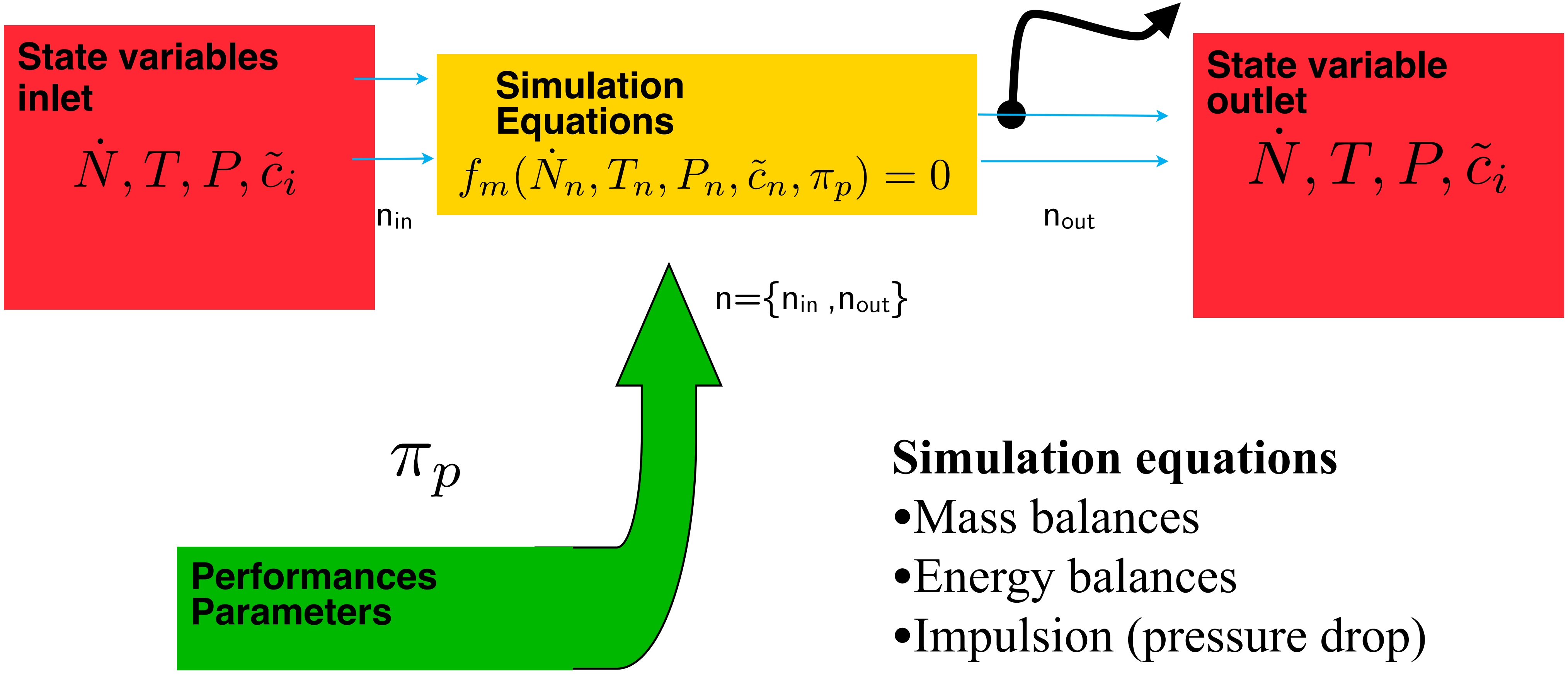
$$s_i = s_i^{0f} + \int_{T_0}^{T} \frac{cp_i(T)}{T} dT - \Re ln\frac{P_i}{P^0}$$

- This shows that the properties can be deduced if we know
  - the correlation equations
  - the data characterising the components
  - the fundamental rules of thermodynamics.

A process unit model : transforming states

A simulation model introduces a set of equations that model the thermo-chemical transformations that occur in the unit with the aim of calculating the the states of the flows leaving the unit as a function of the inlet flows and the physical characteristics of the unit.

