Simultaneous Process Design and Optimal Utility Selection by gPROMS ModelBuilder

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Outline

- Motivation and Objective
- Mathematical Programming of Multi-period Utility Targeting
  - Core issues
- Implementation in gPROMS ModelBuilder
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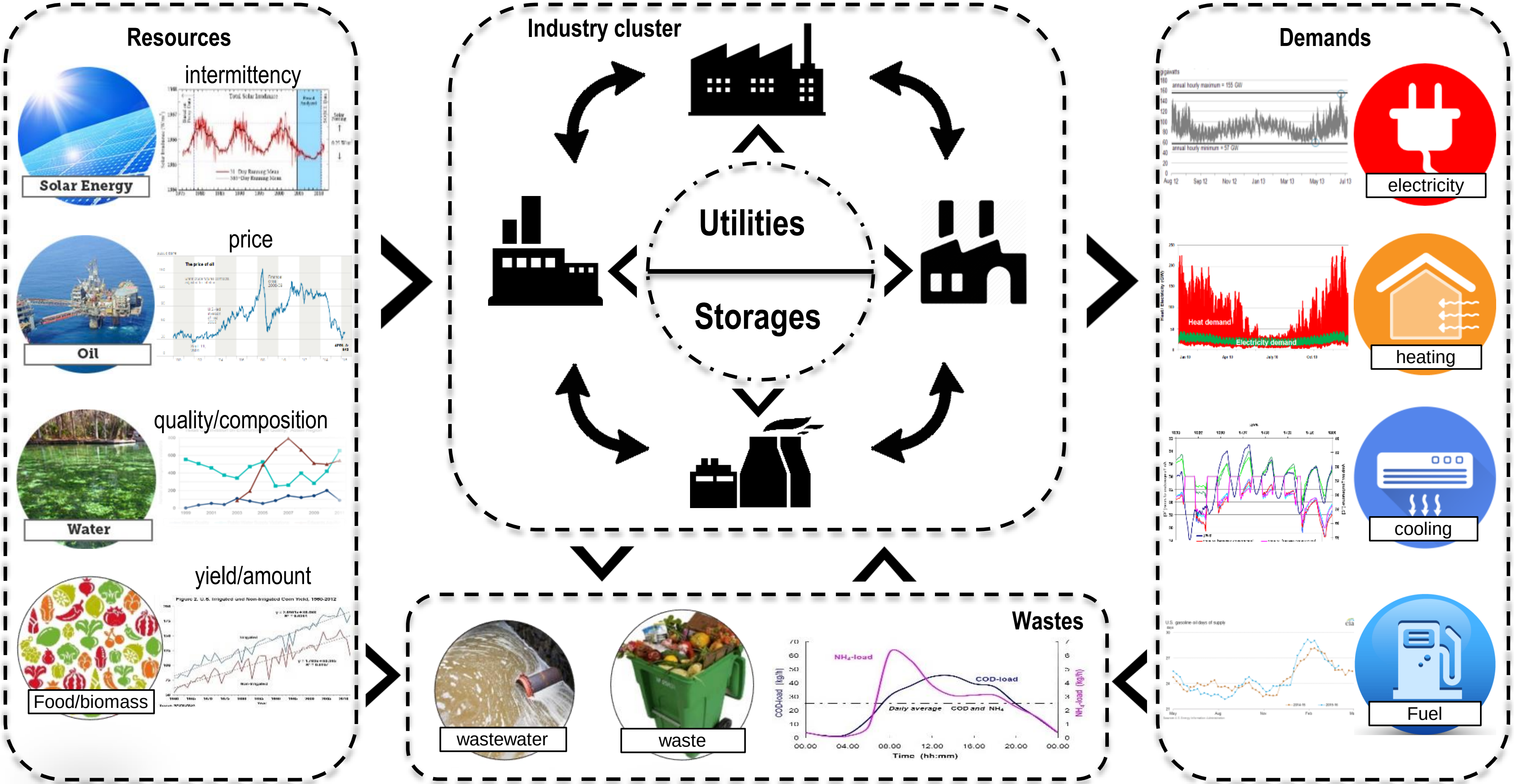
  - gIntegration and Utility Model Specification
  - Case Study
- Perspectives on Process OPTIMIZATION and Optimal Utility Selection
- Conclusions, Problems and Coupling with IPESE Research
- Short Demonstration

Motivation



Problem description:

Input:

- Multi-period (steady-state) information on resources, wastes and demands
- (Partial-load) performance and cost data of processes, utilities and storages

Output:

- Find economically-optimal **sizing and operation profile** of utilities and storages

