gPROMS ProcessBuilder

Advanced Process Simulation for Chemicals & Petrochemicals

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Chemicals & Petrochemicals

gPROMS ProcessBuilder

A new gPROMS family product

gPROMS product family

General mathematical modeling

gMODEL

gPROMS ModelBuilder
Advanced process modeling environment

Sector-focused modeling tools

Chemicals & Petrochemicals

gPROCESS

gPROMS ProcessBuilder
Advanced process simulation

AML: GLC, AML: FBCR, AML: FT, AML: BCR, AML: TBR

Advanced model libraries for reaction & separation

Life Sciences, Consumer, Food, Spec & Agrochem

gSOLIDS
Solids process optimization

gCRYSTAL
Crystallization process optimization

gCOAS
Oral absorption

Power & CCS

gCCS
CCS system modeling

Fuel Cells & Batteries

gFUELCELL
Fuel cell stack & system design

Oil & Gas

gFLARE
Flare networks & depressurization

Wastewater Treatment

gWATER
Wastewater systems optimization

The gPROMS platform

gPROMS

Equation-oriented modeling & solution engine

Materials modeling

gSAFT
INFOCHEM Multiflash
OLI

Model deployment tools

Enterprise
Objects

Deploy models in common engineering software

Motivation

Provide

1. All the power of the gPROMS platform and first-principles modeling
   - *without the need to write models*
2. Custom modeling capability *where necessary*
   - maximize competitive advantage

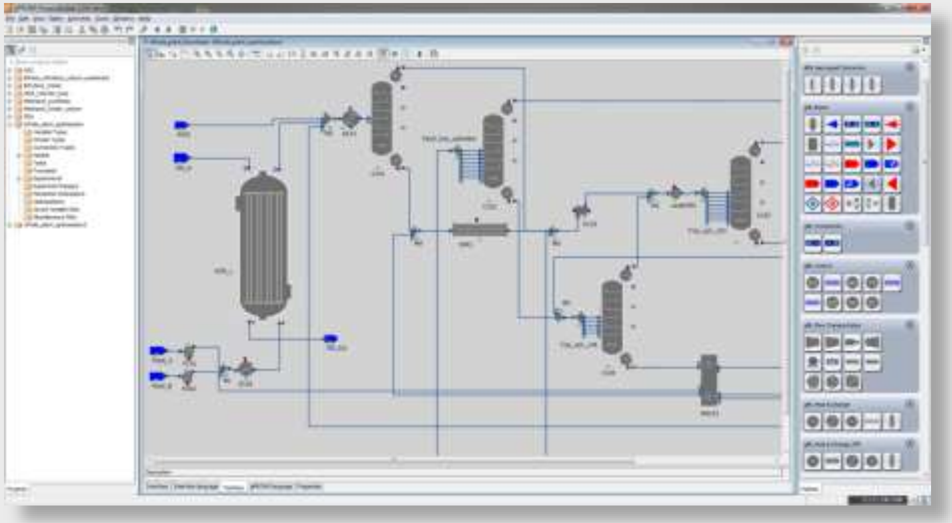
➔ **Ease-of-use** combined with **equation-oriented power**
   - solve full problem scope – rapidly

➔ Full **rigorous optimization**
   - find optima directly – no need for trial & error simulation

➔ gPROCESS

gPROMS ProcessBuilder
"Advanced Process Simulation"