Thermodynamic state
Constitutive equations



Simulation equations

- Mass balances
- Energy balances
- Impulsion (pressure drop)
- Performances equations

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

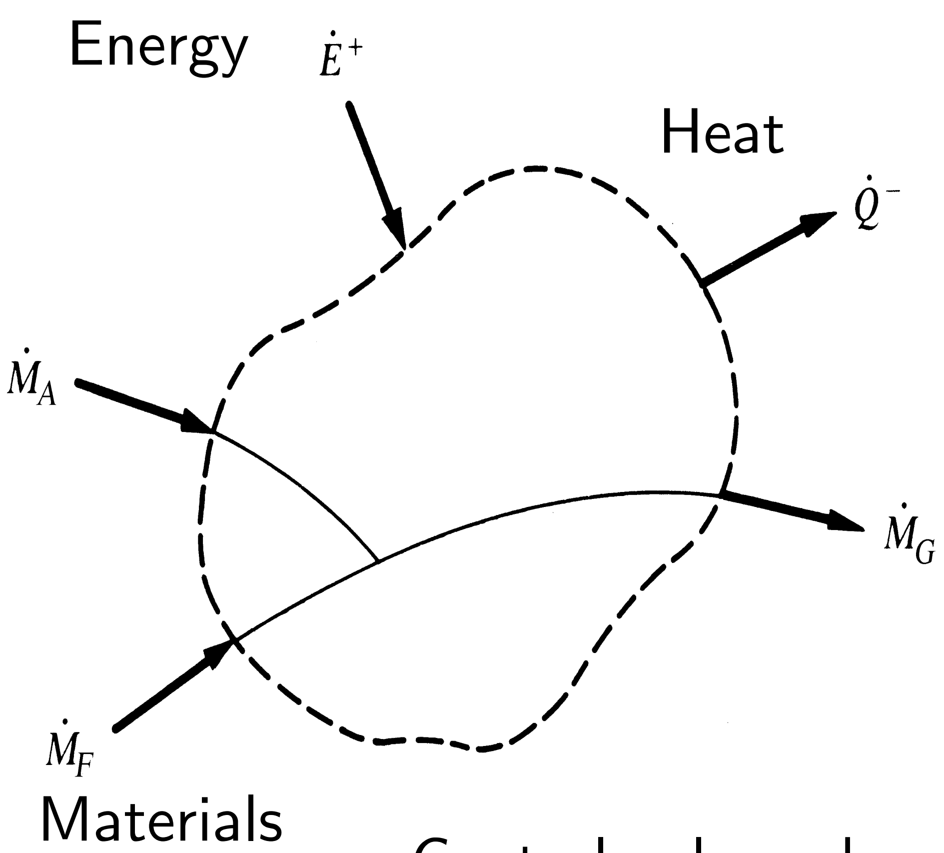
no Accumulation = 0 = in - out + Generation - Consumption

+ 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



Control volume boundary

Mass network

N_c mass balances per network*

1 energy balance

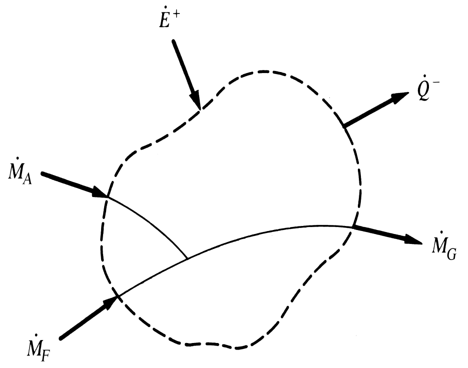
1 impulsion balance (P)

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

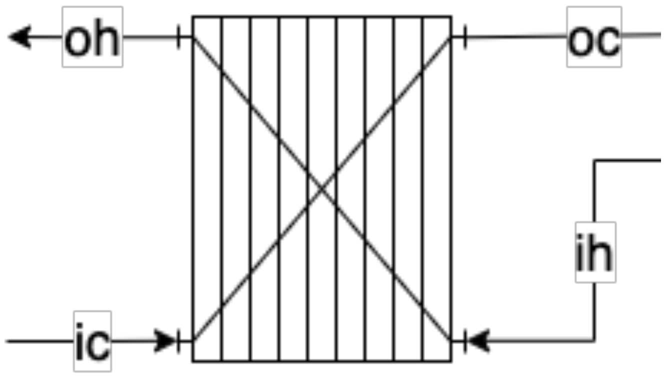
$$\sum_f \dot{m}^+_f \cdot h(T_f, P_f, x_f) + \sum_Q \dot{Q}^+ + \sum_E \dot{E}^+ = \frac{dQ}{dt} = 0$$

