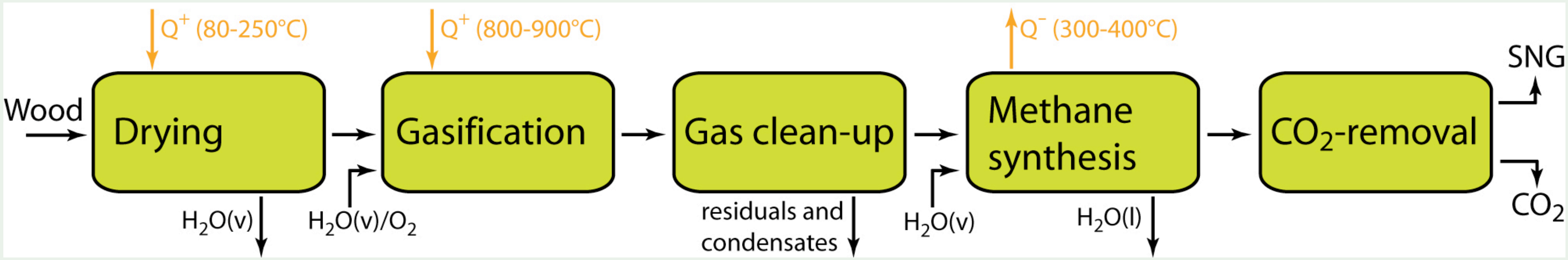
Process design and process integration

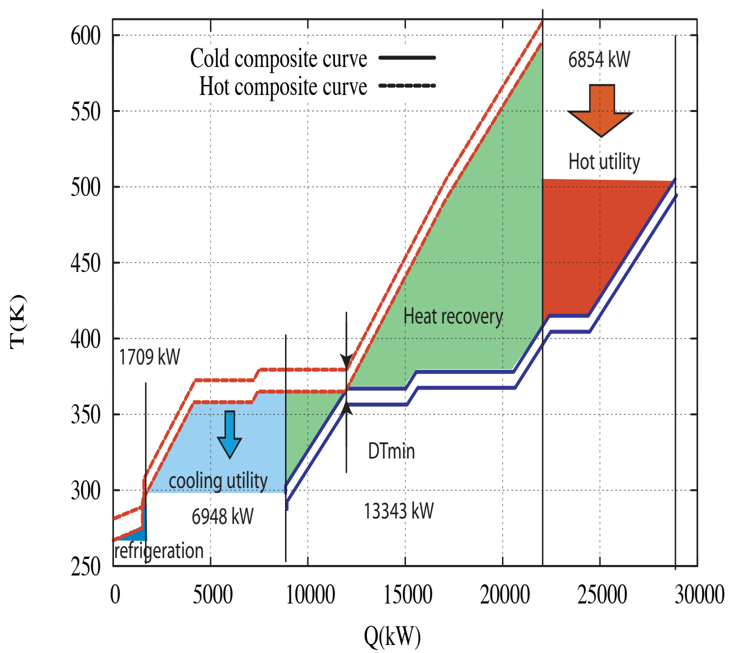
Prof F. Marechal

Process analysis

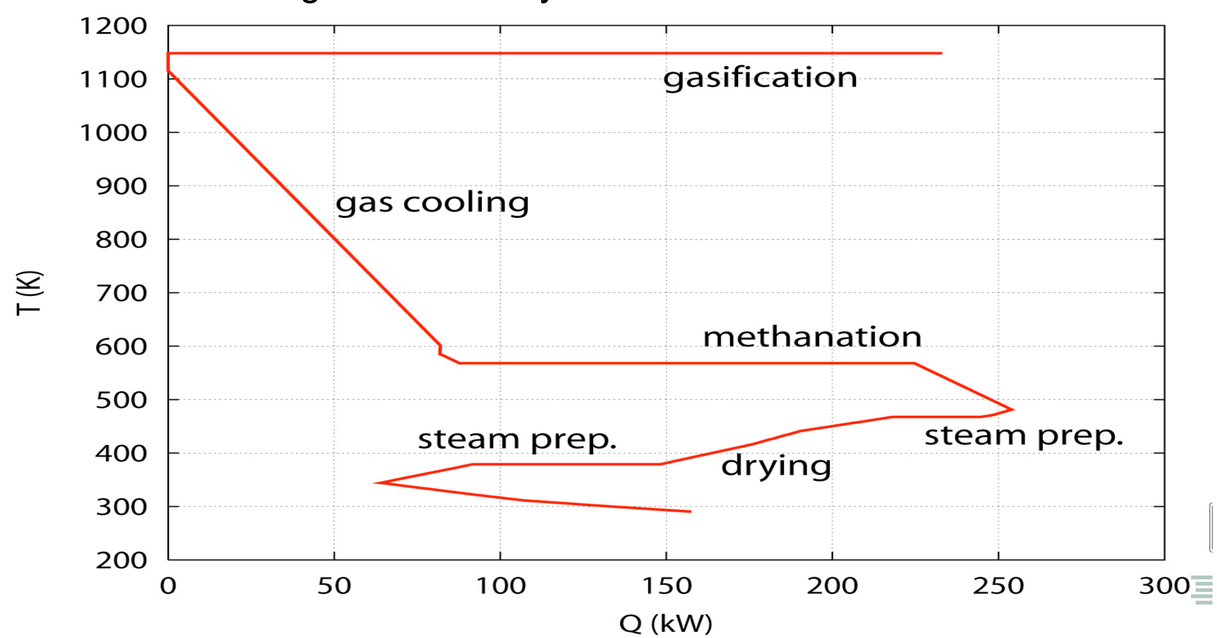
Example: Common wood to SNG route



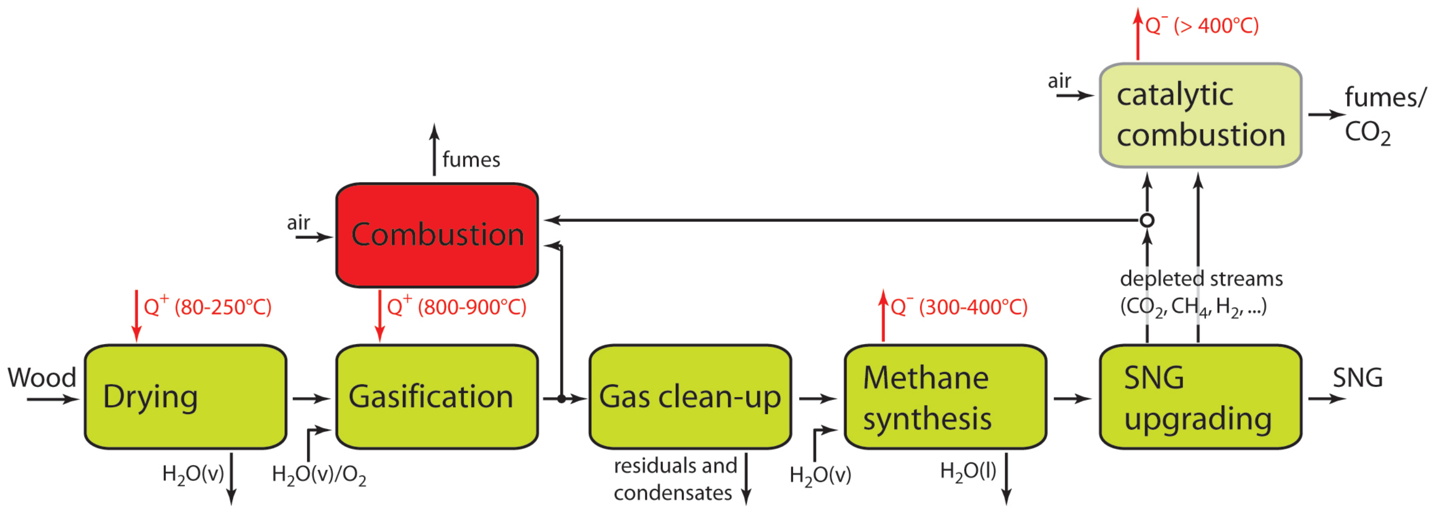
$$CH_{1.35}O_{0.63} + 0.3475H_2O \xrightarrow{\Delta H^0 = -10.5\ kJ/mol_{wood}} 0.51125CH_4 + 0.48875CO_2$$