Motivation

Post-combustion Adsorbent-based CO_2 capture

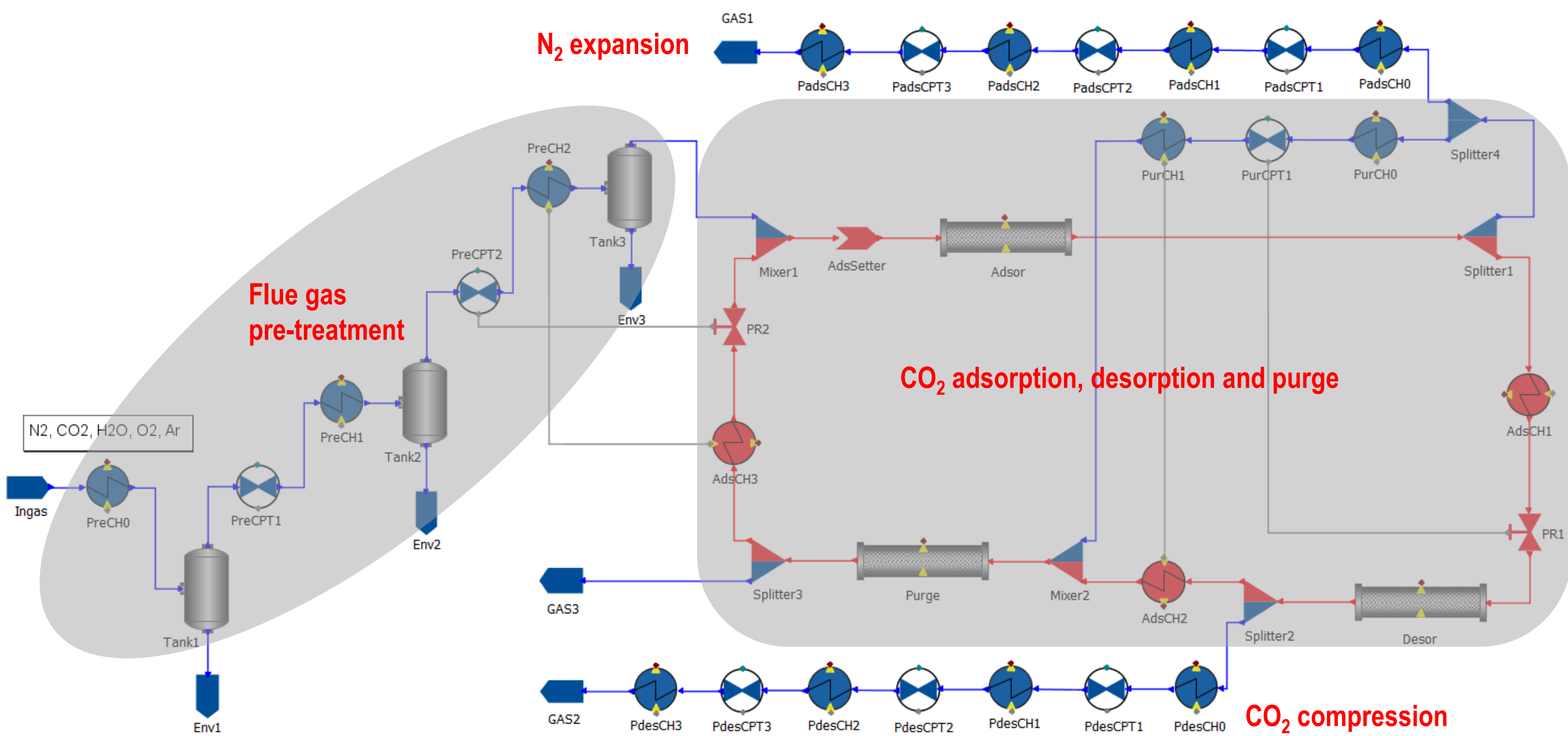
Predesign
adsorbent selection
heat/mass integration
cost estimation

→

Flowsheeting/Unit Design
heat exchanger network
unit design
auxiliaries selection

→

Dynamic Behavior
start-up behavior
load-shifting response
optimal control



Objective

To realize
flexible heat/mass integration,
multi-period utility selection, sizing and operation
in gPROMS software

Mathematical Formulation of Multi-period Utility Targeting

Mixed-integer linear programming problem (Marechal2003)

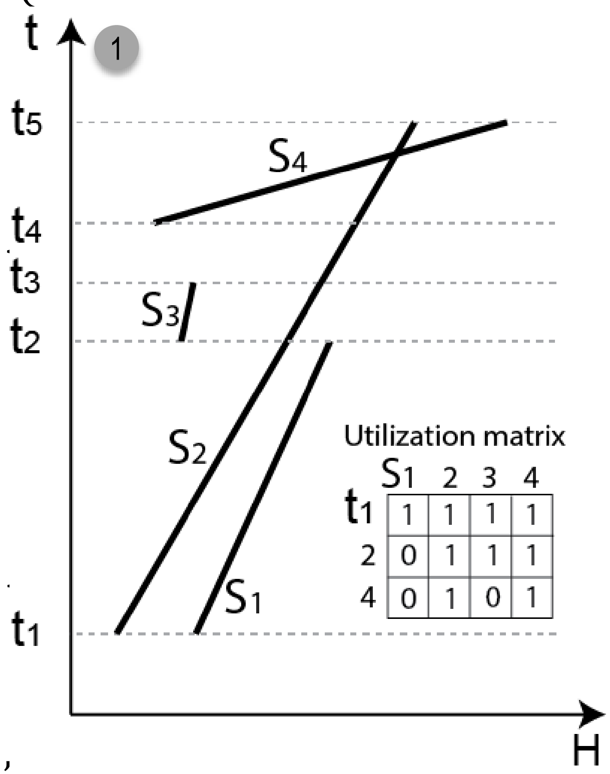
$$\min_{y_{u,i},f_{u,i},Y_u,F_u} \overbrace{\sum_{u=1}^{n_U} a_{u,i} Y_u}^{\text{fixed maintenance}} + \overbrace{\sum_{i=1}^{n_P}\left(\sum_{u}^{n_U}\left(b_{u,i} f_{u,i}\right) + c^{b}_{e,i} W^{b}_{e,i} - c^{s}_{e,i} W^{s}_{e,i}\right)\cdot t_i}^{\text{operating cost}} + \overbrace{\frac{1}{\tau}\sum_{u=1}^{n_U}\left(\alpha_u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

