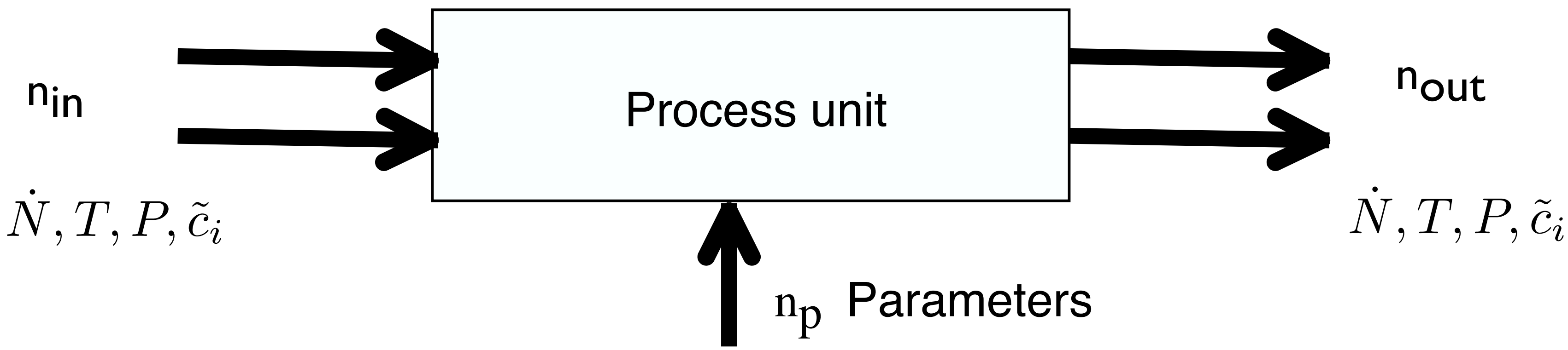
Flowsheets and process unit models

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

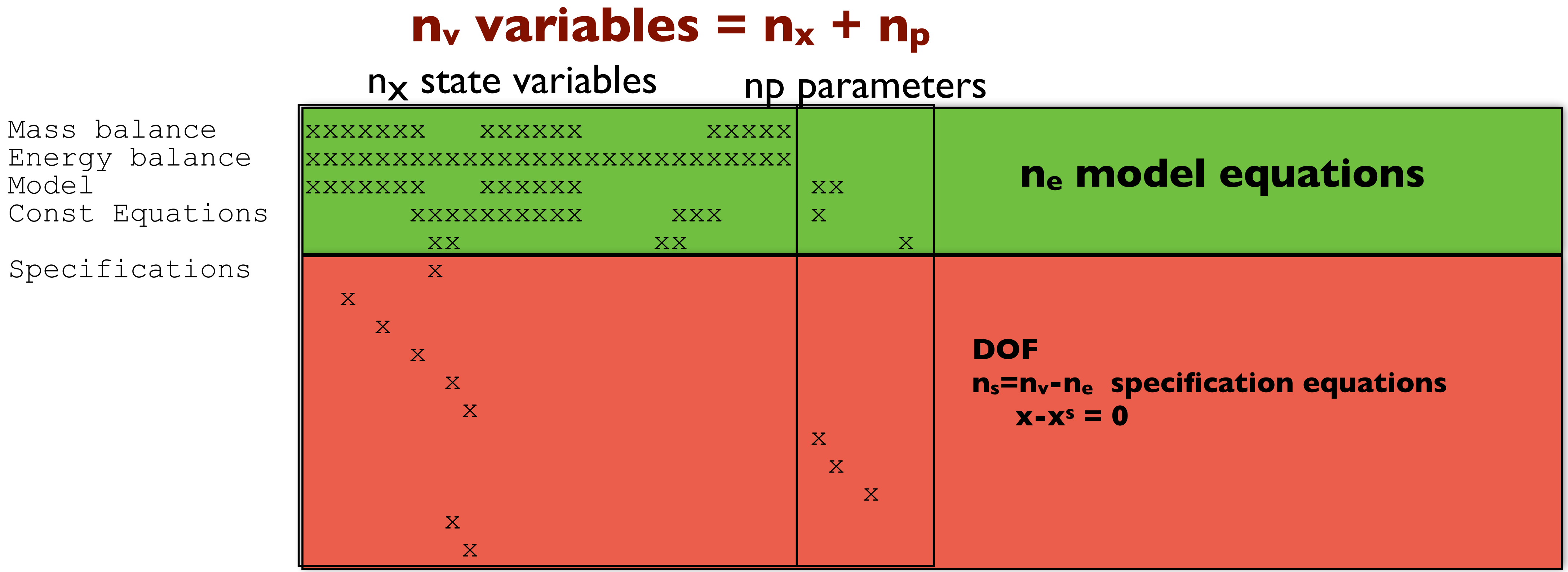
State of the streams	$n_x=(n_{out} + n_{in})*(n_c+2)$
Unit parameters	n_p
Internal variables	n_t

$$DOF = n_v - n_e$$

DOF = number of set points to make the unit calculable

$$n_e + n_s = n_v$$

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)

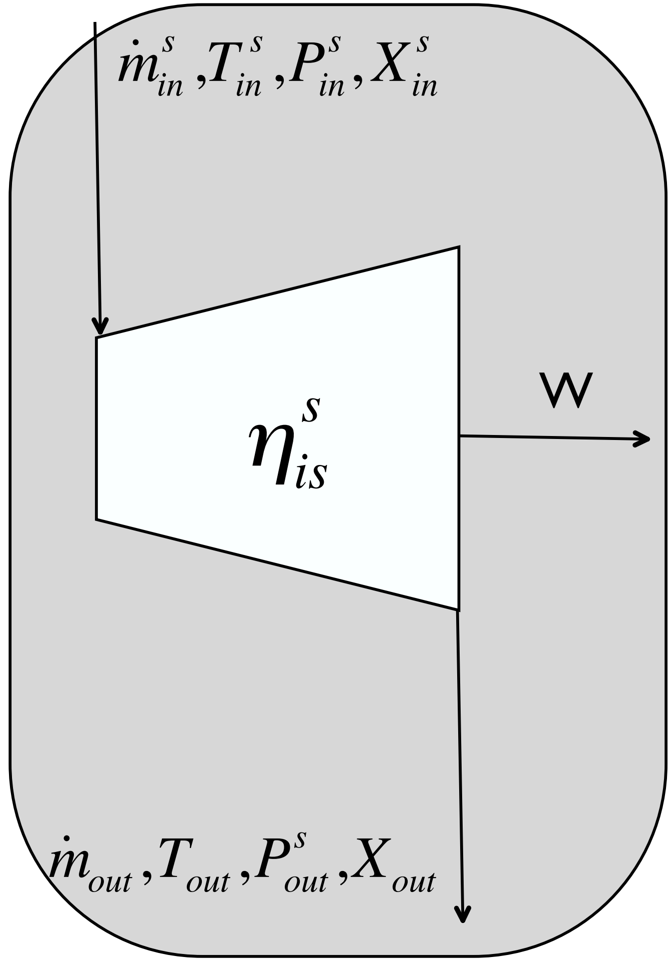
Solving models : turbine model

- **Variables** : state of flows and unit parameters

Inlet conditions		N + 2
Tout (K)	Temperature	1
Pout (bar)	Pressure	1
x_{iout}	Composition	N
$\dot{m}_{out}$	Flow	1
W	Work	1
Wis	Isentropic Work	1
Tis	Isentropic temperature	1
Eff is	Isentropic efficiency	1
Total		2N+9