Accumulation

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

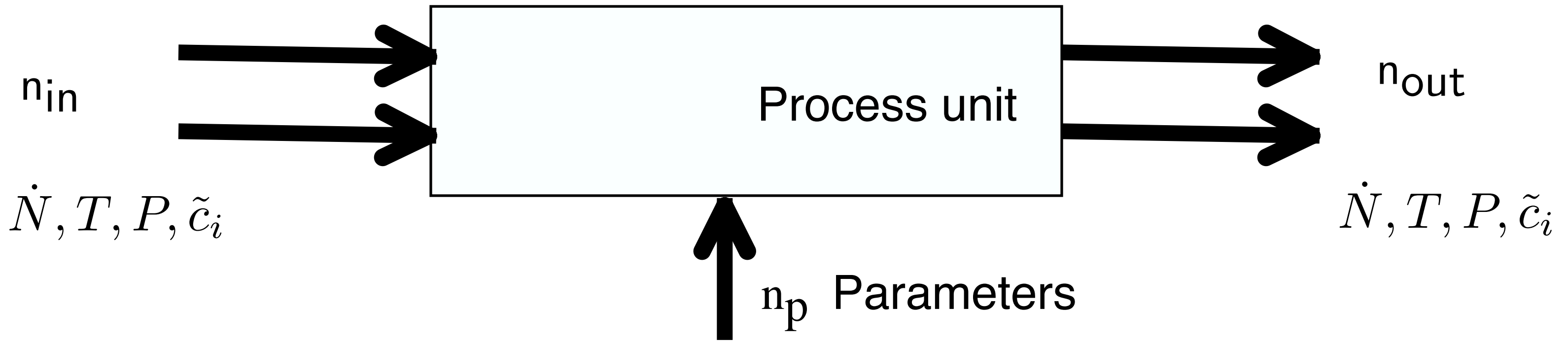
Non linear equations !

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

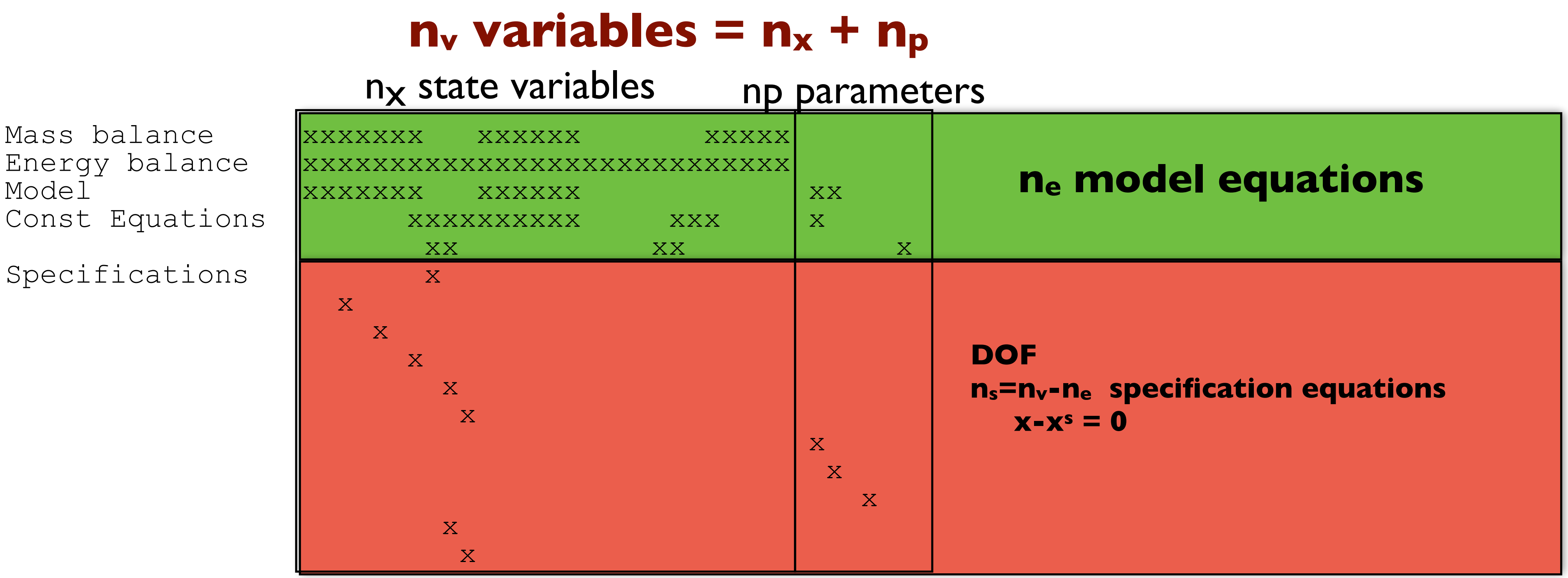
State of the streams	$n_x=(n_{out} + n_{in})*(n_c+2)$
Unit parameters	n_p
Internal variables	n_t