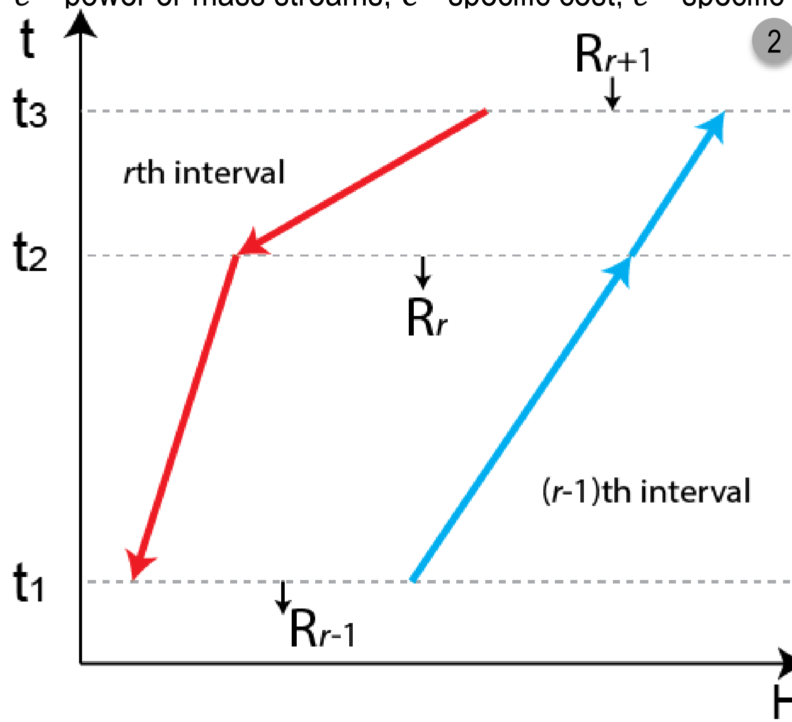
1 **Heat cascade**

$$\begin{cases} \sum_{u}^{n_U} f_u \sum_{j} x_{u,j,r} q_{u,j,r} + \sum_{k}^{n_P} L_k \sum_{j} x_{k,j,r} Q_{u,j,r} = R_r \\ R_1 = 0 \quad R_{n_T} = 0 \quad R_r \geq 0 \end{cases}$$

u—utility index; i—period index; r—inlet temperature index;
k—process index; b, s—resourced purchased and sold;
e—power or mass streams; c—specific cost; c—specific cost;

Power/mass integration





n;
t;
not;

Feasibility

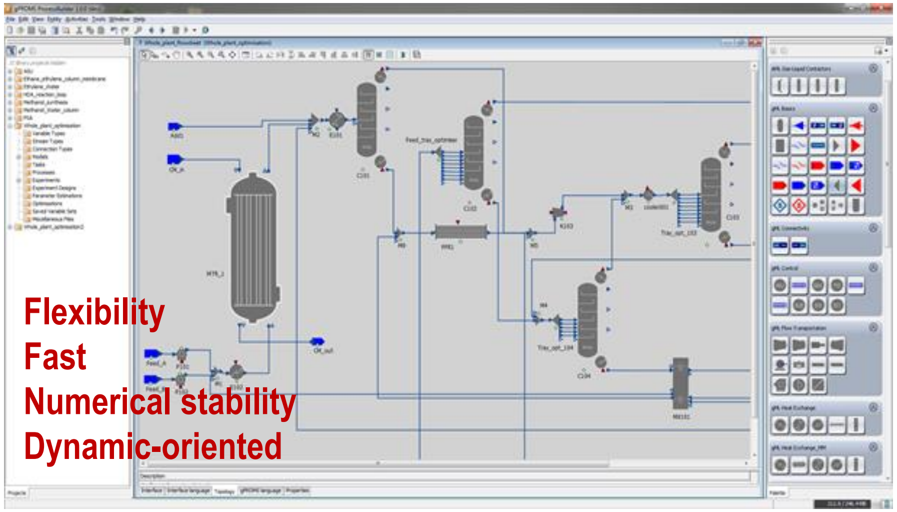
$\forall u = 1, \dots,$

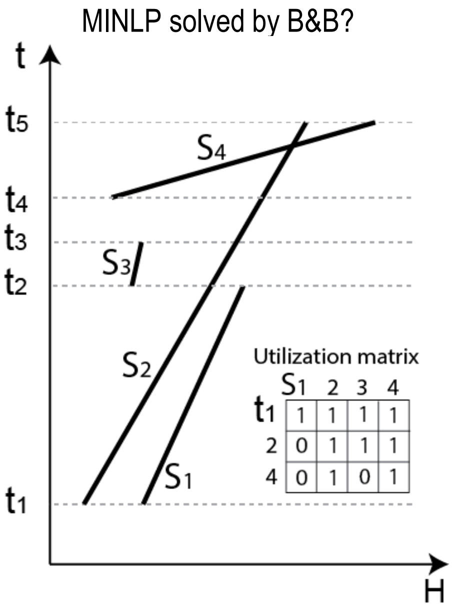
Core Issues

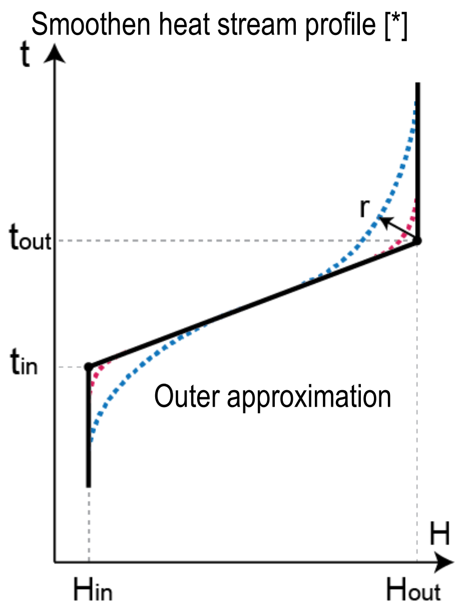
On solving the mathematical problem:

- Flowsheeting/modeling of processes/utilities
- Heat integration and material integration
  - Temperature/material quality
  - Heat requirement/material flow
  - **Data pre-treatment for heat cascade**
    - Possibly sorting temperature/quality intervals
    - Integer utilization matrix of hot/cold streams
    - Estimate/correct H-T profiles
  - **Non-differentiable nature**
    - Difficult to smoothen composite curves

Common issue for all equation-based modeling software







- Multi-period MILP to close the energy and material balance
  - Nominal process variables/efficiency not changing with the size

MILP Implementation?