- **Equations** : specifications + model

Inlet conditions		**N + 2**
Mass bal	$\dot{m}_{in} x_{i,in} = \dot{m}_{out} x_{i,out}$	N
Energy Bal	$\dot{m}_{in} h(T_{in}, P_{in}, X_{in}) - \dot{m}_{out} h(T_{out}, P_{out}, X_{out}) = \dot{W}$	1
Composition	$\sum x_{i,out} = 1$	1
Dim 1	$\dot{W} = \dot{W}_{is} * \eta_{is}$	1
Dim 2	$\dot{W}_{is} = h(T_{in}, P_{in}, X_{in}) - h(T_{out}^{is}, P_{out}, X_{out})$	1
Dim 3	$s(T_{out}^{is}, P_{out}, X_{in}) = s(T_{in}, P_{in}, X_{in})$	1
Total		2N+7



DOF = (2N+9) - (2N+7)= 2

Fix 2 variables to calculate the model

Assumptions : no condensation, inlet specified

N=number of compounds

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

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

Simultaneous resolution

- Turbine model

Model

$$\dot m_{out} - \dot m_{in} = 0$$

$$x^j_{out} - x^j_{in} = 0$$

$$h_{in} - h(T_{in}, P_{in}, X_{in}) = 0$$

$$s_{in} - s(T_{in}, P_{in}, X_{in}) = 0$$

$$h^{is}_{out} - h(s_{in}, P_{out}, X_{out}) = 0$$

$$h_{out} - h_{in} + \eta_{is} * \left(h_{in} - h^{is}_{out}\right) = 0$$

$$T_{out} - T\left(h_{out}, P_{out}, X_{out}\right) = 0$$

$$W - \dot m_{in} * (h_{in} - h_{out}) = 0$$

Specifications

$$\dot m_{in} - \dot m^s_{in} = 0$$

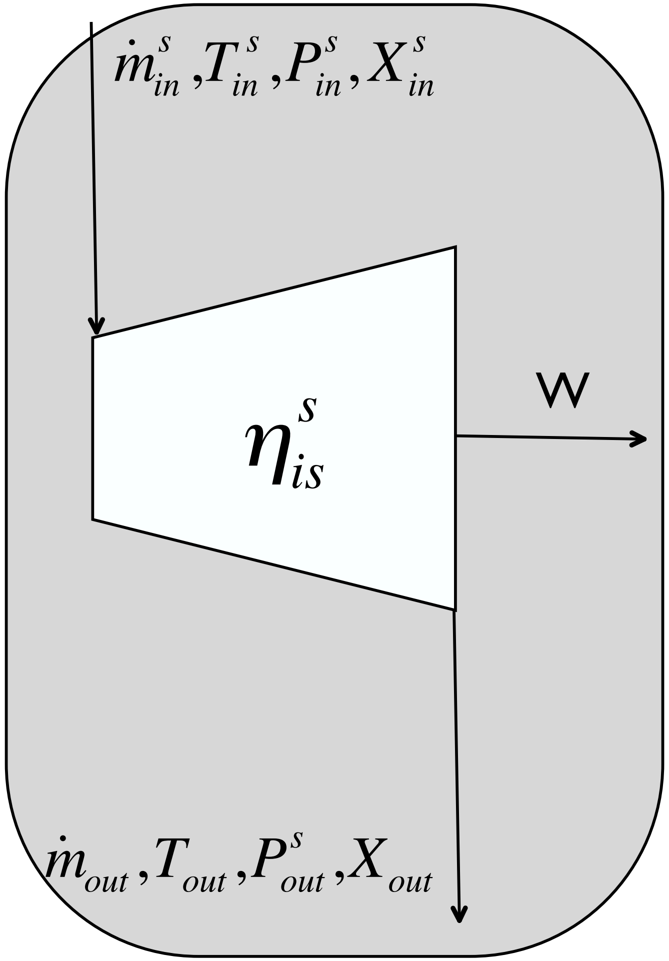
$$x^j_{in} - x^{j,s}_{in} = 0$$

$$T_{in} - T^s_{in} = 0$$

$$P_{in} - P^s_{in} = 0$$

$$P_{out} - P^s_{out} = 0$$

$$\eta_{is} - \eta^s_{is} = 0$$



constitutive equations

Non linear system resolution using Newton Raphson methods

$$\left|\begin{array}{l} F(X,P) = 0 \\ S(X,P) = 0 \\ IN(X) = 0 \end{array}\right. \quad \Rightarrow F(X) = 0 \quad (NxN)$$

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.

Sequential resolution

- Turbine model

Model Eq 7-14

$$\dot m_{out} - \dot m_{in} = 0$$

$$x^j_{out} - x^j_{in} = 0$$

$$h_{in} - h(T_{in}, P_{in}, X_{in}) = 0$$

$$s_{in} - s(T_{in}, P_{in}, X_{in}) = 0$$

$$h^{is}_{out} - h(s_{in}, P_{out}, X_{out}) = 0$$

$$h_{out} - h_{in} + \eta_{is} * \left(h_{in} - h^{is}_{out}\right) = 0$$

$$T_{out} - T\left(h_{out}, P_{out}, X_{out}\right) = 0$$

$$W - \dot m_{in} * (h_{in} - h_{out}) = 0$$

Specifications Eq 1-6

$$\dot m_{in} - \dot m^s_{in} = 0$$

$$x^j_{in} - x^{j,s}_{in} = 0$$

$$T_{in} - T^s_{in} = 0$$

$$P_{in} - P^s_{in} = 0$$

$$P_{out} - P^s_{out} = 0$$

$$\eta_{is} - \eta^s_{is} = 0$$

constitutive equation

Incidence matrix

```
Eq1    x
Eq2     x
Eq3      x
Eq4       x
Eq5        x
Eq6         x
Eq7    x     x
Eq8     x     x
Eq9     xx     x
Eq10    xx      x
Eq11       x    xx
Eq12       x x    x
Eq13       x      xx
Eq14   x   x       xx
```

rearrange 1 var/eq

Explicit form $y(i)=f_i(y(k=1..i-1))$

Sequence definition

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

```
Eq1 -> min     x
Eq2 -> xin      x
Eq3 -> Tin       x
Eq4 -> Pin        x
Eq5 -> Pout        x
Eq6 -> Etais        x
Eq7 -> mout    x     x
Eq8 -> xout     x     x
Eq9 -> Hin      xx     x
Eq10-> Sin      xx      x
Eq11-> Houtis      x    xx
Eq12-> Hout        x x    x
Eq13-> Tout        x      xx
Eq14-> W       x   x       xx
```