$$DOF = n_v - n_e$$

DOF = number of set points (specifications) to make the unit calculable

$$n_e + n_s = n_v$$

Incidence Matrix of a Unit model



To solve the problem :

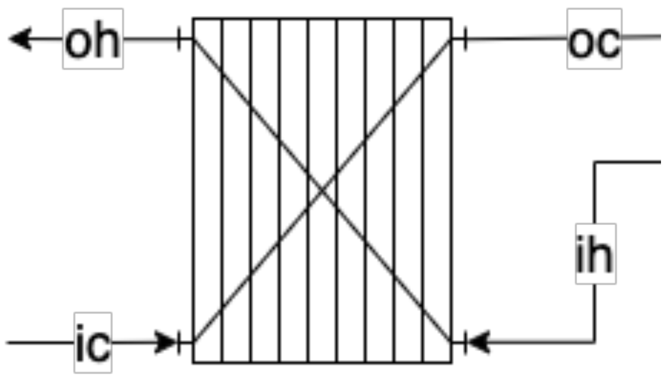
1) square matrix

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)

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

<u>F(X) : Equations</u>

Ne=Ns + Nb + Nm

		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		

<u>X : Variables</u>

Nv state

Ni intermediate

Np parameters

Nx=Nv+Ni+Np

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.

Simultaneous equation solving

		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		

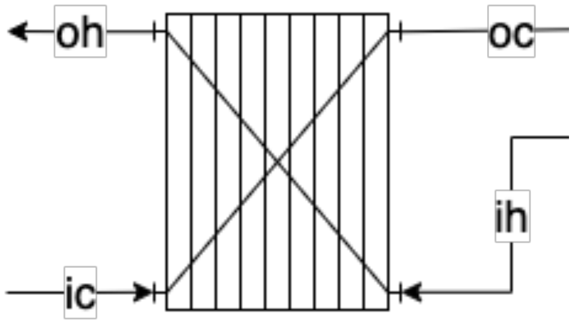
Find X such that

F(X)=0

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)	$\dot{m}_{ci} = \dot{m}^s_{ci}$	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								
14(S)	$A = A^s$													x		
15(S)	$U = U^s$															x

