Advanced Process Modelling Forum 2016, April 20-21 2016, London, UK

Simulatenous Process Design and Optimal Utility Selection

Ligang Wang, François Maréchal

Industrial Process and Energy Systems Engineering, Swiss Federal Institute of Technology in Lausanne, L'industrie 17, 1950 Sion, Switzerland.
ligang.wang@epfl.ch (LW); francois.marechal@epfl.ch (FM)

1. Motatiation and Tasks

Most effective methods for heat and mass network design of industrial processes are based on pinch analysis. However, it is difficult to couple pinch analysis directly in an equation-based simulator, since it features with with non-differentiable nature and requires sorting of temperature arrays. The optimal utility selection is also significant from the whole system and multi-period operation viewpoint. However, these functions have not been included in gPROMS products.

Therefore, a foreign object, **gIntegration**, for heat and mass integration considering both the process design and multi-period utility selections. The information of heat-mass streams of both processes and utilities are collected by connecting to the integration unit to call gIntegration. The pinch analysis and mixed-integer linear programming problems for multi-period utility selection are solved in gIntegration for optimal utility selection. Graphic presentations of pinch analysis and multi-period period operation of utility are grapically presented in the report of the integration unit. The gIntegration is flexible and really easy to use for stead-state problems.

2. Mathematical Formulation of Multi-period Utility Targeting

The utility selection can be formulated as a **mixed-integer linear programming** problem (Maréchal2003):

$$\min_{y_{u,i},f_{u,i},Y_u,F_u} \sum_{u=1}^{n_U} a_{u,i}Y_u + \sum_{i=1}^{n_P}\left(\sum_{u}^{n_U}(b_u f_{u,i}) + c^{b}_{e,i}W^{b}_{e,i} - c^{s}_{e,i}W^{s}_{e,i}\right)\cdot t_i + \frac{1}{\tau}\sum_{u=1}^{n_U}(\alpha_u Y_u + \beta_u F_u)$$

Heat cascade:

$$\begin{cases}\sum_{u=1}^{n_U} f_{u,i}q_{u,r} + \sum_{k=0}^{n} Q_{k,r}L_{k,i} + R_{r+1,i} - R_{r,i} = 0 \\ R_{1,r} = 0 \quad R_{n_R+1} = 0 \quad R_{r,i} \geq 0\end{cases}$$

Power-mass integration:

$$\begin{cases}\sum_{u=1}^{n_U} f_{u,i}w_u + W^{b}_{e} - L_{k,i}W_k \geq 0 \\ \sum_{u=1}^{n_U} f_{u,i}w_u + W^{b}_{e} - W^{s}_{e} - L_{k,i}W_k = 0 \\ W^{b}_{e} \geq 0 \quad W^{s}_{e} \geq 0\end{cases}$$

Feasibility:

$$\begin{cases} y_{u,i} \in 0,1 \quad Y_u \in 0,1 \\ Y_u \geq y_{u,i} \quad F_u \geq f_{u,i} \\ f_u^{\min} y_{u,i} \leq f_{u,i} \leq f_u^{\max} y_{u,i}\end{cases}$$

$$\forall u = 1,\dots,n_U \quad \forall i = 1,\dots,n_P \quad \forall r = 1,\dots,n_R$$

Symbols:
u - utility index; i - period index; r - temperature interval index;
k - process index; b, s - resources purchased and sold;
e - power or mass streams; c - specific cost;
y - utility use fact at period i (if use $y = 1$, else $y = 0$);
Y - utility equiped or not (if equiped $Y = 1$, else $Y = 0$);
f - utility load at period i; F - utility size;
t - length of period i; τ - annulization factor;
a - fixed operating cost; b - variable operating cost;