Solving sequence

Sequential resolution

Transform equations in explicit form : $x_i=f(x_{j<i})$

- Turbine Model

$$\dot{m}_{out} = \dot{m}^{s}_{in}$$

$$x^{j}_{out} = x^{j,s}_{in}$$

$$h_{in} = h(T^{s}_{in}, P^{s}_{in}, X^{s}_{in})$$

$$s_{in} = s(T^{s}_{in}, P^{s}_{in}, X^{s}_{in})$$

$$h^{is}_{out} = h(s_{in}, P^{s}_{out}, X_{out})$$

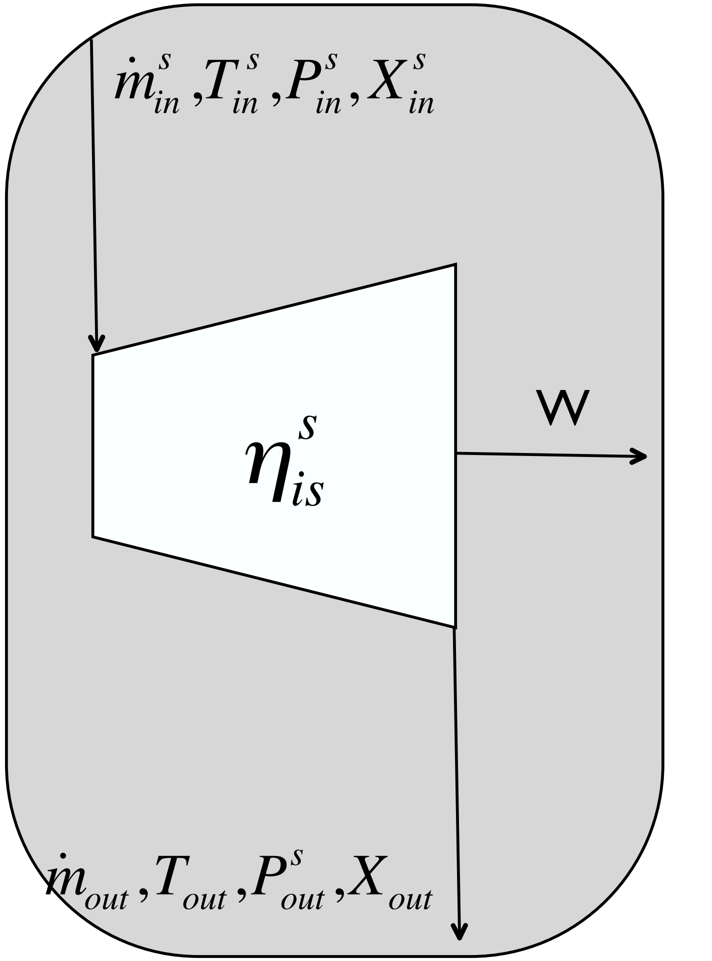
$$h_{out} = h_{in} - \eta^{s}_{is} * \left(h_{in} - h^{is}_{out}\right)$$

$$T_{out} = T\left(h_{out}, P^{s}_{out}, X_{out}\right)$$

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

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

Constitutive equation



Incidence matrix is arranged to be diagonal inferior

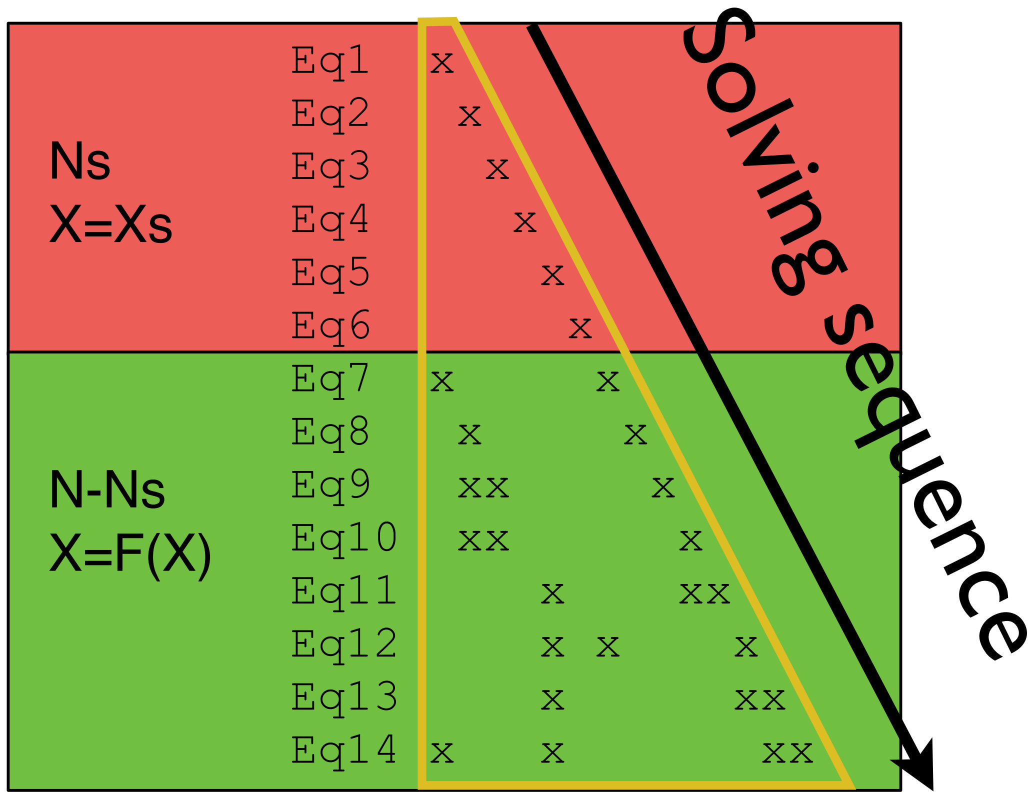
Explicit form $y(i)=f_i(y(k=1..i-1))$

Sequence definition case I

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



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

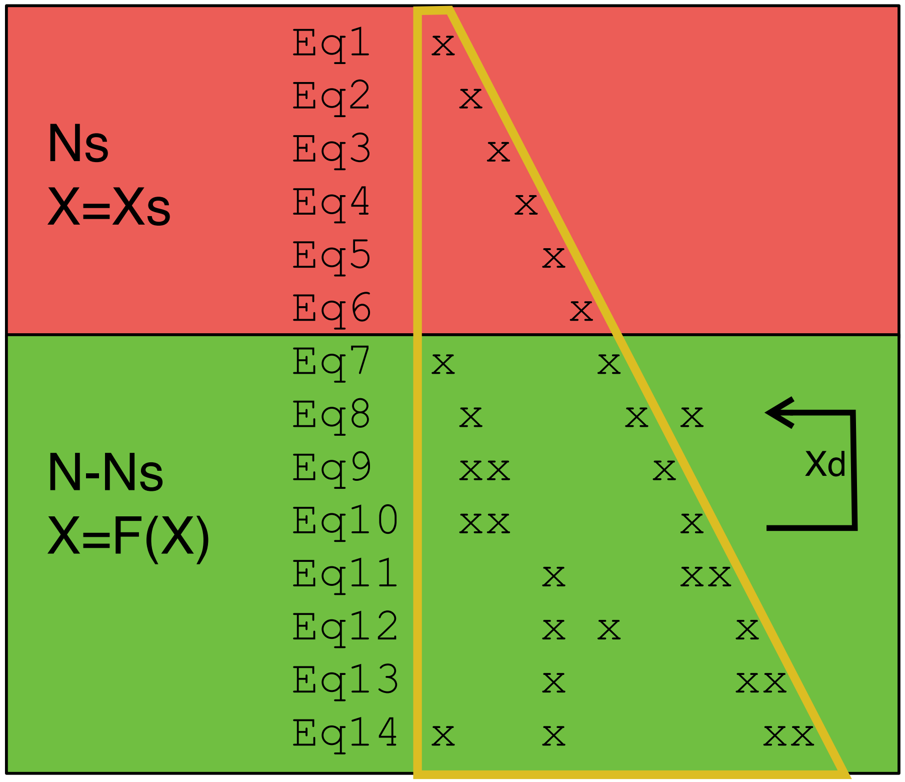
if not $$diag_i = f(diag_k, k = 1, \ldots, i-1)$$