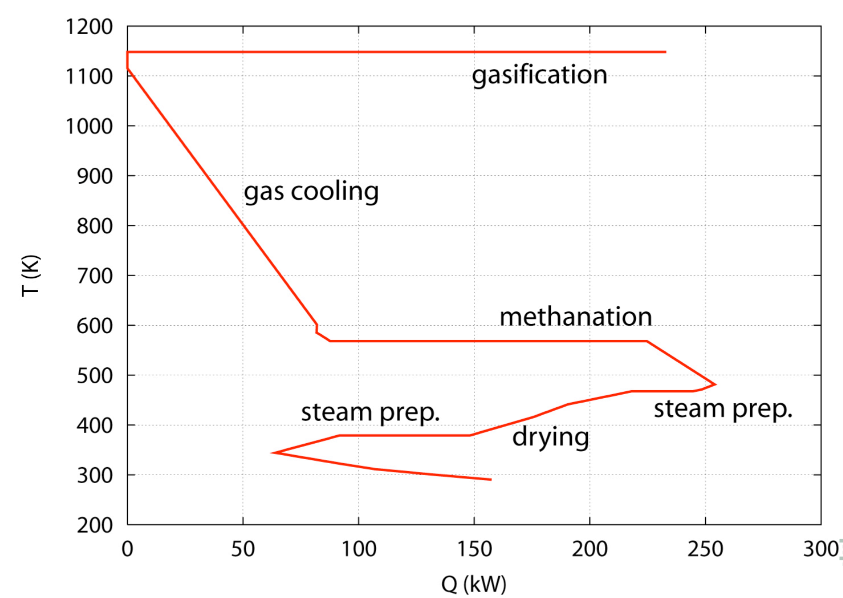
Process Composite Curve including heat recovery



Closing the energy balance

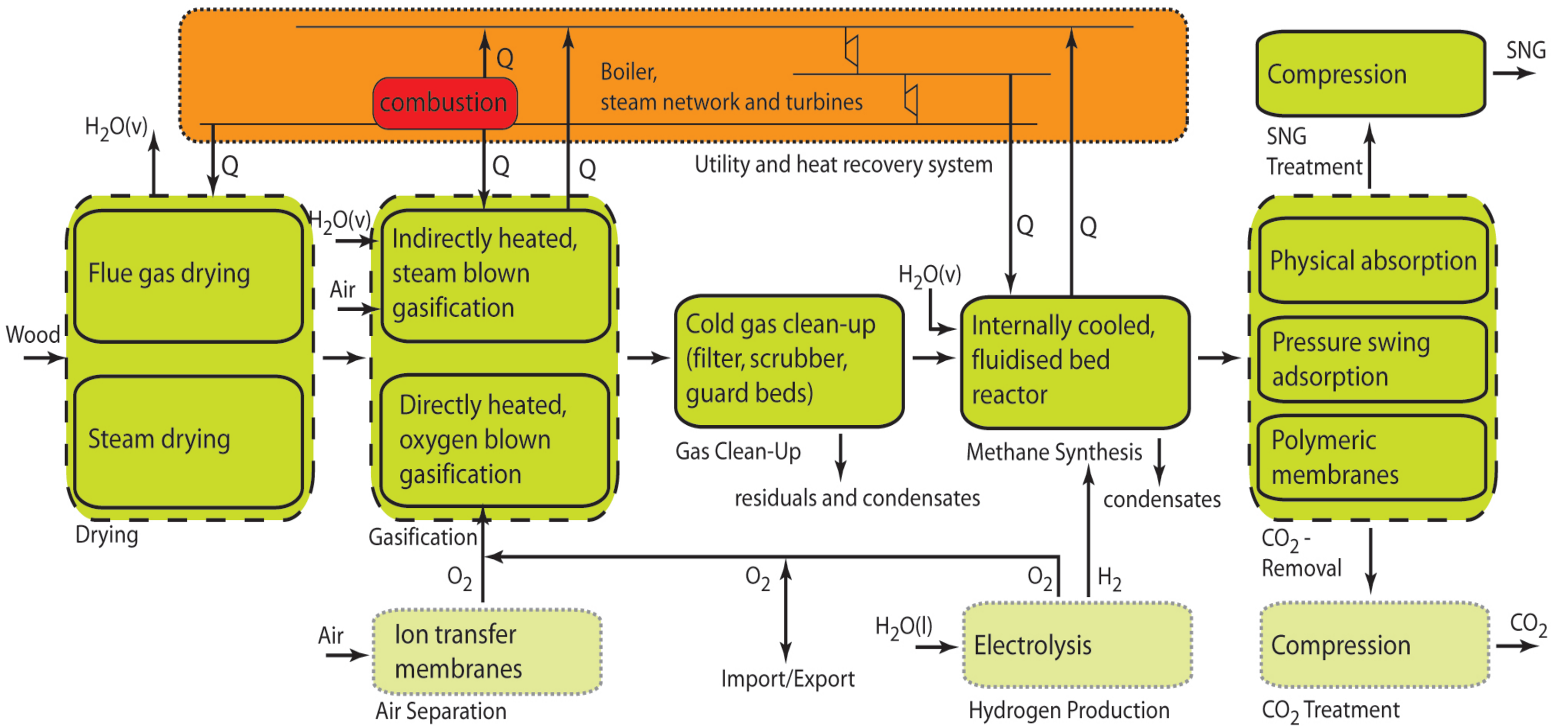


- MER of crude production
- hot utility: combustion
- fuel choice?
  - waste streams
  - intermediate products