Implementation Overview

Key idea: Solve the MILP problem as Post Computation (require no derivative information)

Flowsheeting in gPROMS

- Process modeling
- Utility modeling

Direct utility specification simply by the UTILITY unit:
1. Information of heat and mass streams
2. Utility size bound and minimum load
3. Utility cost data

Information of heat and mass streams

INTEGRATION

INTEGRATION unit calling FO: gIntegration
Problem formulation for FO:gIntegration:
1. Initialize FO: gIntegration
2. Format necessary information
3. Set objective function

Periodic information:
1. Periodic variation of resources, wastes and demands
2. Periodic operation of processes

FO: gIntegration.dll

- Multi-period MIP formulation (refer to sec. 2)
- Utility size and operation
- Heat cascade with given utility sizes or the utility sizes calculated by MILP

Report of unit INEGRATION
1. Utility utilization
2. Utility operation load
3. Heat cascade curves

MILP Solver (GUROBI)

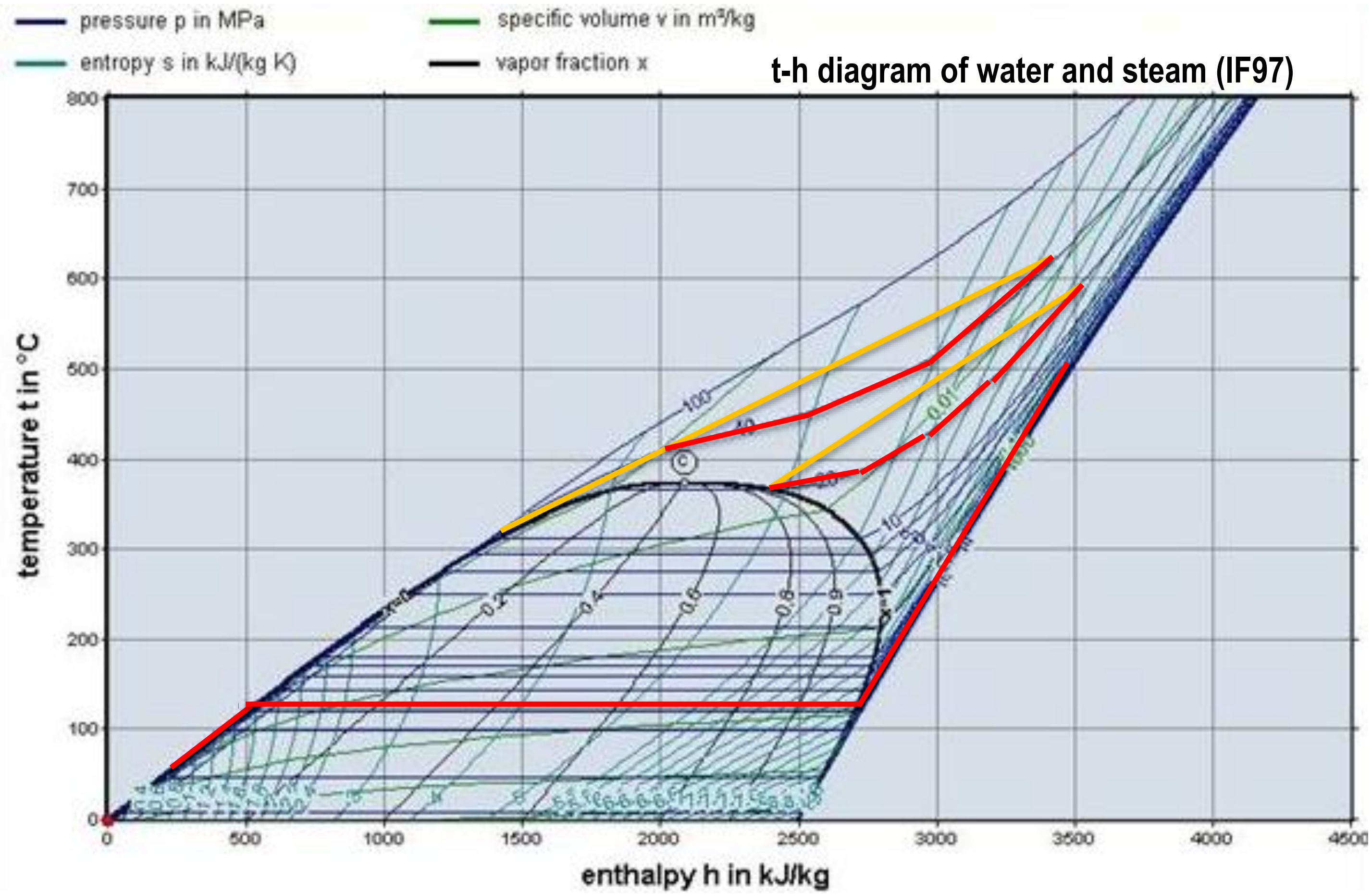
Information Collection: Heat Streams

Estimation of H-T profiles

A robust way of representing a heat stream: $[T_{\text{in}}, H_{\text{in}}, T_{\text{out}}, H_{\text{out}}, \Delta T_{\min}, \alpha]$

Three-section representation of streams crossing two-phase zone

Multi-section representation of high-pressure and -temperature streams, especially those close to the critical point



Information Collection: Connection Types

Heat flow (many): scalar, bi-direction

Heat (IPESE Basics)

Connection parameters

Name	Type	Dimensions	Foreign Object class	Default
unit_id	INTEGER	<scalar>	<Not applicable>	0
Add new				

Distribution domains

Domain name	Lower bound	Upper bound	Dimensions
Add new			

Connection variables

Name	Type	Dimensions
inlet_temperature	temperature	<scalar>
inlet_load	heat	<scalar>
outlet_temperature	temperature	<scalar>
outlet_load	heat	<scalar>
minimum_temperature_difference	no_type_gezero	<scalar>
Add new		