$$OC_u = a_u + b_u \cdot F_u$$

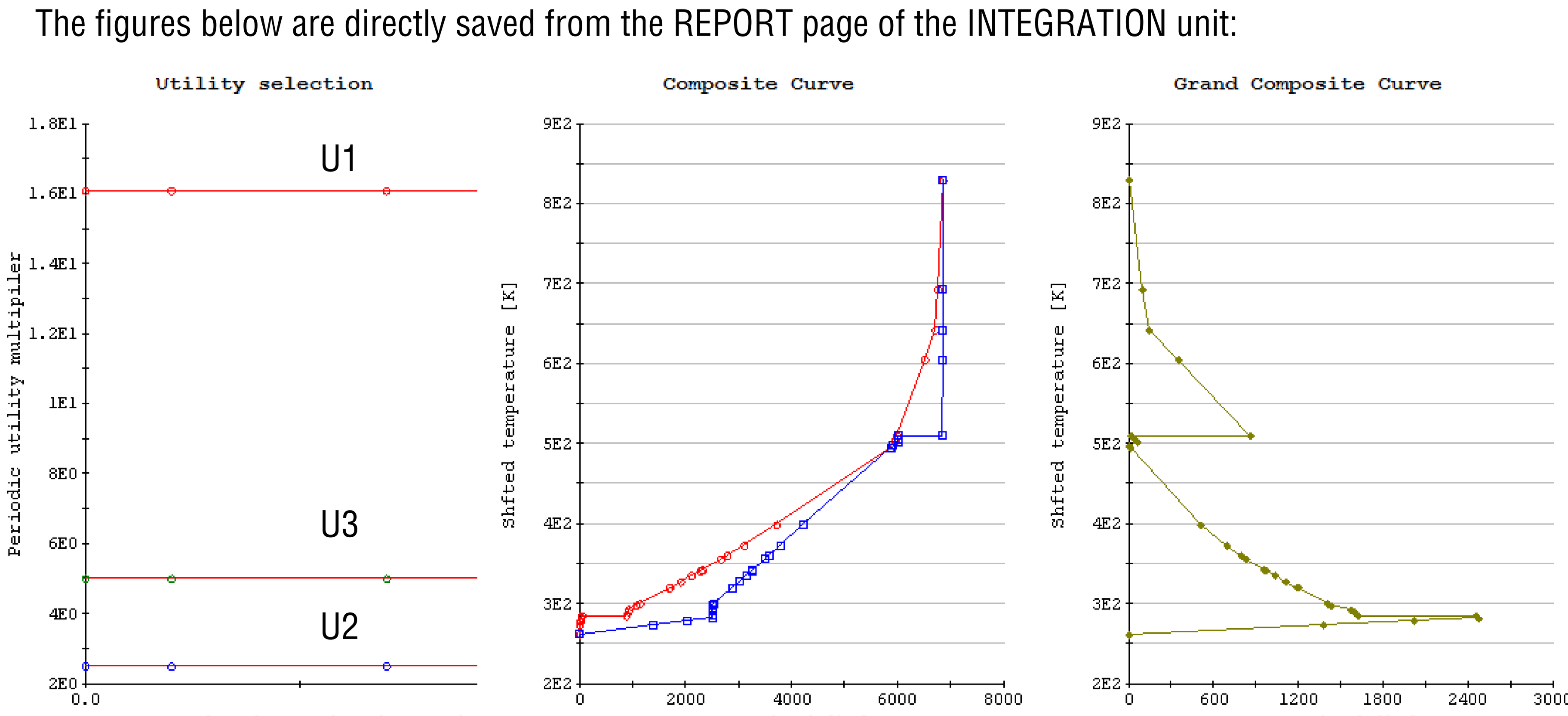
α - fixed investment cost; β - variable investment cost;