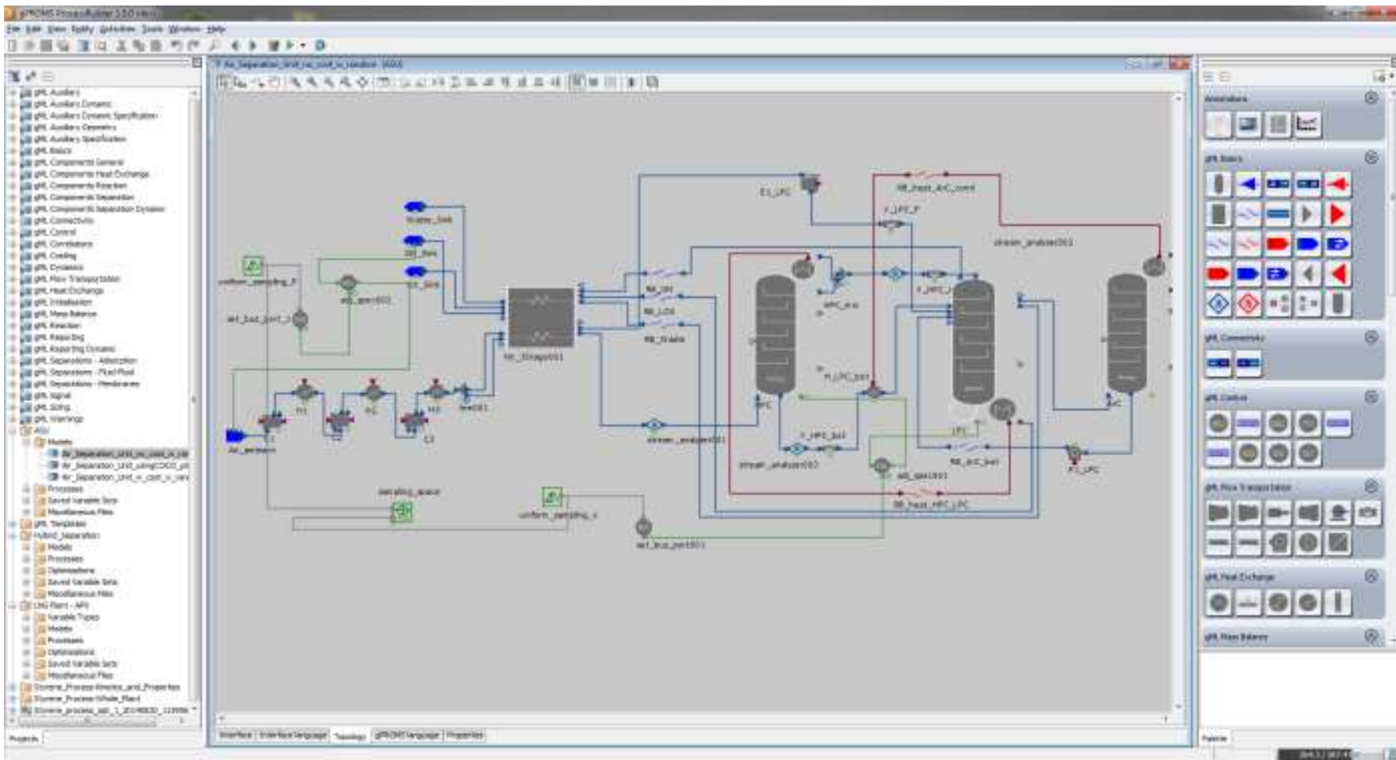
A process modeling tool for chemicals & petrochemicals



gPROMS ProcessBuilder

Basics

- Supports “core” flowsheeting functionality
  - **drag-and-drop flowsheeting** based on **model libraries**
  - analysis of process behavior via **steady-state & dynamic simulation**
  - optimization of design & operation via **steady-state & dynamic optimization**



So what's different?

<u>Advanced</u> Process Simulation

… goes well beyond standard flowsheeting tools

So what's different?

1. Industry-leading model libraries
2. Powerful custom modeling
3. Complex reactor models with standard units
4. Optimization
5. Equation-oriented power
6. State-of-the-art physical properties
7. Instrumentation & control
8. Pre-built modeling solutions for specific sectors
9. … and more

1. Industry-leading model libraries

I. gPROMS Model Libraries (gML)

- common unit operations for chemicals/petrochemicals
- comparable to those provided in other flowsheeting tools
- BUT
  - other key models, e.g. kinetic reactors, adsorption, membranes, control elements
  - steady-state and dynamic, high-fidelity

II. Advanced Model Libraries

- incorporate PSE's state-of-the-art modeling know-how
- AML:GLC – Advanced Model Library for Gas/Liquid Contactors
- AML:FBCR – Advanced Model Library for Fixed-Bed Catalytic Reactors

III. Client/3rd-party model libraries

- can be used together with gML/AMLs, provided they conform to gPROMS ProcessBuilder standard

Separation

Separations – Fluid-Fluid

- Component splitter
- Flash drum
- Decanter
- 3-phase separator
- Distillation column (tray, equilibrium)
- Distillation column (packed-bed, HETP)
- Distillation column (packed-bed, 1D rate-based)
- Distillation column (packed-bed, 2D rate-based)
- Distillation column (reactive)

AML:GLC

Separations – Adsorption*

- Adsorption bed
- Schedule for periodic processes (PSA, TSA)
- Schedule for self-interacting bed approach

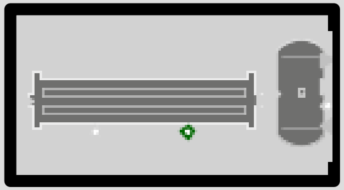
Separations – Membranes*

- Membrane module

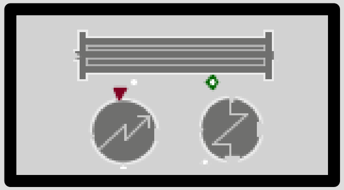
** Unique in general process simulation tools*

Separation

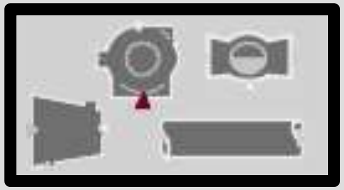
Reaction



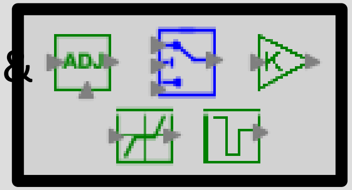
Heat exchange



Flow transportation



Instrumentation & control



Reaction and heat exchange

Reaction

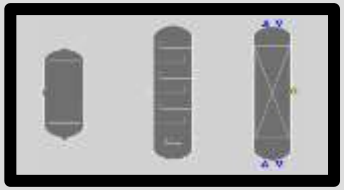
Conversion reactor
Gibbs reactor
CSTR (kinetic & equilibrium reactions)
PFR (kinetic & equilibrium reactions)*
Fixed-bed catalytic reactor (1D)*
Fixed-bed catalytic reactor (2D)*
Fixed-bed catalytic reactor (2D + intra-particle)*