Process superstructure

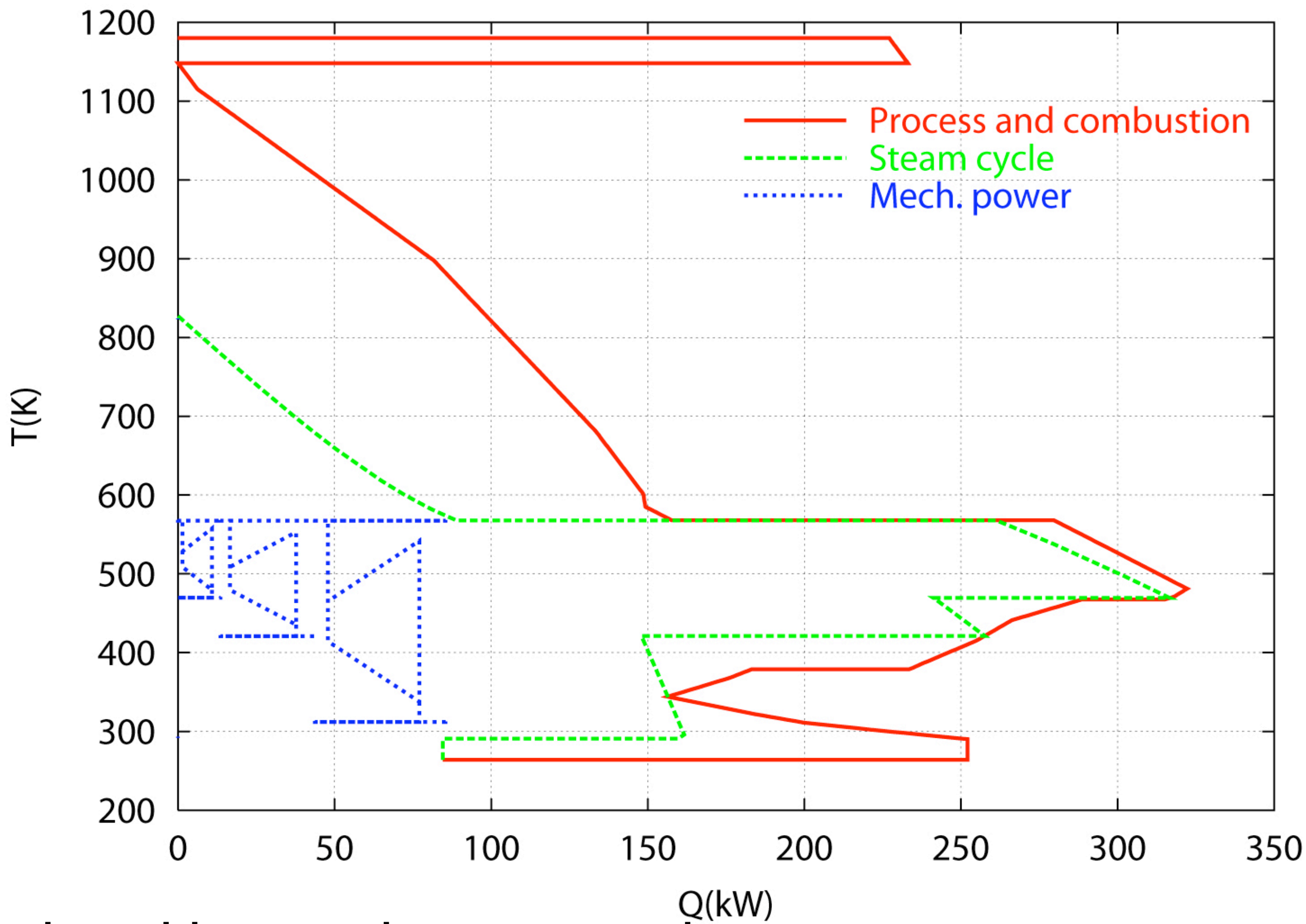
Integrating heat recovery technologies in the superstructure



Each option : y_o, f_o => split : $f_{in} = \sum_{o}^{n_o} f_o$ => mix $\sum_{o}^{n_o} f_o = f_{out}$

Flowsheet generation (2)
Energy-integration model

MILP resolution: ... to an integrated solution



Combined heat and power production

Sizing units

$$Size_u(x, \pi^*)$$

$$where \quad x \in \{x_u^+, x_u^-, \pi_u\} \quad : \text{ problem state variable}$$

x_u^+ Streams entering the unit u

x_u^- Streams leaving the unit u

π_u Parameters of the unit u

π_u^* sizing model parameters the unit u

- Sizing function may be complex and heuristics
  - sequence of calculation
  - see for example Ulrich et al.

Ulrich, K.T., and S.D. Eppinger, others. *Product design and development*. Vol. 384. McGraw-Hill New York, 1995.

see also : http://www.mech.utah.edu/senior_design/07/uploads/Main/Lect12-ConceptSelection.pdf.

Estimating investment cost based on reference data

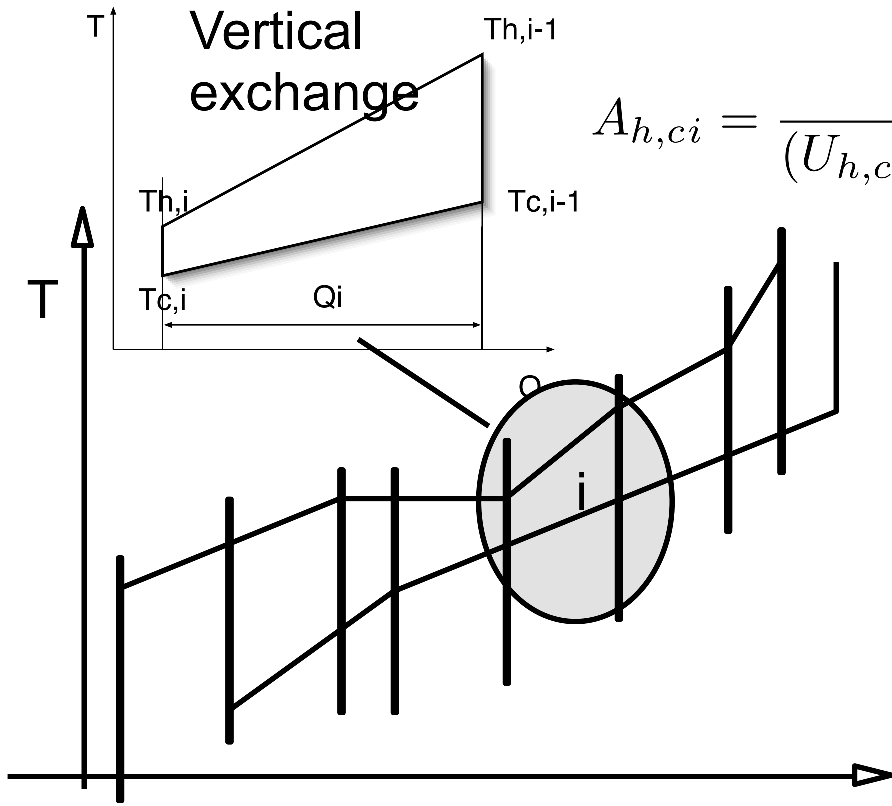
$$C_p = C_{p,ref} \cdot \left(\frac{A}{A_{ref}}\right)^{\gamma} \cdot \frac{I_t}{I_{t,ref}}$$