$$IC_u = \alpha_u + \beta_u \cdot F_u$$

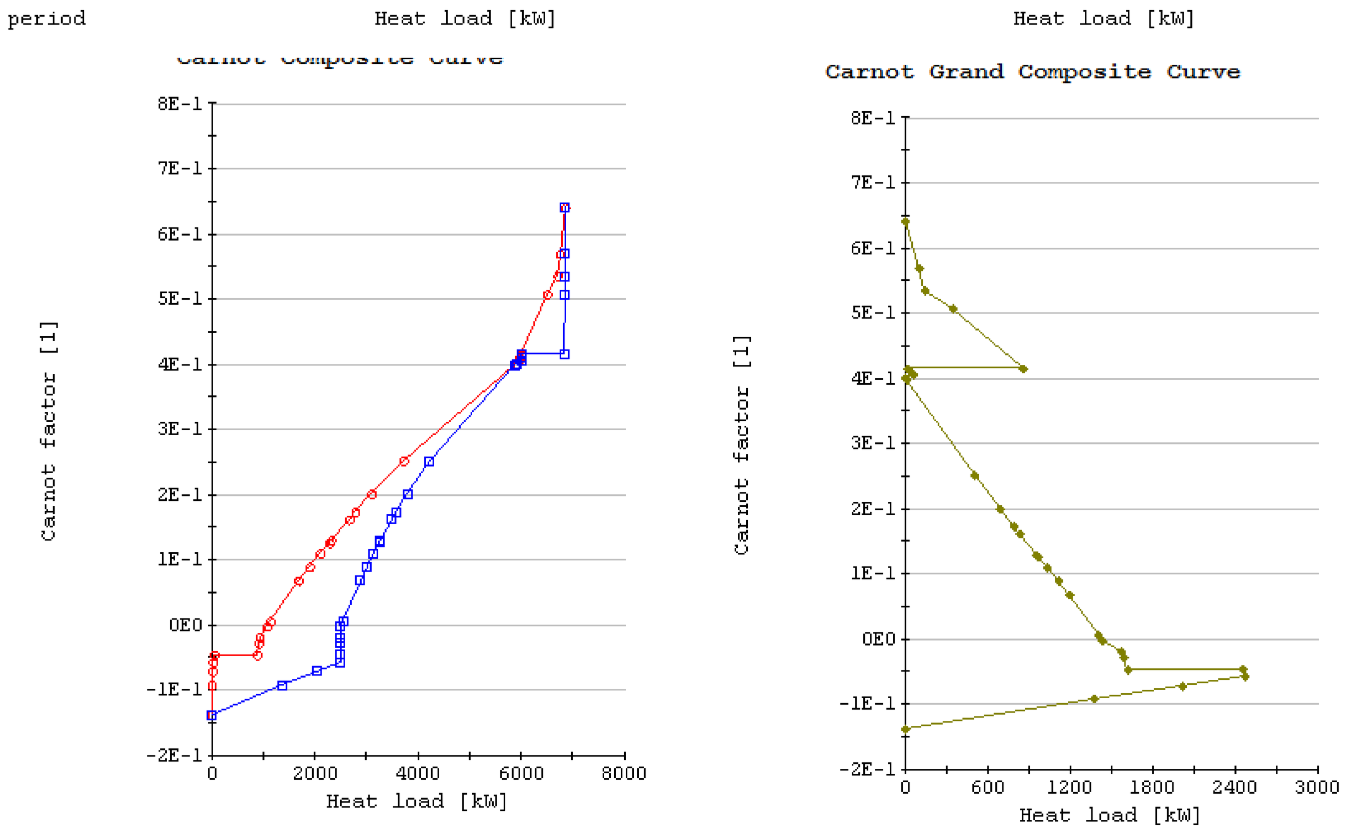
q, Q - utility and process heat at temperature interval r;
L - process operation level at period i;
R - heat transfer from the higher temperature interval;
w, W - utility and process power or mass flows;
$f_u^{\min}$ - lower bound of utility size;
$f_u^{\max}$ - upper bound of utility size;

5. Results of the Exemplary Illustration

The figures below are directly saved from the REPORT page of the INTEGRATION unit:



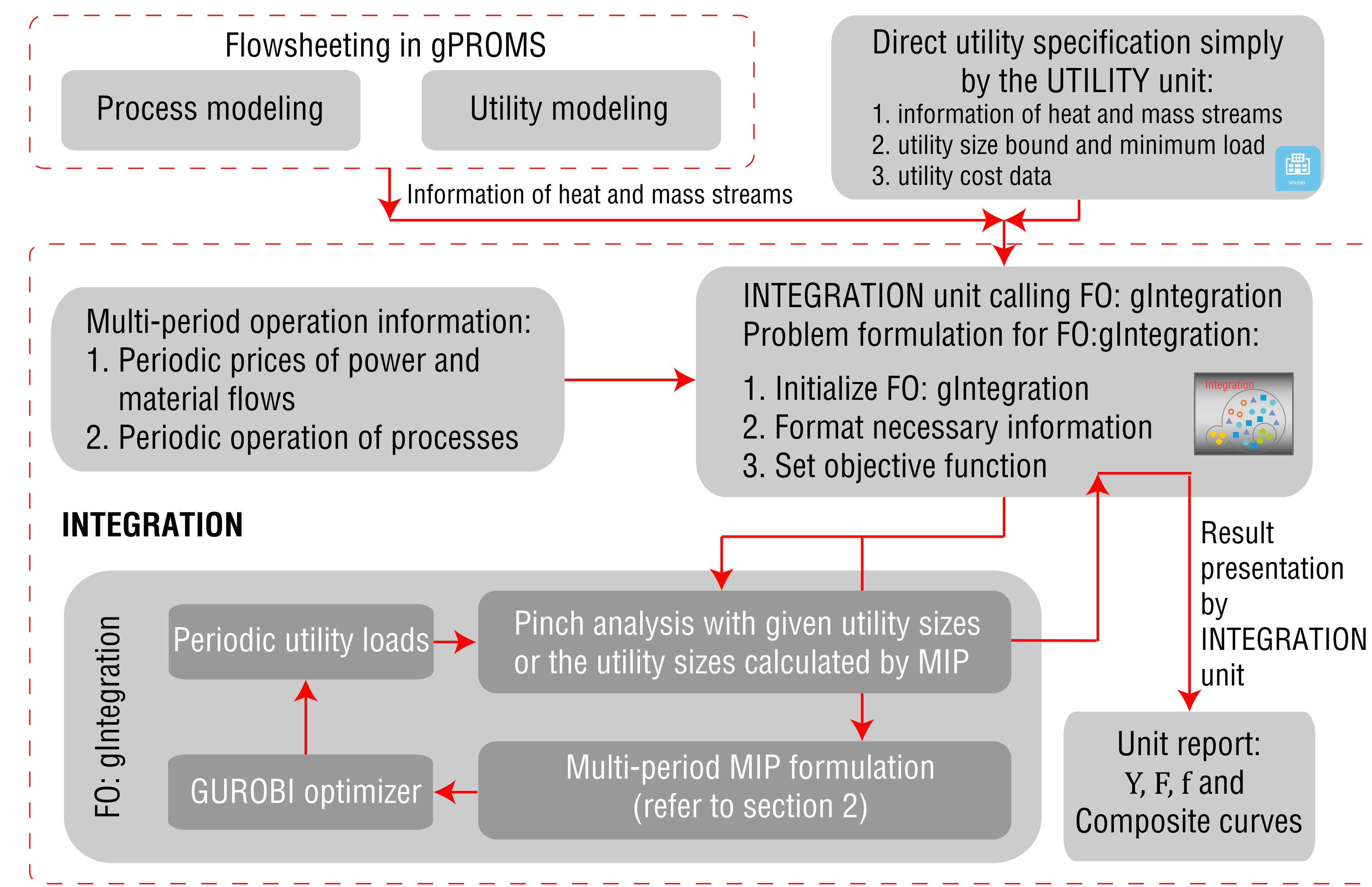
Note:
The graphs presented are based on the base-case process design without process optimization. Here we only illustrate the ability of gIntegration.