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
     $Xd^k \mathrel{?=} Xd^{k-1}$
   - 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 $Xd^k - Xd^{k-1} = 0$

More complicated model : $X_i = f(X_i, X_{k \neq i})$

Detailed modeling of the expansion using empirical equations

$$\dot{m}_{out} = \dot{m}_{in}^{s}$$

$$x_{out}^{j} = x_{in}^{j,s} \qquad \forall j$$

$$h_{in} = h(T_{in}^{s}, P_{in}^{s}, X_{in}^{s})$$

$$s_{in} = s(T_{in}^{s}, P_{in}^{s}, X_{in}^{s})$$

$$h_{out}^{is} = h(s_{in}, P_{out}^{s}, X_{out})$$

$$\tau = \frac{P_{in}^{s}}{P_{out}^{s}}$$

$$\bar{v} = \frac{v(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) + v(T_{out}^{k}, P_{out}, X_{out})}{2}$$

$$\eta_{is} = a * \tau + b * \dot{m}_{in} * \bar{v} + c * \left(\dot{m}_{in} * \bar{v}\right)^{2} + d$$

$$h_{out} = h_{in} - \eta_{is} * \left(h_{in} - h_{out}^{is}\right)$$

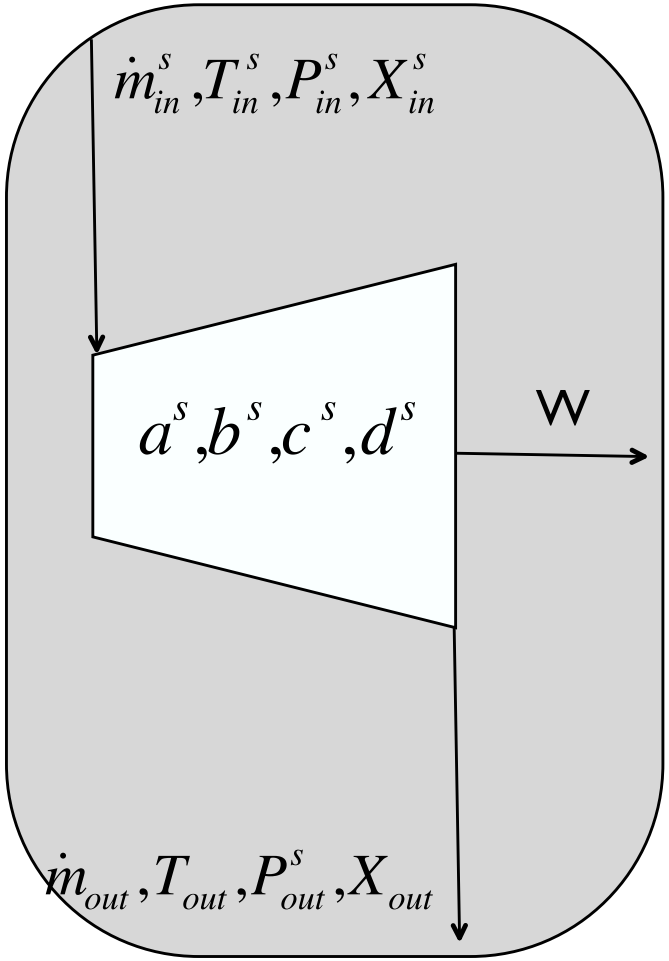
$$T_{out}^{k+1} = T\left(h_{out}, P_{out}^{s}\right)$$

$$\left|T_{out}^{k} - T_{out}^{k+1}\right| \leq \frac{EPS_{T}}{\left|T_{out}^{k}\right| + \varepsilon_{T}} ?$$

$\leftarrow$ *non* *oui*

$$\downarrow$$

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



Use of another mode of calculation

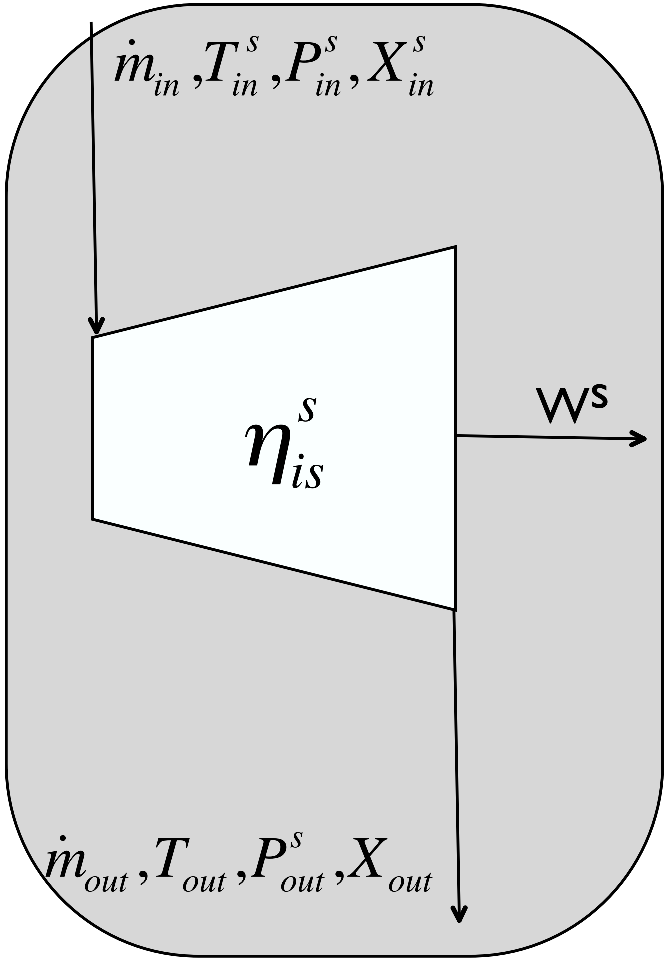
- E.g. calculate the flow for a given Pressure and Work
- simultaneous solving : change the specs