Sequential resolution

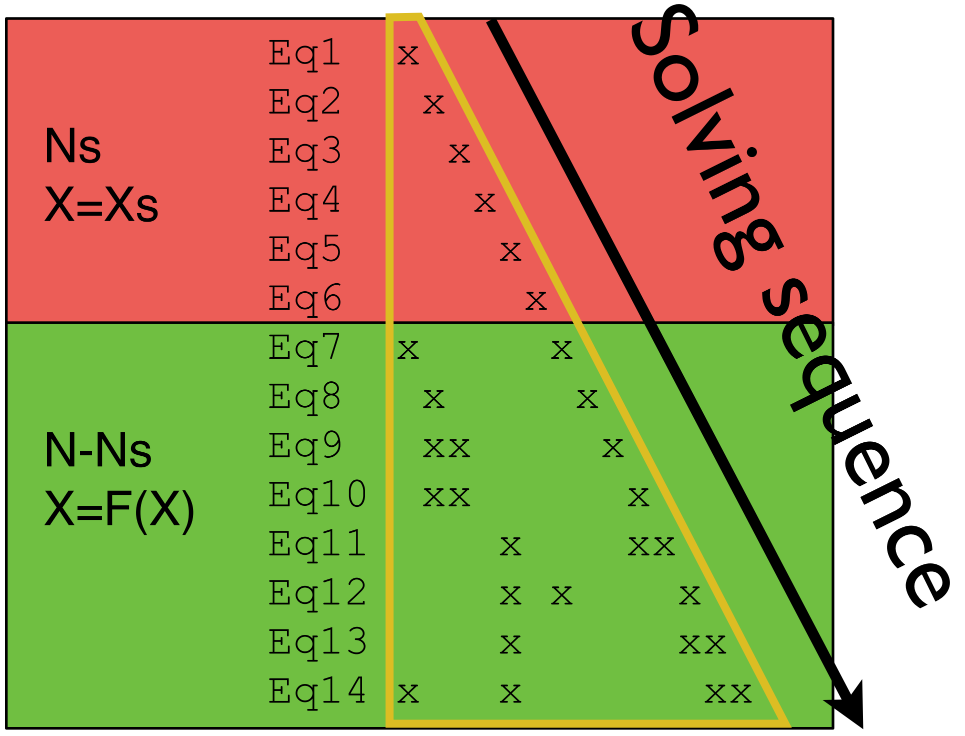
- Reorganise the equations such that :
  - one equation has one unknown => $x_i = f(x_{j<i})$

Sequence definition case 1

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 each equation one after the other in sequence



Sequence definition case 2

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

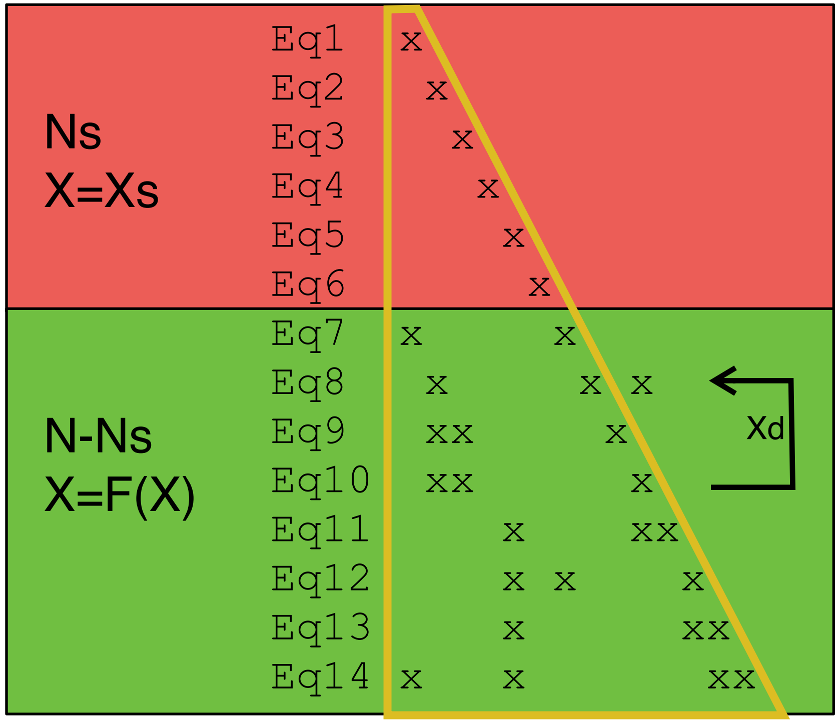
if not $$diag_i = f(diag_k, k = 1, \ldots, i-1)$$