Parameters & variables | Style | Port categories | Value table attributes | Value table style | Properties

Power flow (one): scalar, bi-direction

Power (IPESE Basics)

Connection parameters

Name	Type	Dimensions	Foreign Object class	Default
unit_id	INTEGER	<scalar>	<Not applicable>	0
Add new				

Distribution domains

Domain name	Lower bound	Upper bound	Dimensions
Add new			

Connection variables

Name	Type	Dimensions
in_power	power	<scalar>
out_power	power	<scalar>
Add new		

Parameters & variables | Style | Port categories | Value table attributes | Value table style | Properties

Mass flow (many): scalar, bi-direction

Mass (IPESE Basics)

Connection parameters

Name	Type	Dimensions	Foreign Object class	Default
unit_id	INTEGER	<scalar>	<Not applicable>	0
Components	ORDERED SET	<scalar>	<Not applicable>	
Add new				

Edit to add a new entr

Distribution domains

Domain name	Lower bound	Upper bound	Dimensions
Add new			

Connection variables

Name	Type	Dimensions
mass_fraction	mass_fraction	Components
inlet_mass_flowrate	mass_flowrate	<scalar>
outlet_mass_flowrate	mass_flowrate	<scalar>
Add new		

Parameters & variables | Style | Port categories | Value table attributes | Value table style | Properties

Utility info

Utility (IPESE Basics)

Connection parameters

Name	Type	Dimensions	Foreign Object class	Default
unit_id	INTEGER	<scalar>	<Not applicable>	
Fmin	REAL	<scalar>	<Not applicable>	
Fmax	REAL	<scalar>	<Not applicable>	
ICost1	REAL	<scalar>	<Not applicable>	
ICost2	REAL	<scalar>	<Not applicable>	
OCost1	REAL	<scalar>	<Not applicable>	
OCost2	REAL	<scalar>	<Not applicable>	
Add new				