Model

$$\dot m_{out} - \dot m_{in} = 0$$
$$x^j_{out} - x^j_{in} = 0$$
$$h_{in} - h(T_{in}, P_{in}, X_{in}) = 0$$
$$s_{in} - s(T_{in}, P_{in}, X_{in}) = 0$$
$$h^{is}_{out} - h(s_{in}, P_{out}, X_{out}) = 0$$
$$h_{out} - h_{in} + \eta_{is} * \left(h_{in} - h^{is}_{out}\right) = 0$$
$$T_{out} - T\left(h_{out}, P_{out}, X_{out}\right) = 0$$
$$W - \dot m_{in} * (h_{in} - h_{out}) = 0$$

Specifications

$$W - W^s = 0$$
$$x^j_{in} - x^{j,s}_{in} = 0$$
$$T_{in} - T^s_{in} = 0$$
$$P_{in} - P^s_{in} = 0$$
$$P_{out} - P^s_{out} = 0$$
$$\eta_{is} - \eta^s_{is} = 0$$



Changing the specification set means changing the set of specification equation without changing the set of modeling equations

Use of another mode of calculation

- E.g. calculate the flow for a given Pressure and Work
- sequential solving : redefine the sequence !
-

$$x^{j}_{out} = x^{j,s}_{in}$$

$$h_{in} = h(T^{s}_{in}, P^{s}_{in}, X^{s}_{in})$$

$$s_{in} = s(T^{s}_{in}, P^{s}_{in}, X^{s}_{in})$$

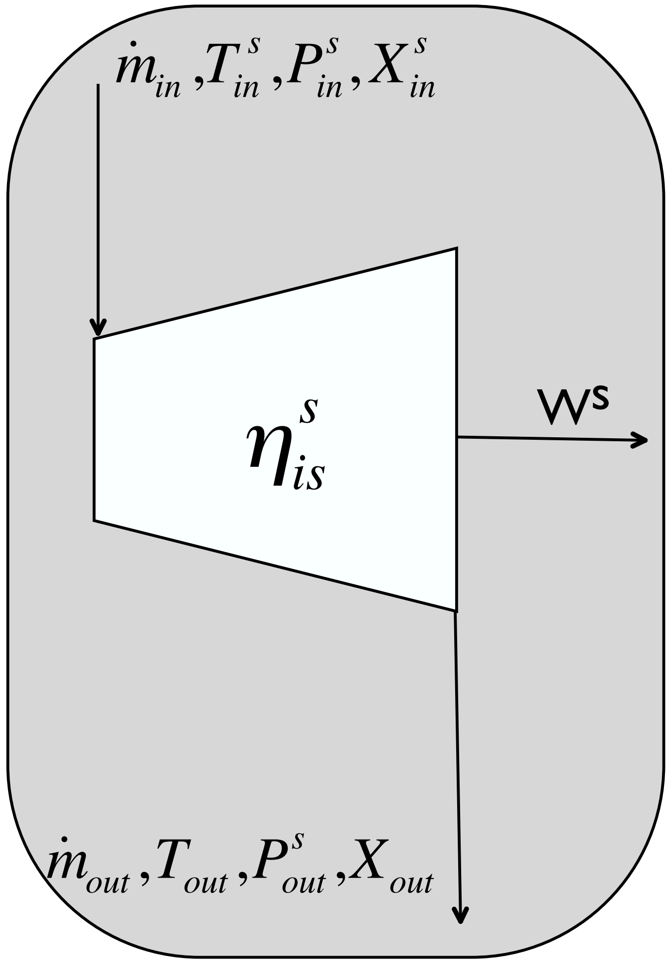
$$h^{is}_{out} = h(s_{in}, P^{s}_{out}, X_{out})$$

$$h_{out} = h_{in} - \eta^{s}_{is} * \left(h_{in} - h^{is}_{out}\right)$$

$$T_{out} = T\left(h_{out}, P^{s}_{out}, X_{out}\right)$$

$$\dot{m}_{in} = \frac{W^{s}}{(h_{in} - h_{out})}$$

$$\dot{m}_{out} = \dot{m}_{in}$$



A new sequence means a new code => more calculation modes = more codes

Use of another mode of calculation

- E.g. calculate the flow for a given Pressure and Work
- sequential solving : use iterations !

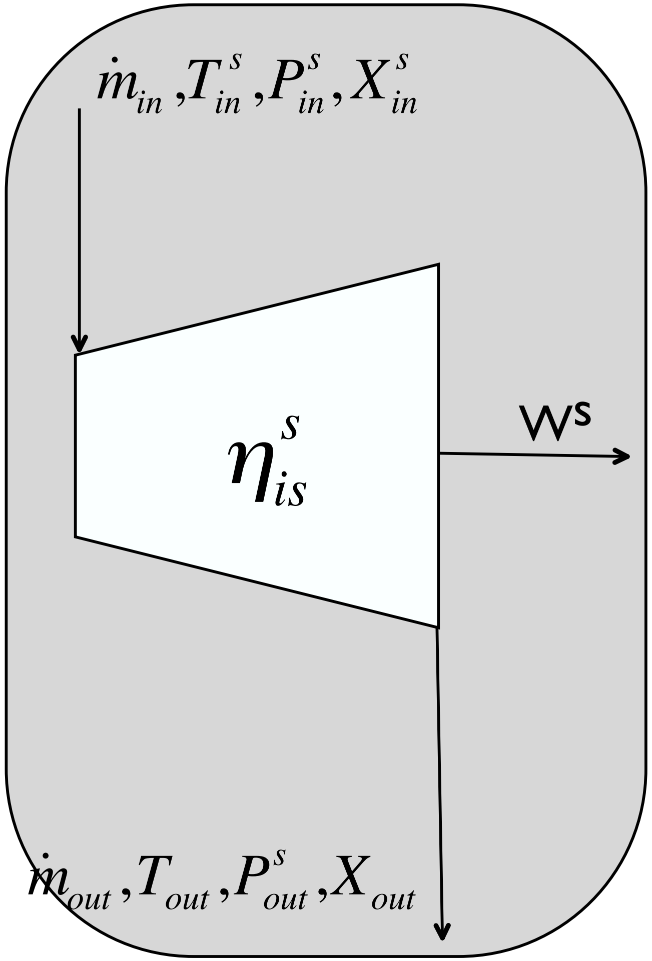
$$\dot{m}_{in}^{k} \rightarrow$$

$$
\begin{aligned}
\dot{m}_{out} &= \dot{m}_{in}^{s} \\
x_{out}^{j} &= x_{in}^{j,s} \\
h_{in} &= h(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) \\
s_{in} &= s(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) \\
h_{out}^{is} &= h(s_{in}, P_{out}^{s}, X_{out}) \\
h_{out} &= h_{in} - \eta_{is} * \left(h_{in} - h_{out}^{is}\right) \\
T_{out} &= T\left(h_{out}, P_{out}^{s}, X_{out}\right) \\
W &= \dot{m}_{in}^{s} * (h_{in} - h_{out})
\end{aligned}
$$

$$\left|W^{k} - W^{s}\right| \le \frac{EPS_{e}}{\left|W^{s}\right| + \varepsilon_{e}} ?$$

$$\left|\dot{m}_{in}^{k} - \dot{m}_{in}^{k+1}\right| \le \frac{EPS_{m}}{\left|m_{in}^{k}\right| + \varepsilon_{m}} ?$$

$$\dot{m}_{in}^{k+1}$$



The advantage is that the model and the resolution sequence does not need to be redefined. This has the advantage of code maintenance.