3. Guess off-diagonal terms Xd

4. Define the order of resolution
5. Solve the sequence

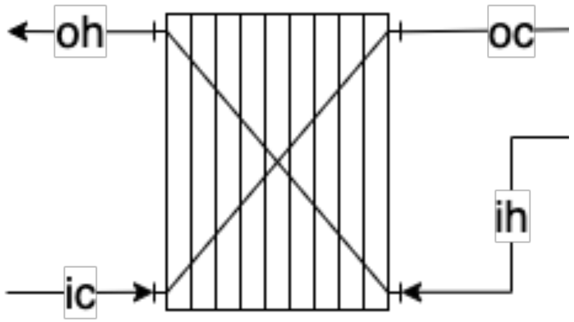
6. Iterate on the value of Xd
   6.1 test convergence
   $Xd^k ?= Xd^{k-1}$
   6.2 if NO : $Xd^{k+1} = Xd^k$
   6.3 back to 5

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									
14(S)	$A = A^s$							x								
15(S)	$U = U^s$								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			
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

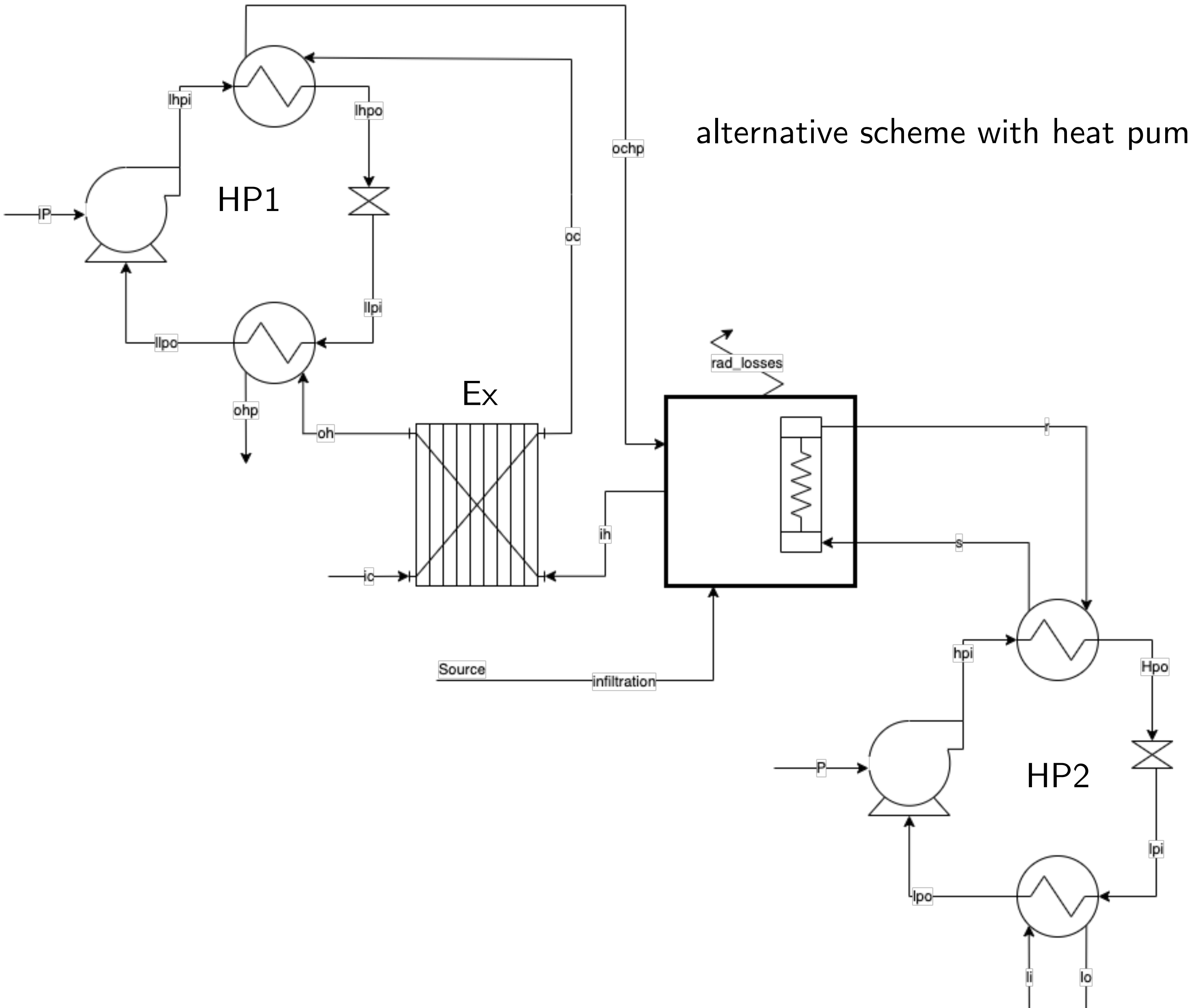
$x_i = f(x_{j<i})$

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

Flowsheets

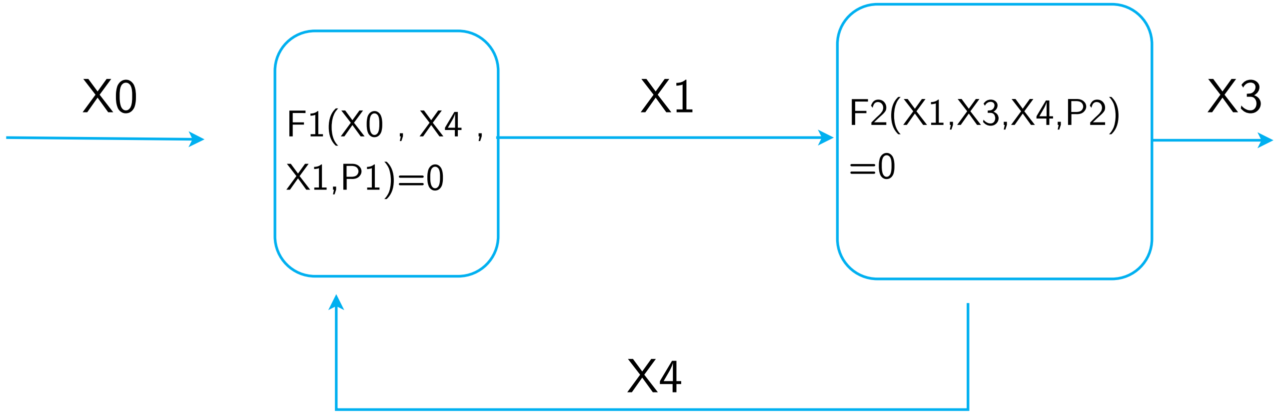
- Process models
  - Process Units
  - Interconnections

alternative scheme with heat pump



Solving Flowsheets : simultaneous approach

- Flowsheet = interconnected modules



N_e : Equations

$F_u(X_f, \pi_u) = 0 \quad \forall u \in \{1..n_u\}, \forall f \in \{1..n_f\}$: Unit models

$X_{f^s} - S_{f^s} = 0$: Specifications (flows)

$\pi_{u^s} - S_{u^s} = 0$: Specifications (unit parameters)

$X^-_{u_i} - X^+_{u_j} = 0$: Links (unit interconnections)

outlet of u_i enters u_j:

N_v : Variables

X_f : $n_f*(2+n_{c,f})$ state of the flows

π_u : $n_u*n_{p,u}$ parameters of unit models

n_f	nb of flows
$n_{c,f}$	nb of compound in flow f
n_u	nb of units
$n_{p,u}$	nb of parameters in unit u

Degrees of freedom : N_{DOF} : N_v - N_e

EPFL

Conclusions

1. Draw the flowsheet
2. Identify the states to calculate the state of the system
   - list of flows with a **name** and **thermodynamic properties**
3. Calculate the degrees of freedom for the system
   - number of specifications
   - identify the variables to specify
   - define the values for the specifications
4. Define the list of states for the system design
   - Operating conditions (list of specifications) seen by the system over its lifetime
5. Define a solving strategy
   - Simultaneous
   - Sequential (with iterations if needed)

Degrees of freedom : 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
- 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 transformations
  - Flowsheet introduce the unit interconnection equations
- Specifications
  - Variables that needs to be fixed to fix the degrees of freedom