$C_{p,ref}$	purchase cost of the reference case
A	equipment attribute
A_{ref}	equipment reference attribute
γ	capacity exponent
$I_{t,ref}$	cost index for the reference year
I_t	cost index for the actual year

– Index :

- Marshall & Swift Equipment Cost Index
- CEPCI : Chemical Engineering Plant Cost Index

Estimating heat exchanger network Area



$$A_{h,ci} = \frac{(Q_{h,c})_i}{(U_{h,c})_i * \Delta(T_{lm})_i} = \left(\frac{1}{h_{i,h}} + \frac{1}{h_{i,c}}\right) * \frac{Q_i}{\Delta(T_{lm})_i}$$

With

$$(\Delta T_{lm})_i = \frac{(T_{h,i} - T_{c,i}) - (T_{h,i-1} - T_{c,i-1})}{ln(\frac{T_{h_i} - T_{c,i}}{T_{h,i-1} - T_{c,i-1}})}$$

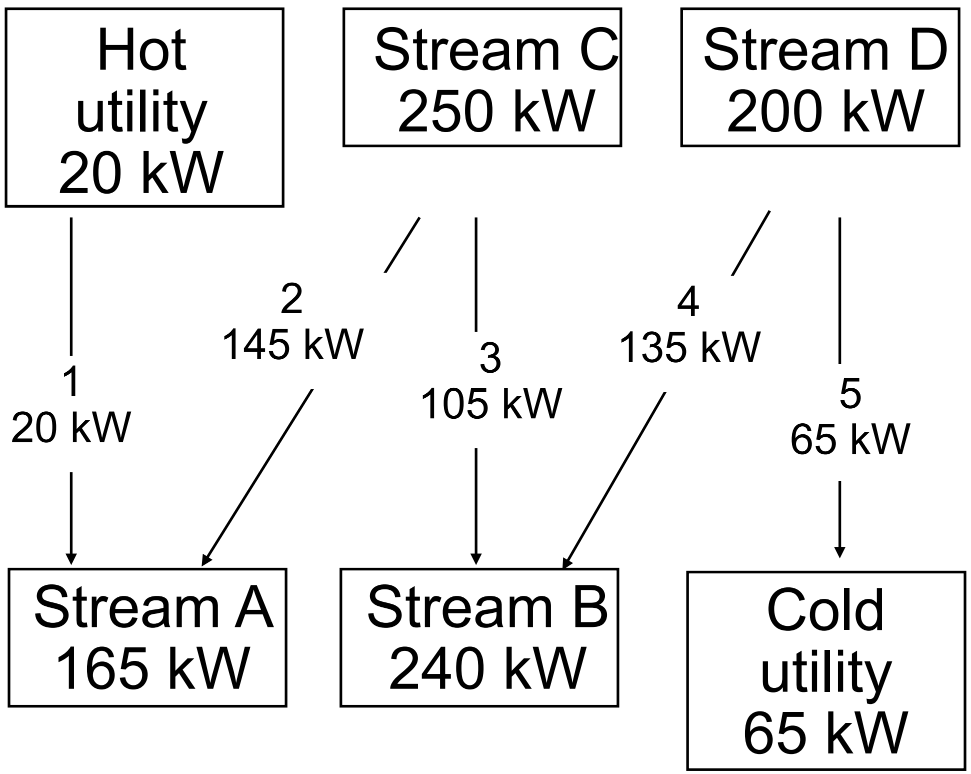
Real temperatures

Overall exchange area : $$A_{HX} = \sum_{i=1}^{n_v} A_i = \frac{Q_i}{(\Delta T_{lm})_i} * (\sum_{j=1}^{(n_{streams})_i} * \left(\frac{1}{h_{i,j}}\right))$$

Fluid dependent DTmin/2 for the heat cascade calculation

Minimum number of units

from the graph theory



3 Sources : hot streams

TOTAL = 470 KW

3 Sinks : Cold streams

TOTAL = 470 KW

Number of Exchangers = **Number of streams** + **Number of Utilities** - **Number of independent system**

$$5 = 4 + 2 - 1$$

This is by applying the graph Theory from Leonhard Euler (1707-1783).
When the overall system is balanced, there is at least one independent sub-system

Pinch point = two independent sub-systems

Number of Independent sub-systems above the pinch point

Number of Independent sub-systems below the pinch point

$$U_{\min,MER} = (N_{above} - 1 - S_{above}) + (N_{below} - 1 - S_{below})$$

Number of streams above the pinch point

Number of streams below the pinch point

$$U_{\min,MER} = (N_{total} + N_{utility} - 1) + (N_{pinch} - 1) - (S_{above} + S_{below})$$

Number of Independent sub-systems below and above the pinch point

Total number of streams, including the utilities

Number of streams crossing the pinch point

Estimating the heat exchanger network cost

Overall exchange area : $$A_{HX} = \sum_{i=1}^{n_v} A_i = \frac{Q_i}{(\Delta T_{lm})_i} * (\sum_{j=1}^{(n_{streams})_i} * \left(\frac{1}{h_{i,j}}\right))$$

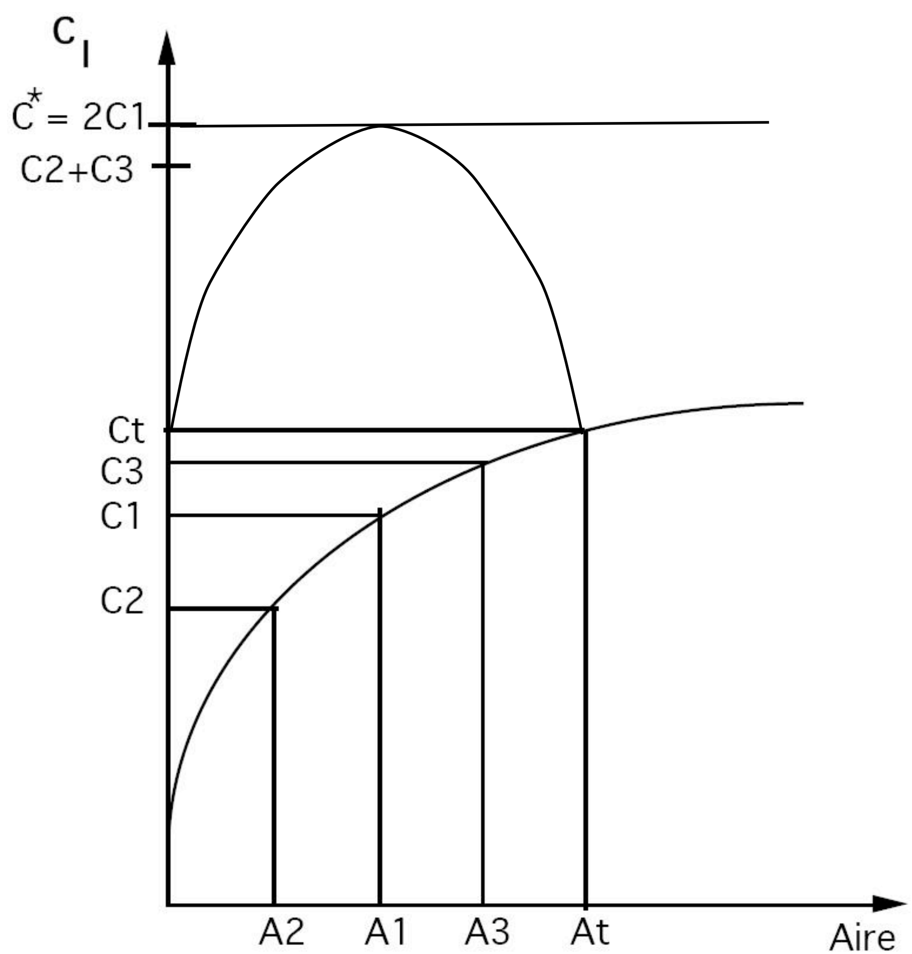
Number of heat exchangers : $$U_{min,mer} = N_{streams} - 1 + \sum_{p=1}^{n_{pinch}} (n_{streams,p} - 1)$$