6. Conclusions

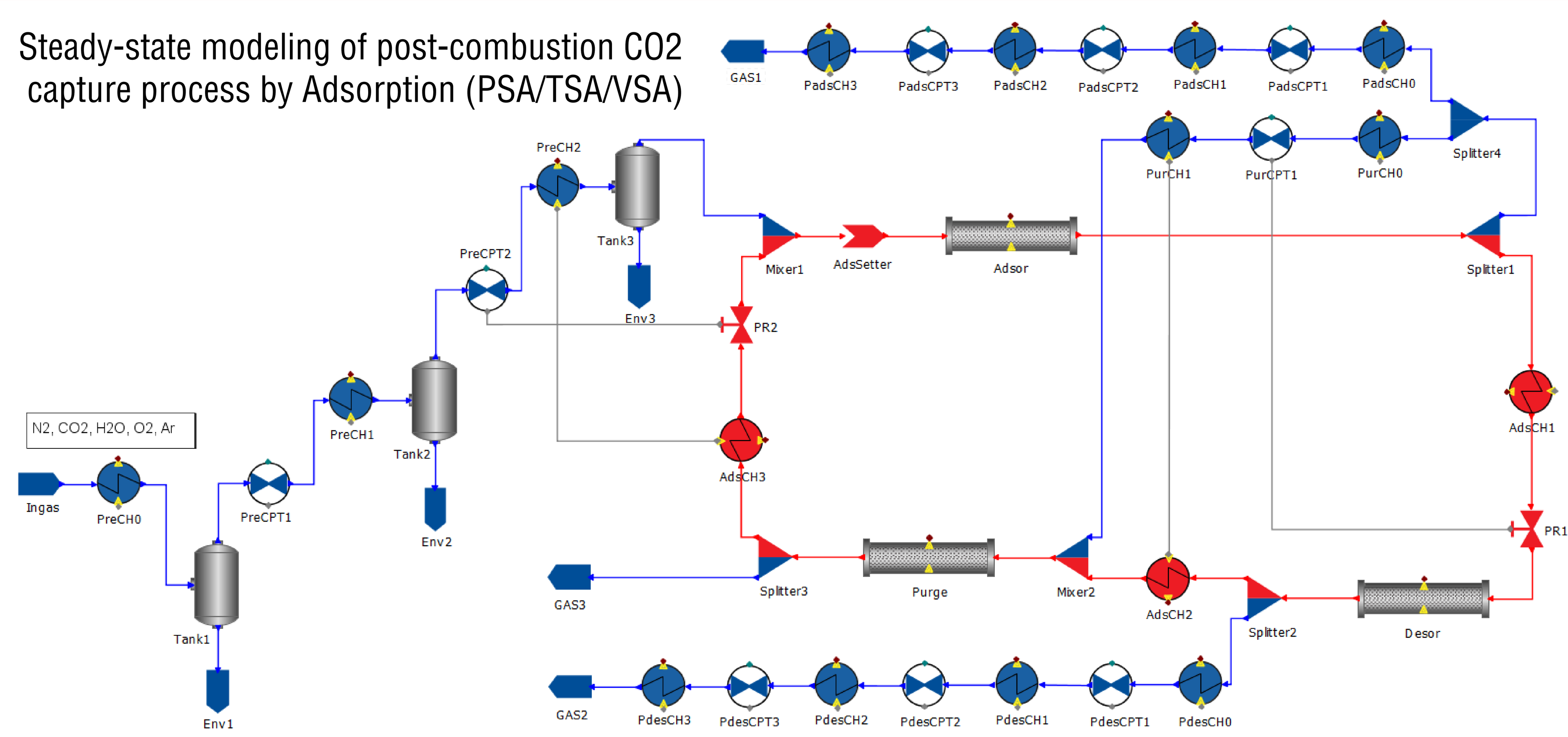
1). The feature of gPROMS of Allowing dynamic and zero-dimension arrays offers great flexibility for multiple or zero connections of heat/mass/power streams.
2). Pinch analysis can not provide derivatives, thus not straightforward for simulatenous process optimization and optimal utility selection. The optimization by gPROMS for the processes coupled with gIntegration needs to be tested!
3). gIntegration needs to be further developed to consider:
   a. Energy and mass storage
   b. Material integration with material pinch
   c. Direct presentation of heat exchanger network