Different use of the model

- 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

- Identification

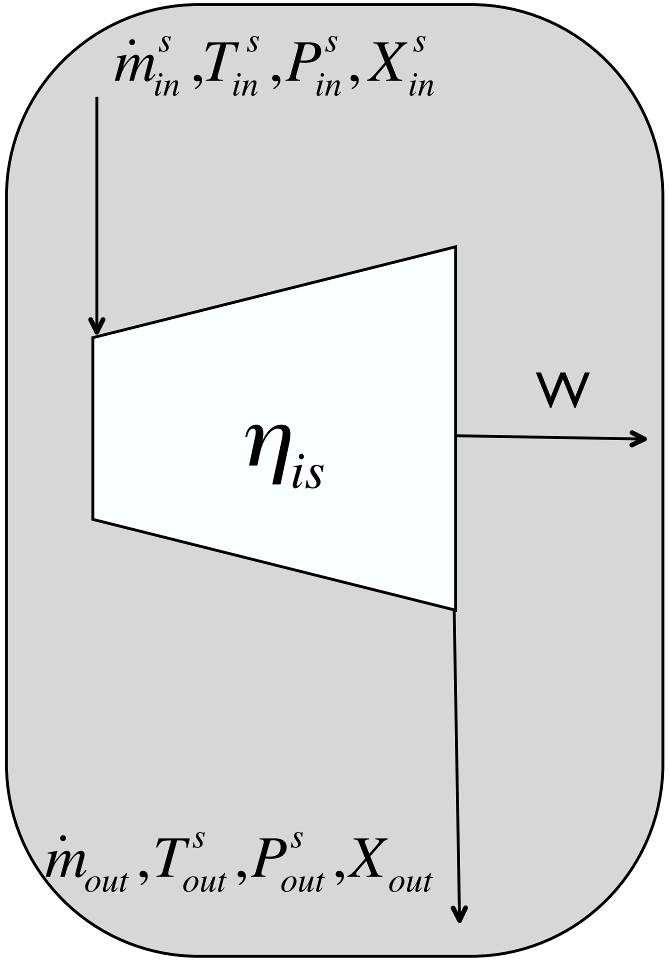
$$U = \frac{Q}{A \Delta T_{lm}}$$ T measured

  – Identify the heat transfer coefficient from measurement

Parameter identification

- Other model

$$\dot{m}_{out} = \dot{m}^s_{in}$$
$$h_{out} = h\left(T^s_{out}, P^s_{out}\right)$$
$$h_{in} = h(T^s_{in}, P^s_{in})$$
$$s_{in} = s(T^s_{in}, P^s_{in})$$
$$h^{is}_{out} = h(s_{in}, P^s_{out})$$
$$\eta_{is} = \frac{h_{in} - h_{out}}{h_{in} - h^{is}_{out}}$$
$$W = \dot{m}^s_{in} * (h_{in} - h_{out})$$



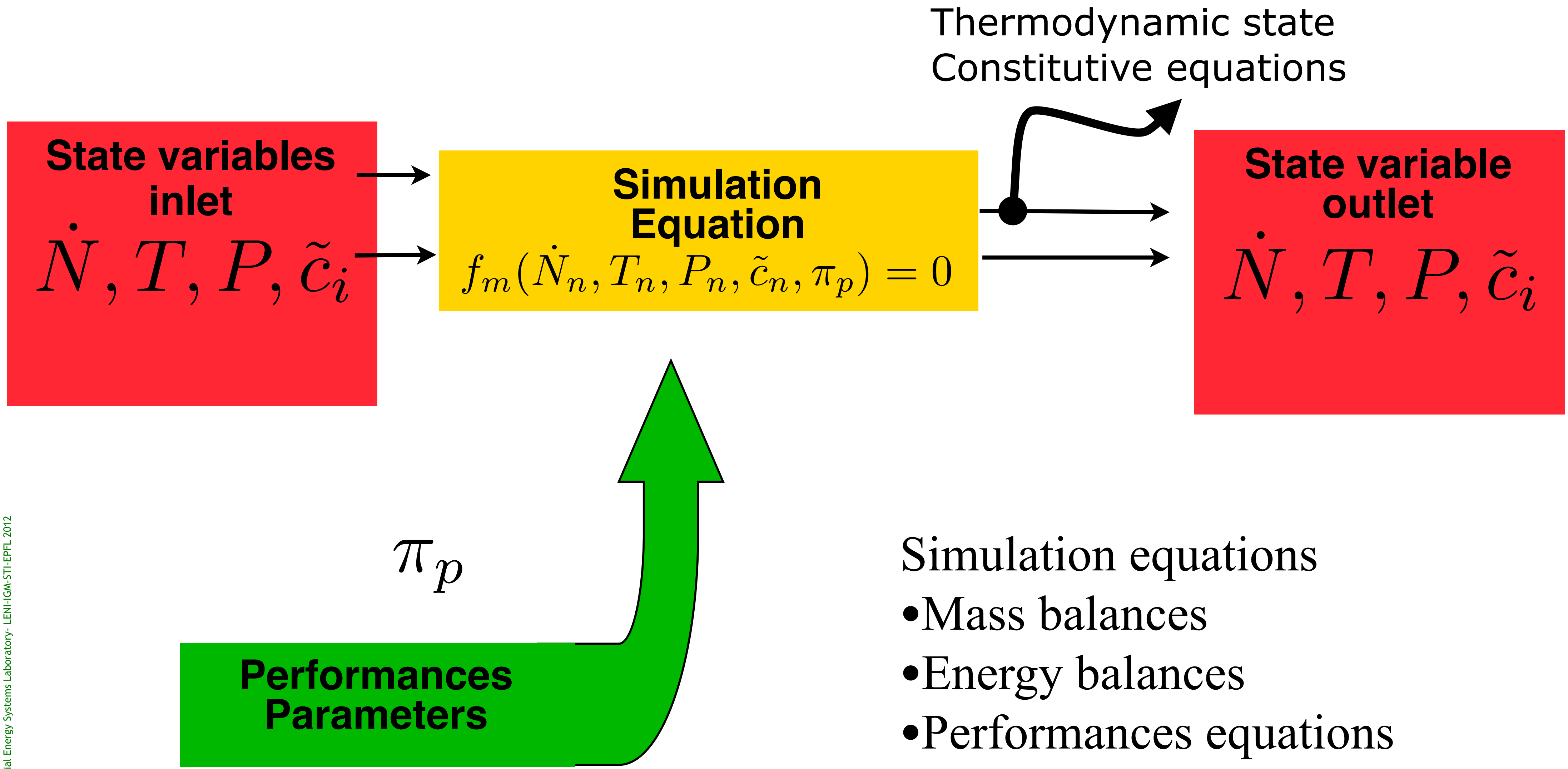
What is the efficiency ?