Heat exchange area for one heat exchanger $$A_h = \frac{A_{HX}}{U_{min,mer}}$$

Estimated investment for the heat exchanger network $$I_{HX} = U_{min,mer}(\frac{I_{today}}{I_{ref}}(a_{h_{ref}} + b_{h_{ref}}(A_h)^{c_{h_{ref}}}))$$

Bolliger, Raffaele, Francesca Pallazzi, and Francois Marechal. “Heat exchanger network (hen) costs and performances estimation for multi-period operation.” In *Computer aided chemical engineering, Proceedings of ESCAPE 18, 18th European Symposium on Computer Aided Process Engineering*. ESCAPE18 conference proceedings, 2008.

Cost estimation : over estimation



by assuming an equal repartition of the area over all the heat exchangers, we will overestimate the heat exchangers total cost.

EPFL

Fluid dependent ΔTmin value

If A and Q are constant

If U increases : ΔT decreases

If U decreases : ΔT increases

=> ΔTmin is related to the streams involved

-> to the film heat transfer coefficient

Temperature difference

$$\dot{Q}_{ex} = U_{ex} A_{ex} \Delta T_{lm}$$

$$\frac{1}{U_{ex}} = \frac{1}{\alpha_{cold}} + \frac{e}{\lambda} + \frac{1}{\alpha_{hot}}$$

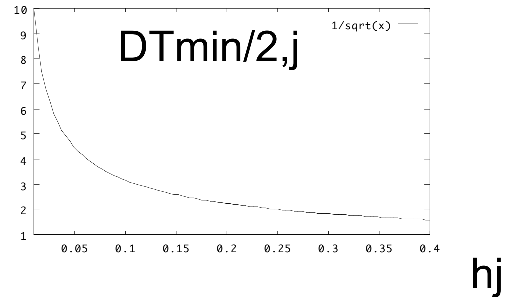
The ΔTmin is related to the type of fluids

Heat exchange: ΔT ≥ ΔTmin/2,h + ΔTmin/2,c

DTmin as a function of heat transfer

Remaining parameter => 1 DOF

$$\Delta Tmin/2_j = K_{\Delta Tmin} \cdot (\frac{\dot{Q}_j \cdot h_{ref}}{h_j \cdot \dot{Q}_{ref}})^{\frac{c}{c+1}}$$



Convective heat transfer coefficient

c is the cost exponent in the heat exchanger cost estimation formula

Table 1: Typical values for the $\Delta T_{min}/2$ as a function of the heat transfer film coefficient

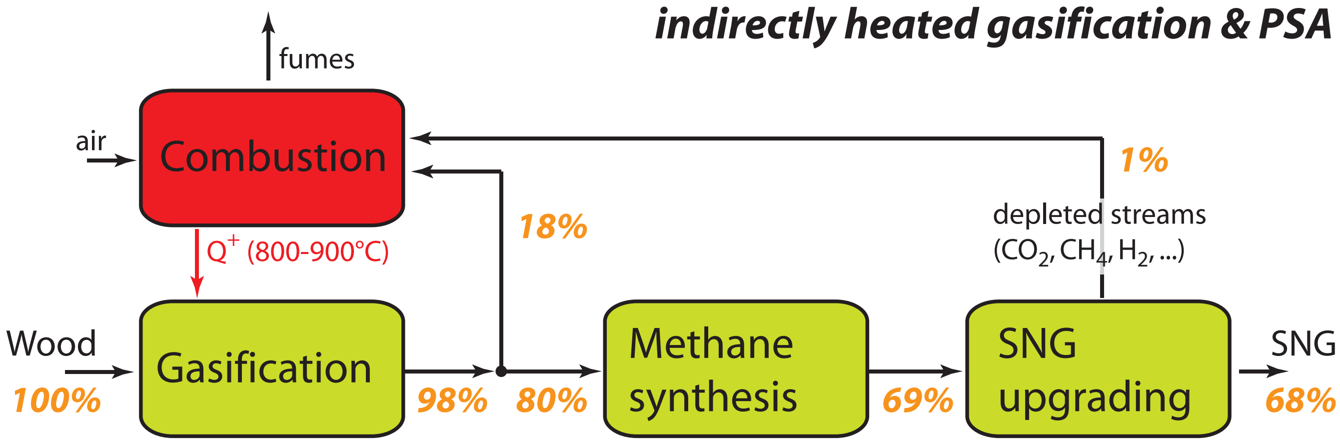
Type	Heat transfer coefficient $W/m^2/C$	$\Delta T_{min}/2$
Gas stream	60	15
Liquid stream	560	5
Condensing stream	1600	3
Vaporizing stream	3600	2

Total cost

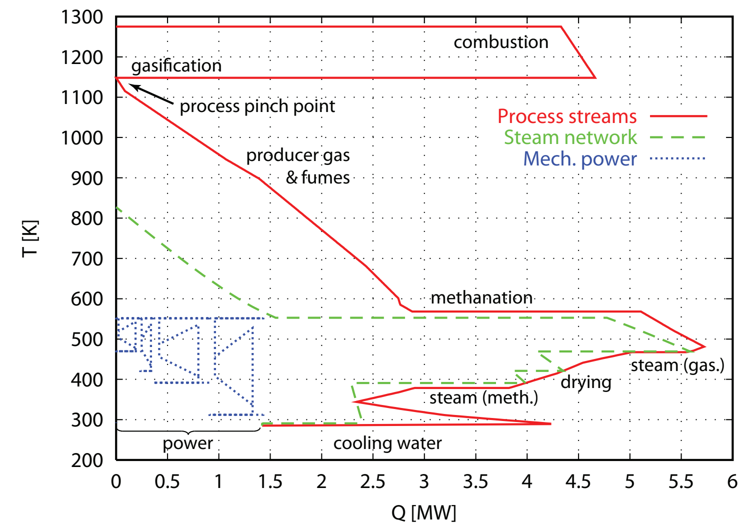
$$TotalCost \quad [\$/year] = \sum_{p=1}^{n_p} OPEX(p) + F + \frac{i(1+i)^{n_y}}{(1+i)^{n_y}-1} \cdot CAPEX$$