3. Implementation in gPROMS ModelBuilder



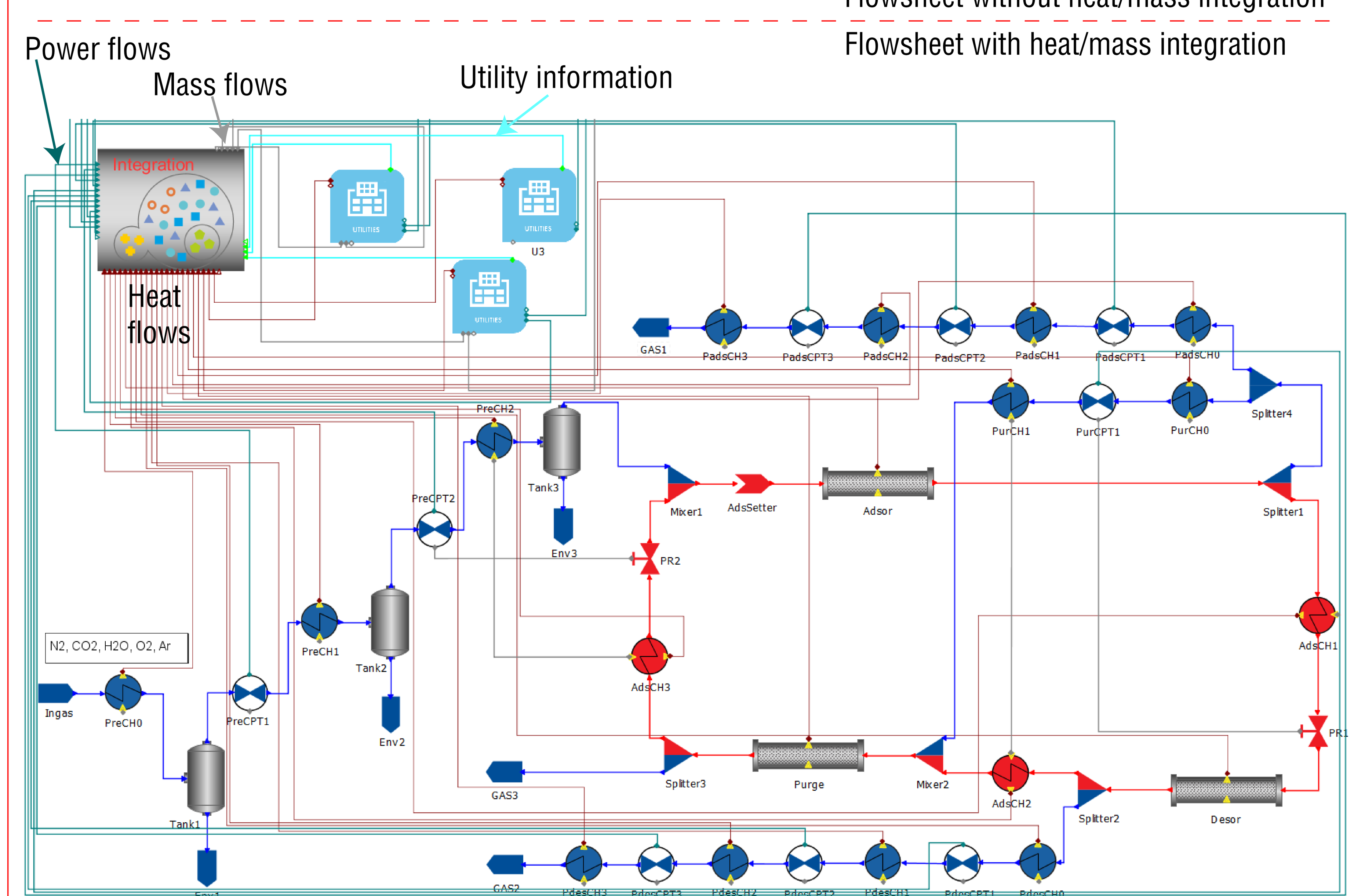
4. Exemplary Illustration (The flowsheeting)