or iterative loop

Conclusions

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

A process unit model

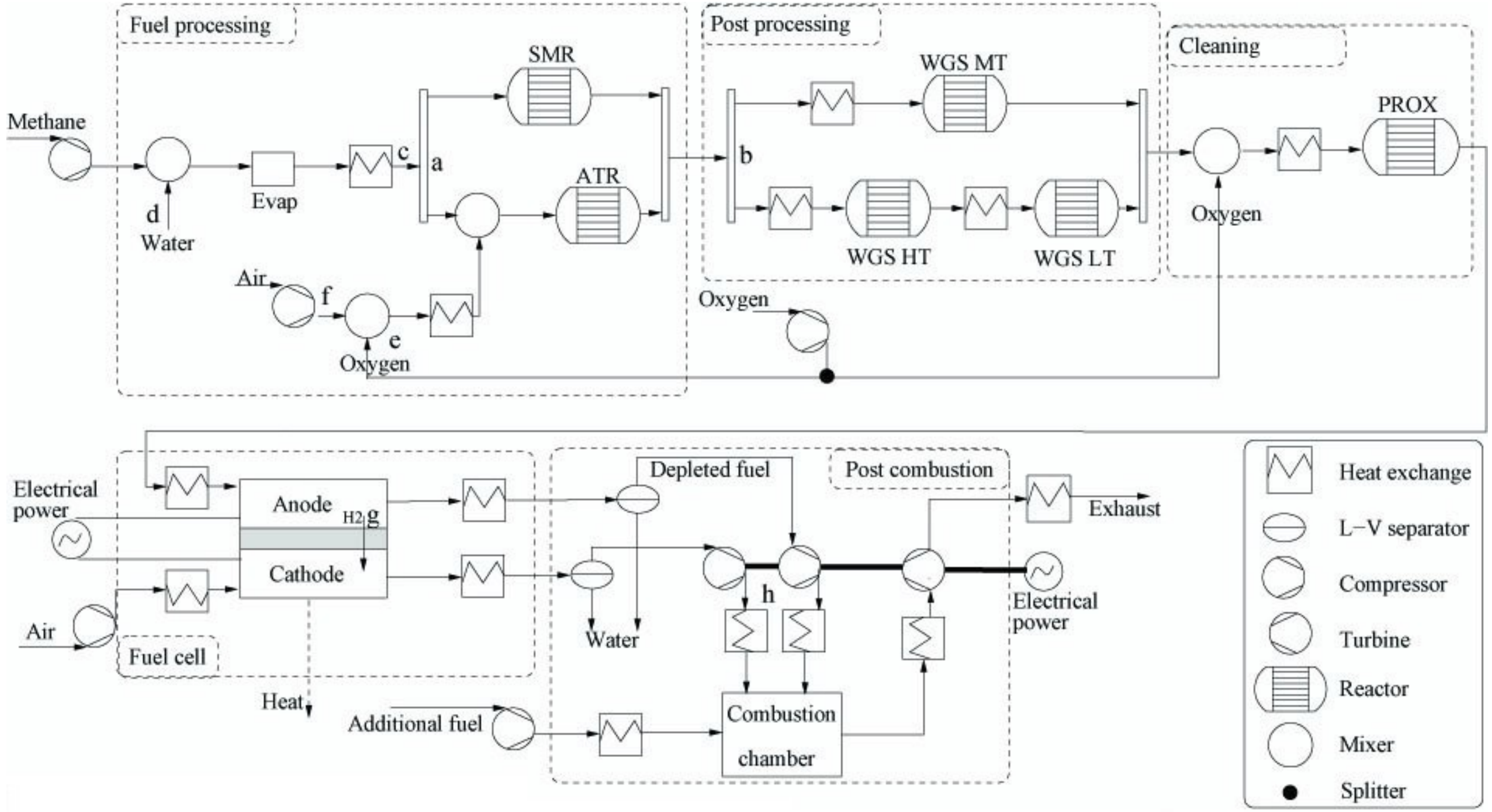


Simulation equations

- Mass balances
- Energy balances
- Performances equations

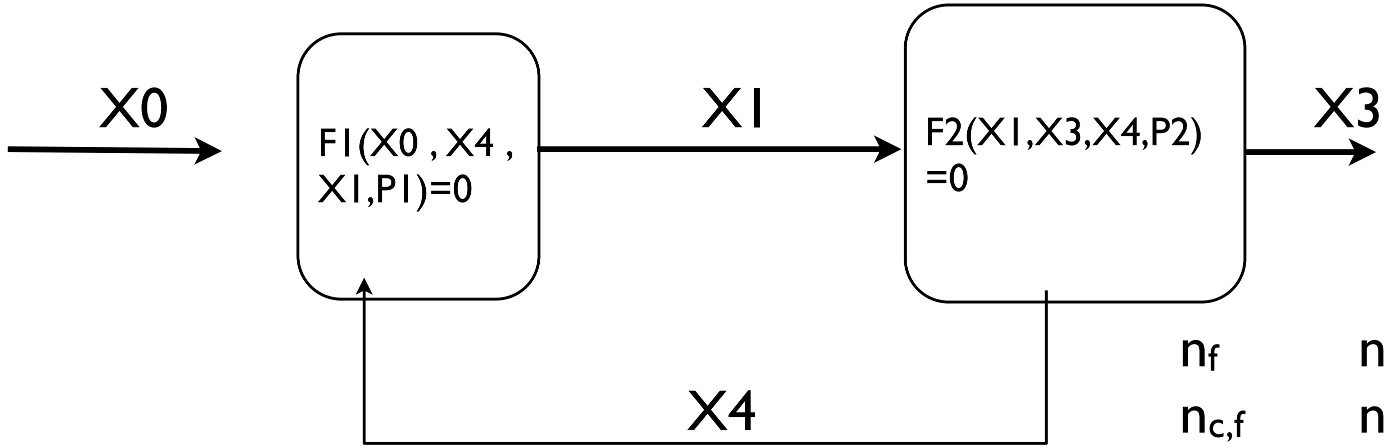
Flowsheeting

- Process models
  - Process Units
  - Interconnections



Solving Flowsheets : simultaneous approach

- Flowsheet = interconnected modules



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

N_e : Equations

$F(X,P)=0$: Models
$X_s-X^*=0$: Specifications (system)
$P_s-P^*=0$: Specifications (unit parameters)
$X_i-X_j=0$: Links (unit interconnections)