$OPEX(p)$	$[\$/period]$	operating cost during period p
n_p		number of operating periods during the year
i	$[-]$	interest rate for the capital investment
n_y	$[year]$	expected life time for the capital investment
$CAPEX$	$[\$]$	Capital investment
F	$[\$/year]$	yearly fixed cost

Some (non-optimised) scenarios for conventional SNG production:



(only the chemical energy flow of the main product conversion is shown)



input: $20\ MW_{th,wood}$

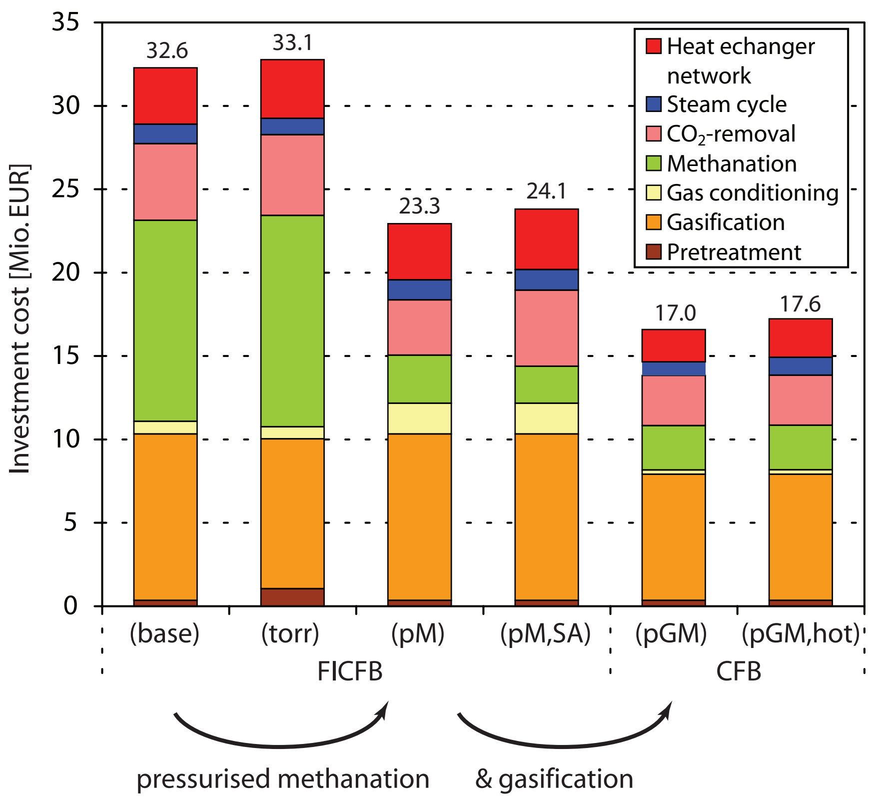
		FICFB				CFB	
		(base)	(torr)	(pM)	(pM, SA)	(pGM)	(pGM, hot)
Consumption	Wood	100%	100%	100%	100%	100%	100%
	Biodiesel	1.8%	1.6%	1.8%	1.8%	0.1%	-
	Electricity	-	0.5%	-	-	0.9%	-
Production	SNG	67.7%	72.1%	67.5%	67.8%	74.0%	74.0%
	Electricity	2.9%	-	2.6%	3.3%	-	1.6%
Overall efficiency		69.4%	70.7&	68.8%	69.8%	73.2%	75.6%

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

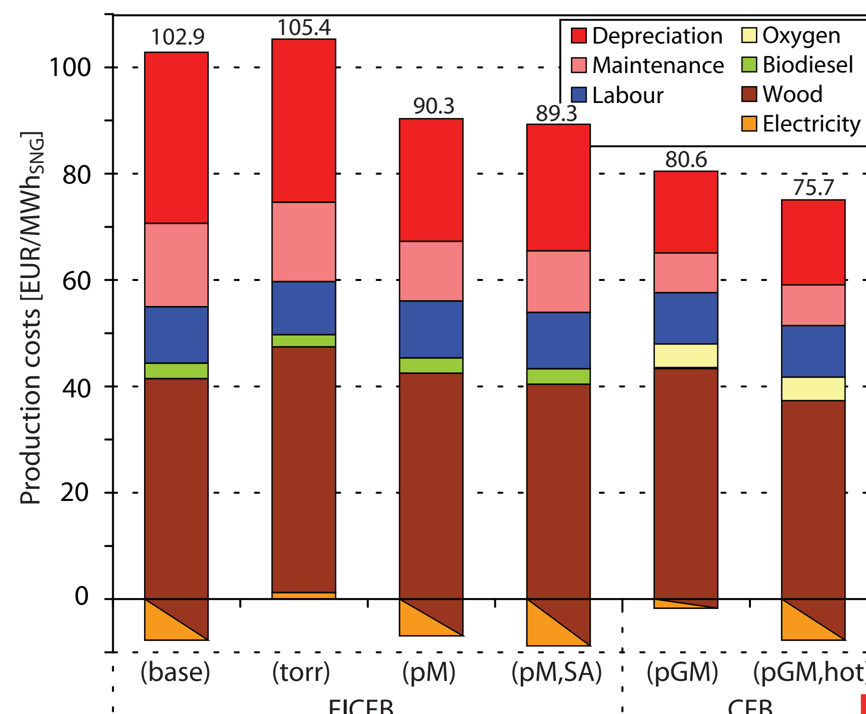
Process performance
conventional SNG

Some (non-optimised) scenarios for conventional SNG production:

Investment cost

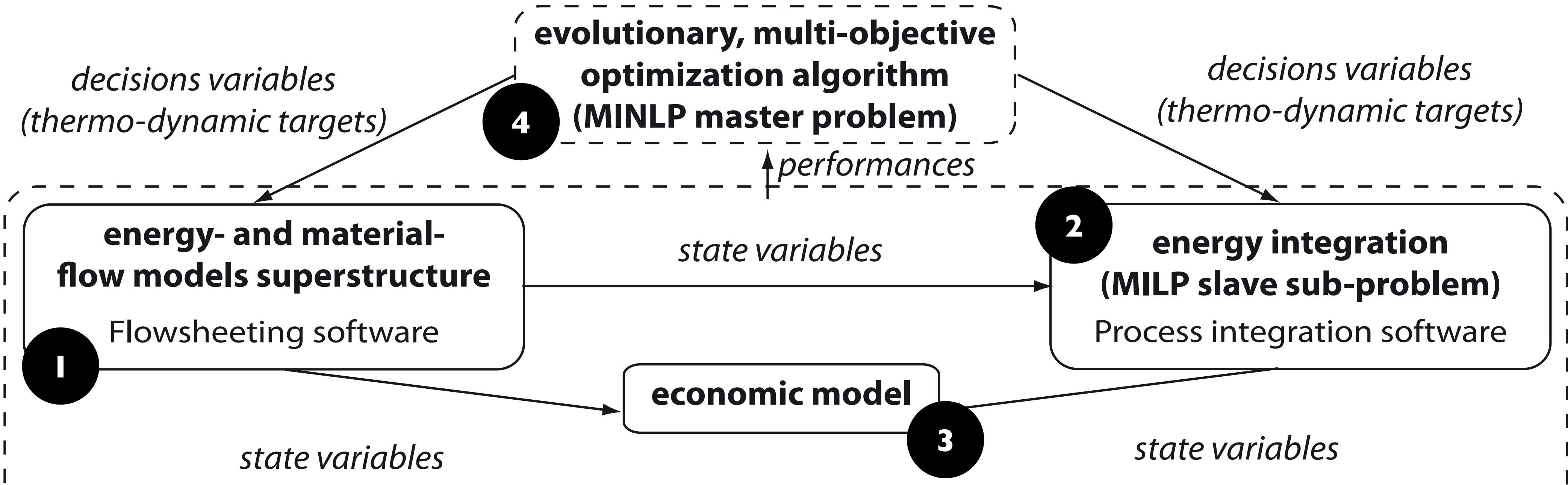


Total production costs



Gassner, Martin, and François Maréchal. "Thermo-economic process model for thermochemical production of Synthetic Natural Gas (SNG) from lignocellulosic biomass." *Biomass and Bioenergy* 33, no. 11 (November 2009): 1587-1604.

Using optimisation to extract solutions



Gerber, Léda, Martin Gassner, and François Maréchal. "Systematic Integration of LCA in Process Systems Design: Application to Combined Fuel and Electricity Production from Lignocellulosic Biomass." *Computers & Chemical Engineering* 35, no. 7 (December 9, 2010): 1265–1280. http://linkinghub.elsevier.com/retrieve/pii/S0098135410003595.

MINLP : decomposition problem

- Master (M) -Slave (S) decomposition

$$\begin{array}{ll} \min\limits_{X_M} & Obj(X_M, X_S(X_M), \pi) \\ s.t. X_S(X_M) & \min\limits_{X_S} Obj_S(X_S, X_M, \pi) \\ s.t. & H(X_S, X_M, \pi) = 0 \\ & H(X_S, X_M, \pi) \geq 0 \end{array}$$

=> partition variabl

=> Simple to solve

$$\begin{array}{ll} X_M & \text{Master Variables} \\ X_S & \text{Slave Variables} \\ \pi & \text{Parameters} \end{array}$$

Black Box strategy

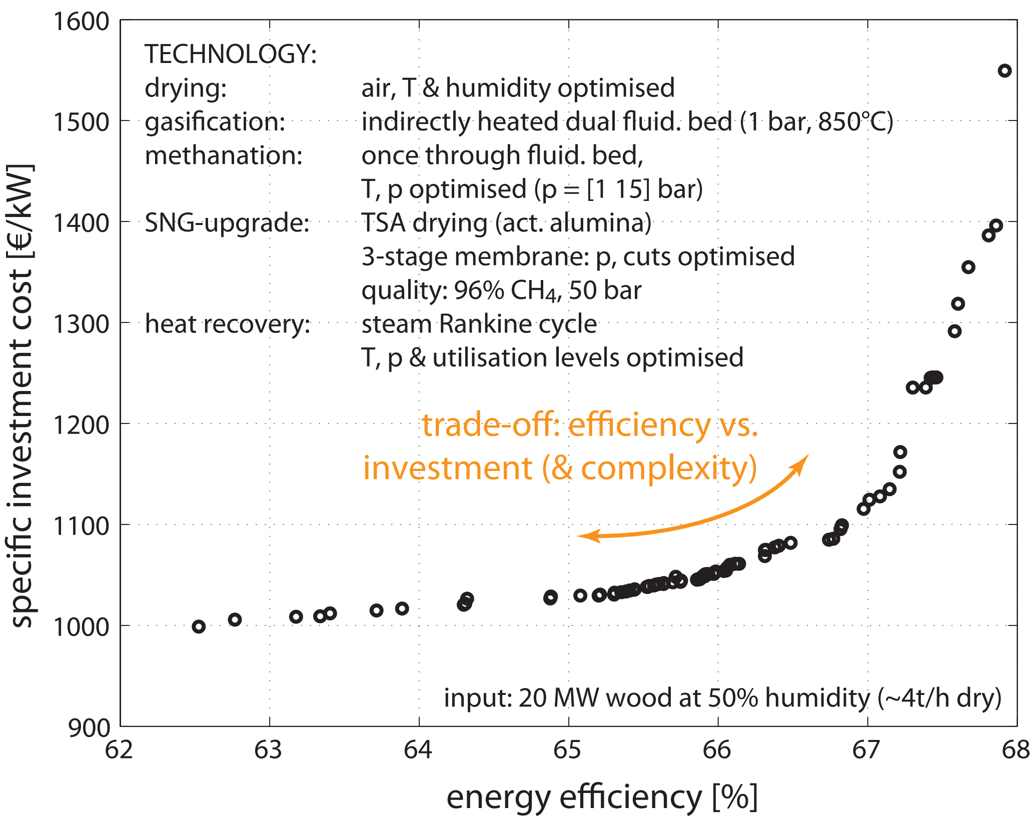
$$
\begin{aligned}
\min_{X^*_{decision}} \quad & TotalCost(X^*_{decision}, X(X^*_{decision})) \\
s.t. \quad & G(X^*_{decision}, X(X^*_{decision})) \leq 0 \quad \text{inequality constraints} \\
where \quad & \\
& X^*_{decision} = \{x_{decision}, y_{decision} \epsilon \{0,1\}\} \\
X(X^*_{decision}) \quad & \text{Calculated by solving:} \\
& F(X_{state}) = 0 \Rightarrow \text{equipment model} \\
& L(X_{state}) = 0 \Rightarrow \text{linking equations} \\
& T(X_{state}) = 0 \Rightarrow \text{constitutive equations} \\
& S(X_{state}) = 0 \Rightarrow \text{Specification equations} \\
& X_{decision} - X^*_{decision} = 0 \Rightarrow \text{Specification of the value of decision variables} \\
where \quad & \\
& X_{state} = \{x_{StateVariables}, x_{UnitParameters}, y_{decision} \epsilon \{0,1\}\}
\end{aligned}
$$

Heuristic methods to systematically generate optimal configurations

- Applies only on black box strategy
- Exploring the search domain
  - systematically
  - based on some analogy
- Simulated annealing
  - based on the analogy with metallurgy
    - heating/cooling of metal to minimize the energy content
- Evolutionary algorithm
  - genetic algorithms
    - based on the analogy of the evolution
      - Best fitted individuals have a higher probability to survive and reproduce
      - Reproduction based on sharing gene info
- Particle swarm
  - initial speed + communication between agents
- Ants colony