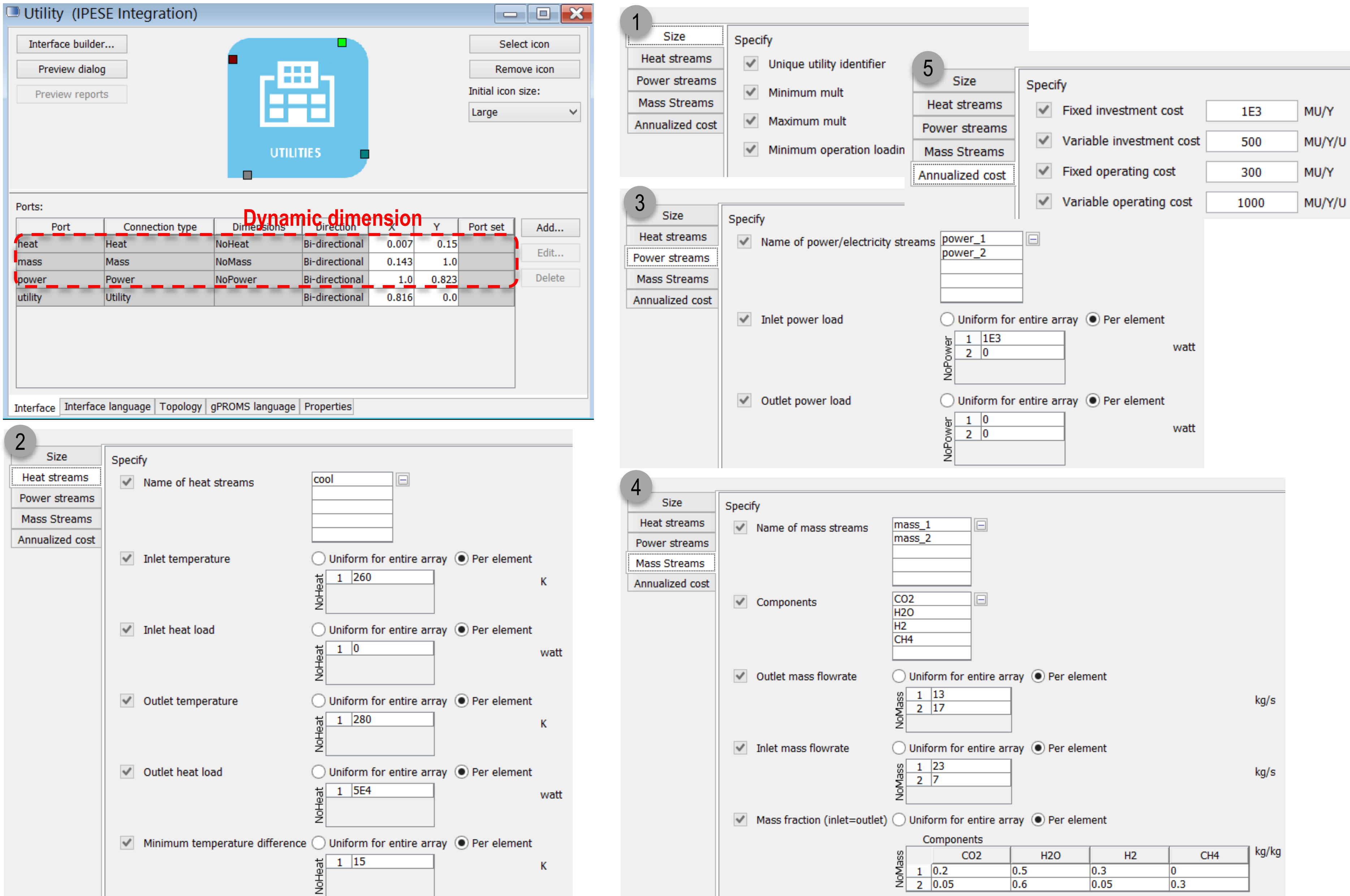
Distribution domains

Domain name	Lower bound	Upper bound	Dimensions
Add new			

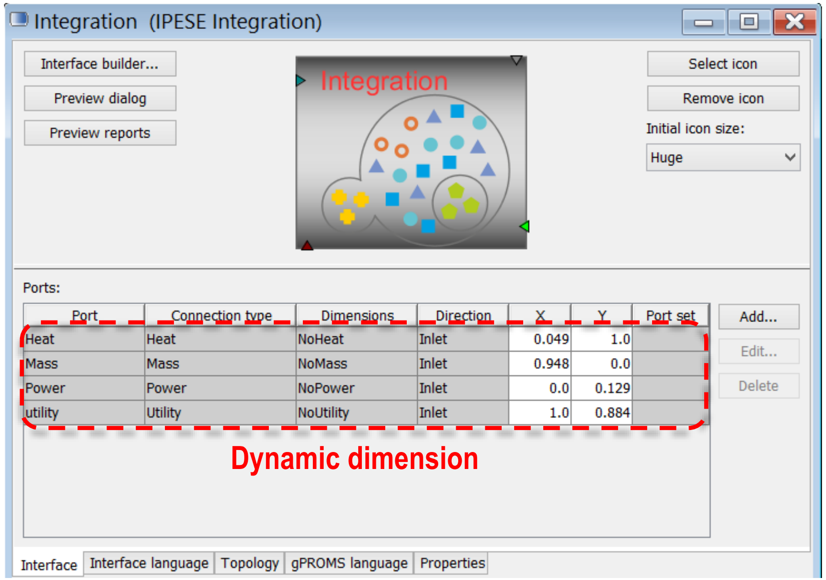
Connection variables

Name	Type	Dimensions
Add new		

Specification: Black-box Utility Modeling



Specification: gIntegration



Initializing FO for parsing input array:

gIntegration:: P1, P2, P3, P4, P5, P6

P1--NoPeriod: Number of period in a year

P2--NoHeat: Number of heat streams

P3--NoPower: Number of power streams

P4--NoMass: Number of mass streams

P5--NoUtility: Number of utilities

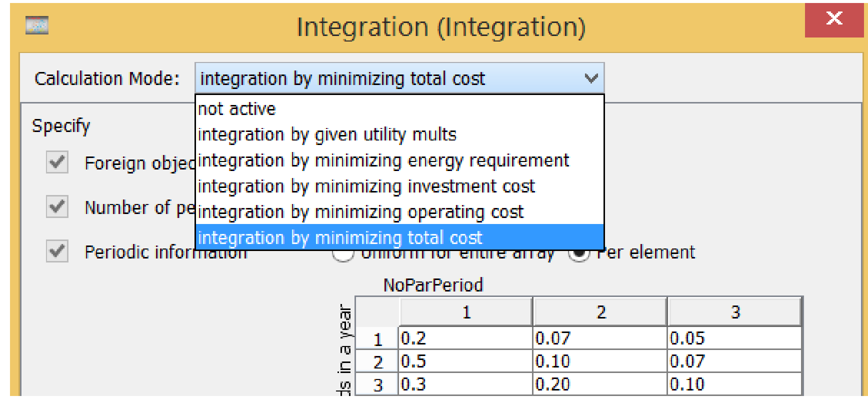
P6--IdPerid4Pinch: Index of period for heat cascade presentation

-1: No presentation after solving MILP

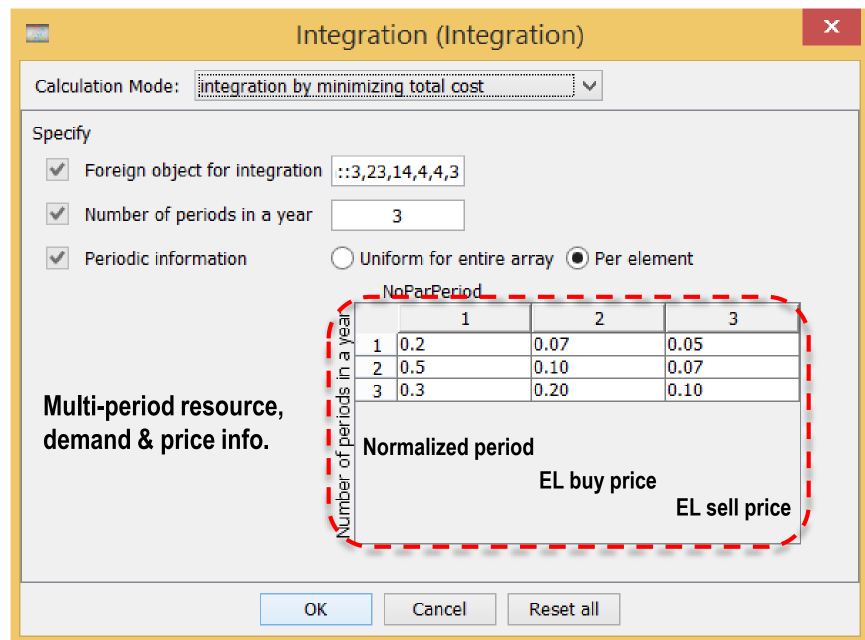
1--NoPeriod: Present heat cascade of the given period

>NoPeriod: Present heat cascade of the NoPeriod

Different objectives implemented:



Multi-period information specification:

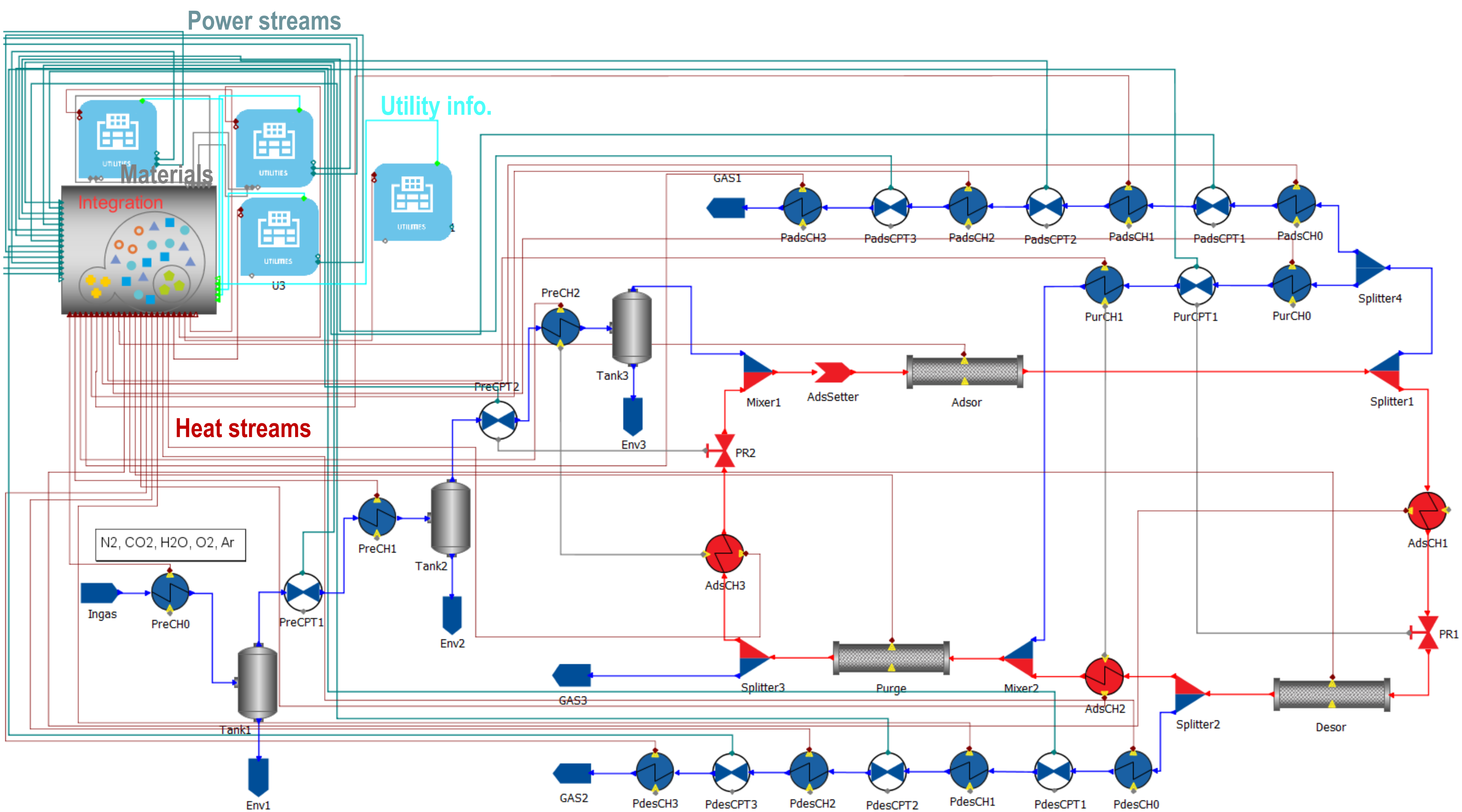


Case Study: Adsorbent-based CO2 Capture (PSA/TSA/VSA)

gIntegration Initialization

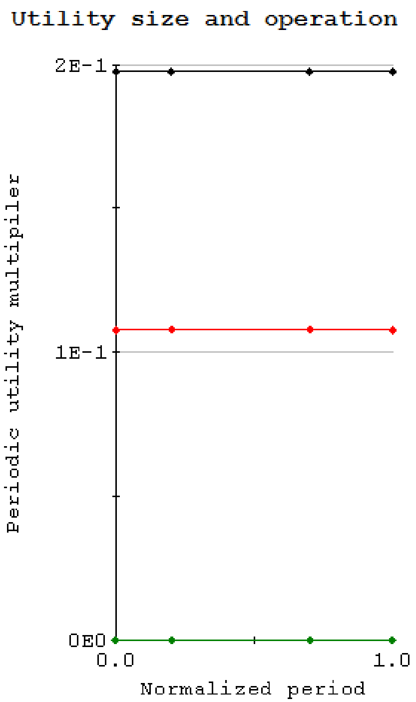
3 periods; 23 heat streams; 14 power streams; 4 mass streams, 4 utilities, heat cascade for period 3

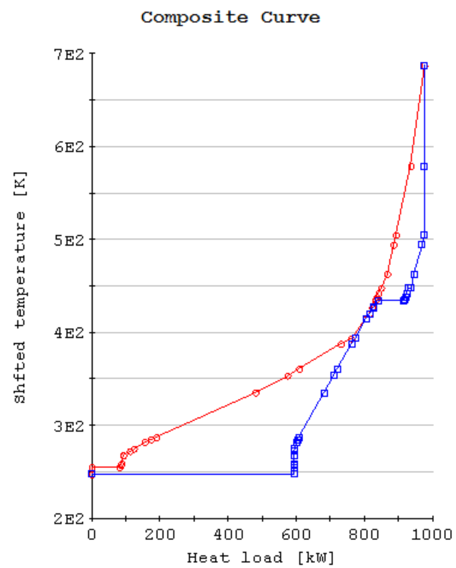
Utility Considered: Parabolic trough (no variation), boiler fluegas, chiller, lake