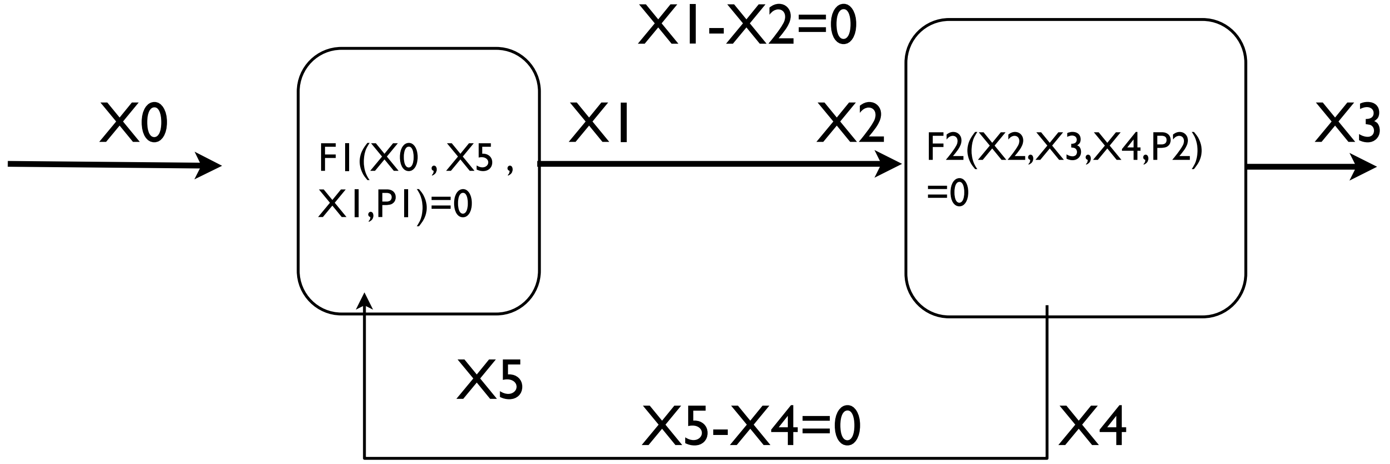
N_v : Variables

$n_f*(2+n_{c,f})$ state of the flows
$n_u*n_{p,u}$ parameters of unit models

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

Solving Flowsheets : simultaneous approach

- Flowsheet = interconnected modules



Simultaneous resolution : Solve a set of non linear equations

$F(X,P)=0$: Models (= a set of concatenated equations)
$X_s-X^*=0$: Specifications (= a set of specifications for fixing the system DOF)
$P_s-P^*=0$: Specifications (= a set of unit parameters specs)
$X_i-X_j=0$: Links (unit interconnections (reduces the DOF of system))

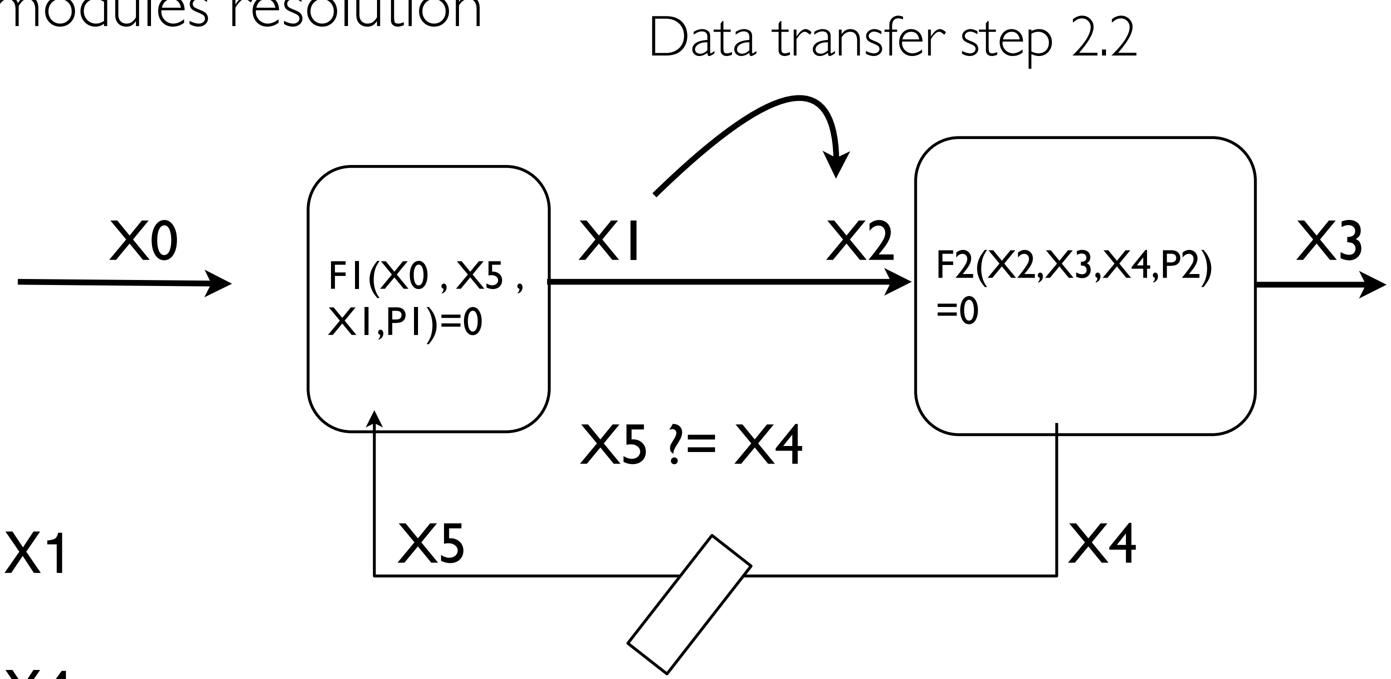
Solving method => Newton Raphson : solve a set of non linear equation

In reality X1=X2 is solved explicitly and only X1 is used
F2((X2,X3,X4,P2)=0 and X1-X2=0 becomes F2(X1,X3,X4,P2)=0

Solving Flowsheets : sequential

- **sequential approach = interconnected modules**
  - calculate output knowing inputs and parameters
  - define a sequence of modules resolution
  - explicitly solve links

Loops (recycle in flowsheets)

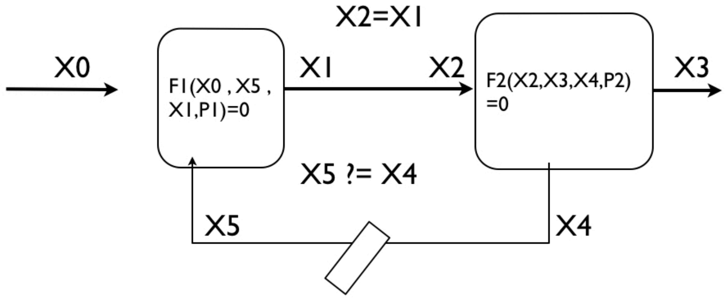


0. Locate X5
1. Guess X5
   2. 2.1 Solve unit 1 => X1
      2.2 X2=X1
   3. 3.1 Solve unit 2 => X4
   4. 4.1 Test X5 ?= X4
      4.2 yes : => out
      4.2 No : goto 5
   5. Propose a new value to X5
   & Goto 2.

Tearing loops
Loops are identified when a value that is needed by a module is the result of the calculation of the module in the sequence

Conclusions

- Flow sheet can be solved
  - simultaneously
  - in sequence



- Open Questions
  - sequential resolution : Defining a resolution sequence
    - define an ordered list of equation solving
    - Identify loops (i.e. calculated values that are needed to solve the sequence)
      - » **Tear the loops and guess an initial value**
      - » **Iterate (do the sequence of internal loop) until convergence of the loop by solving x=f(x)**
  - Simultaneous resolution : Find X^0 to solve $F(X) = 0$
    - this is typically done by using resolution sequence :
      - » **X^0 is built up progressively**
        more X^0 are calculated while adding $F_i(X)=0$ in the list of equations