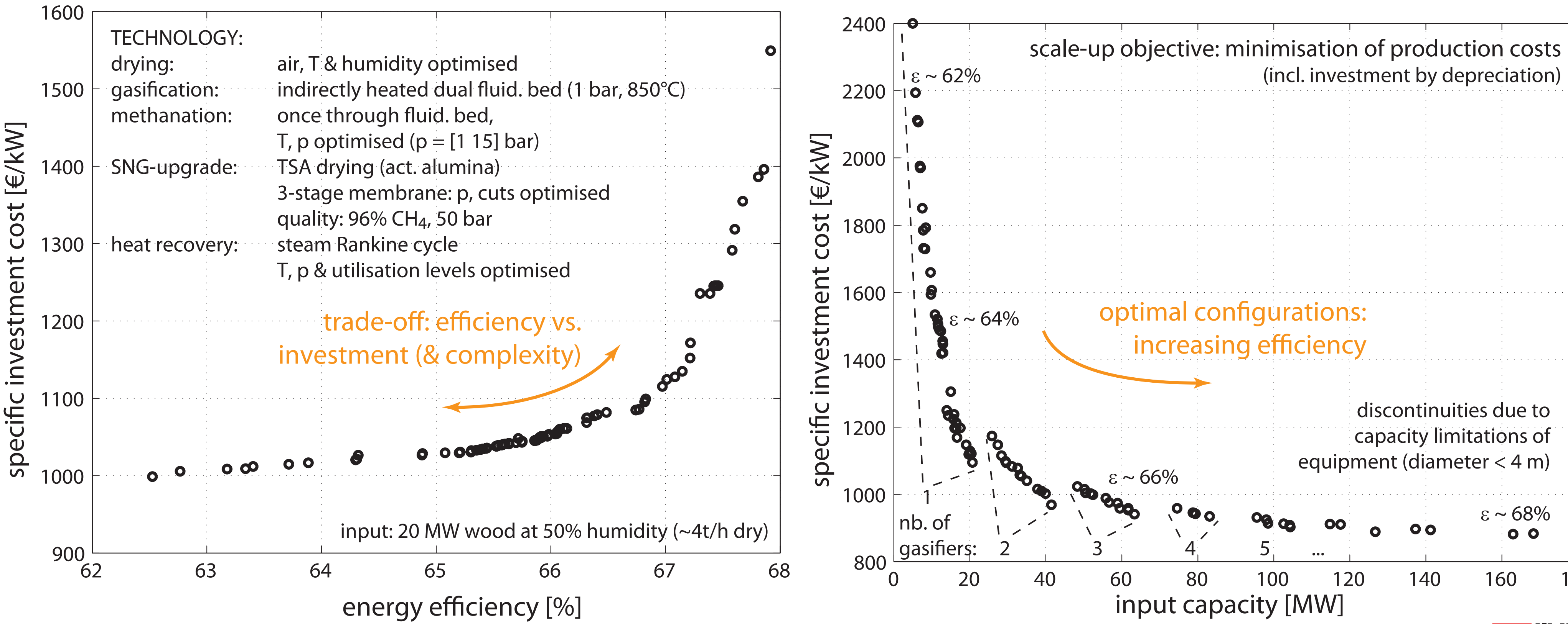
Thermo-economic optimisation
Trade-offs: efficiency and scale vs. investment

Efficiency vs. investment:



ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

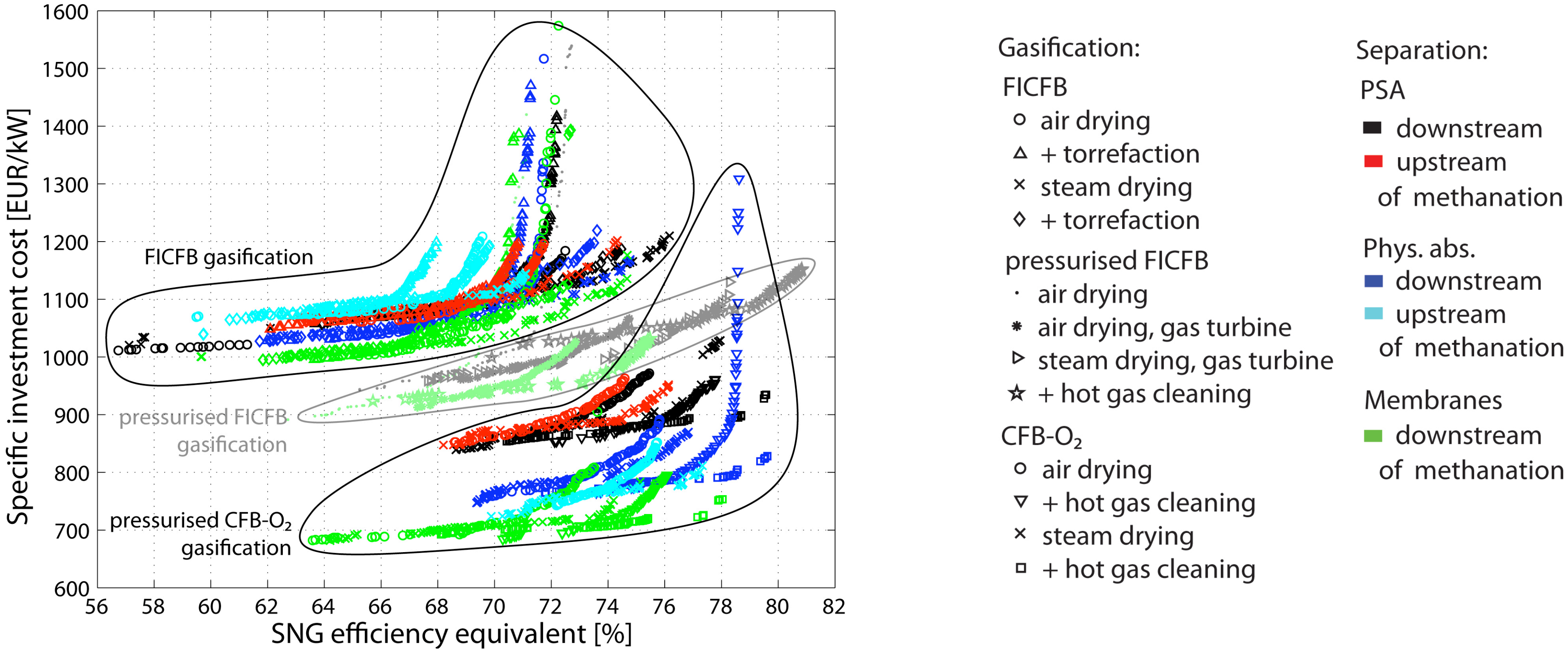
Efficiency vs. investment and optimal scale-up:



8. Analysing the results

- Each point of the Pareto is a process design

Thermo-economic Pareto front (cost vs efficiency):



→ *The best solution is the pressurised directly heated gasifier*

Martin Gassner , Ph D Thesis, EPFL, 2010