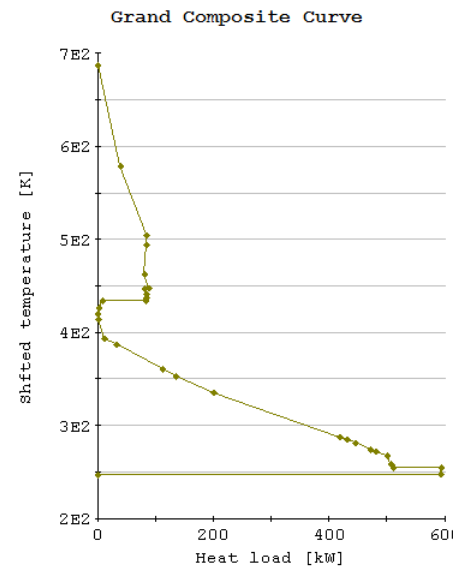


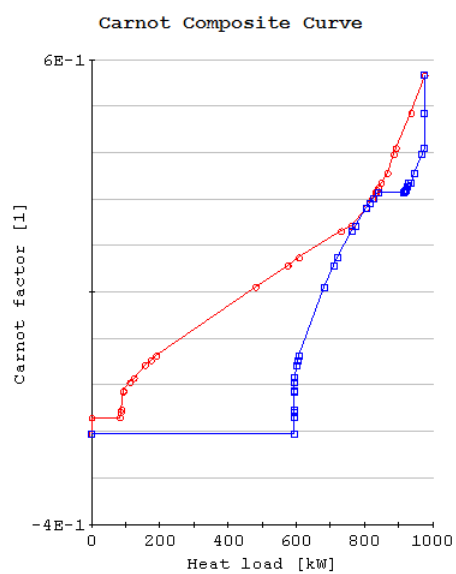
Case Study: Adsorbent-based CO2 Capture (PSA/TSA/VSA)

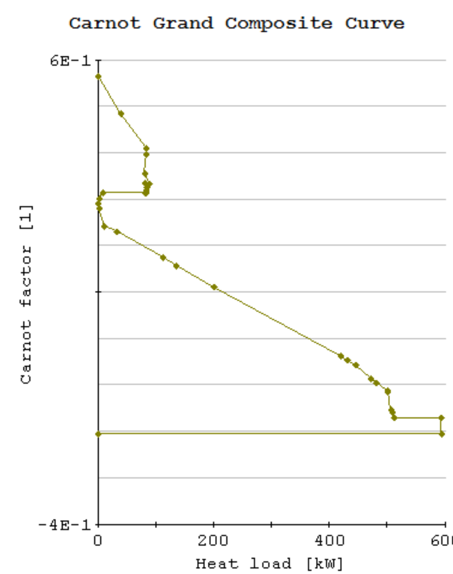
Heat cascade and Utility Selection



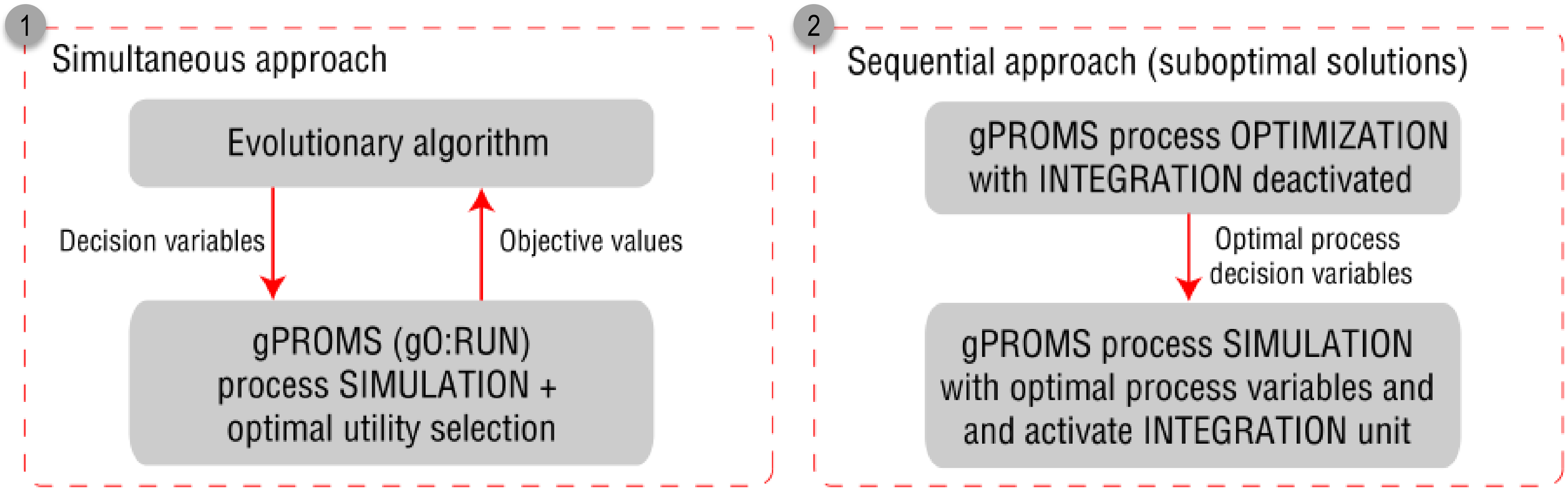








Perspective for Process OPTIMIZATION and Utility Selection



Conclusions, Problems and Coupling with IPESE Research

- Conclusions
  - ✓ Multi-period targeting for optimal utility selection and process design
  - ✓ High flexibility in flowsheeting: dynamic and zero-dimension arrays for connection
  - ✓ Easy-to-use interface

- Problems
  - Can NOT use the original time scale
  - Coupling with original LP/MIP solvers (currently Gurobi)
  - NOT very flexible in reporting utility operation
  - NOT available to graphically present network design

- Possible further coupling with IPESE research
  - Extend with material cascade
  - Extend with multi-period energy storage management
  - Extend with steam network design
  - Extend for dynamic problems?

IPESE
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Thank you for your attention!

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