Steady-state modeling of post-combustion CO2 capture process by Adsorption (PSA/TSA/VSA)

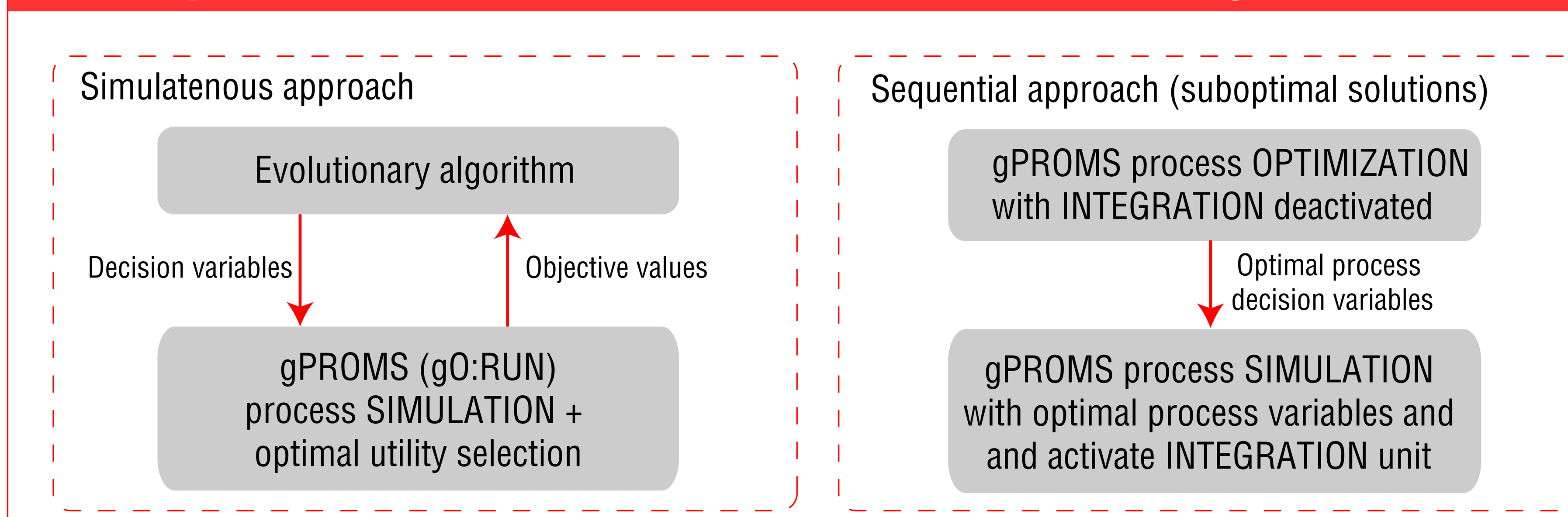


Flowsheet without heat/mass integration

Flowsheet with heat/mass integration



7. Perpective for Process OPTIMIZATION and Utility Selection



Maréchal2003: François Maréchal, Boris Kalitventzeff, Targeting the integration of multi-period utility systems for site scale process integration, Applied Thermal Engineering 23, 2003:1763–1784.