AML:FBCR

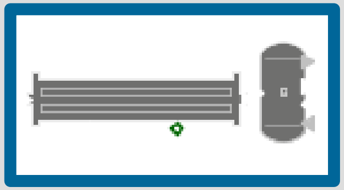
Reaction mechanisms

- Arrhenius
- Langmuir-Hinshelwood
- Michaelis-Menten
- User-specified

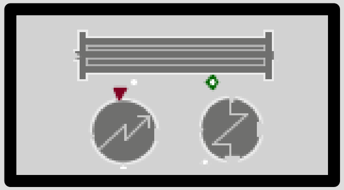
Separation



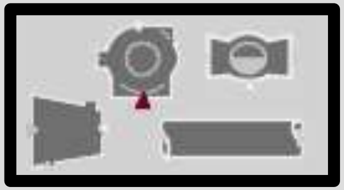
Reaction



Heat exchange



Flow transportation



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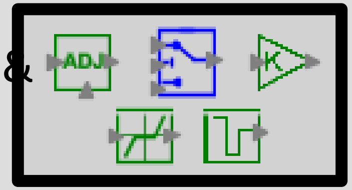


* Unique in process simulation tools

Heat exchange, flow transportation, compression

Heat exchange

- Heater
- Cooler
- Two-stream heat exchanger
- Multi-stream heat exchanger
- Air cooler
- Evaporator
- Condenser

Flow transportation

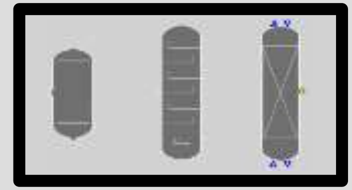
- Pipe
- Pump
- Valve

Compression

- Compressor
- Expander
- Compressor section
- Electric drive
- Surge valve

Developed with Rolls-Royce

Separation



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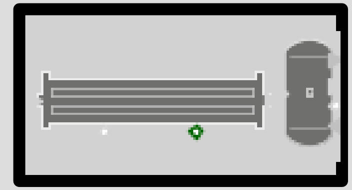
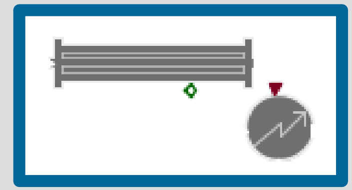
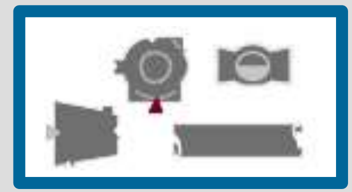


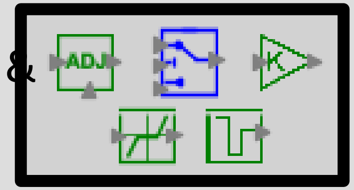
Heat exchange



Flow transportation



Instrumentation & control



1. Industry-leading model libraries

Instrumentation & control

Instrumentation & control

Controllers
- Gain, PID, delays

Logic
- Switches

Linear systems
- Transfer function, state-space model

Discrete
- Dead zone, hysteresis, saturation

Mathematics
- Functions, basic operations

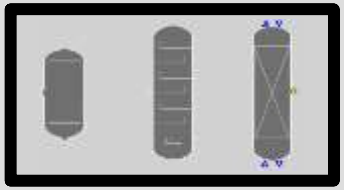
Signal Sources
- Constant, ramp, step signal, function generator, time signal

Signal Sinks
- Display, plot, X-Y plot

Data
- Lookup table, file read, file write

Functionality
- System identification, linearization
- Mixed-integer optimization

Separation



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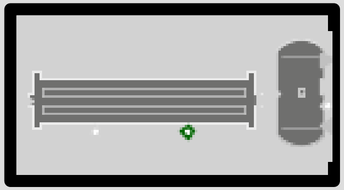
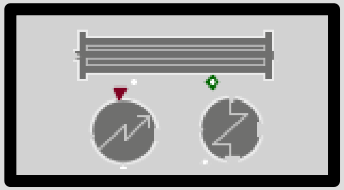
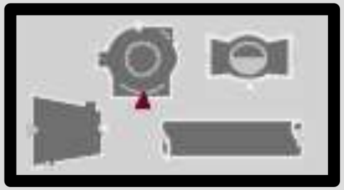


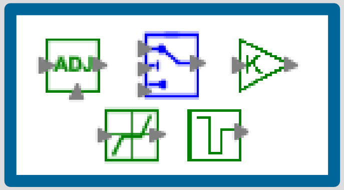
Heat exchange



Flow transportation



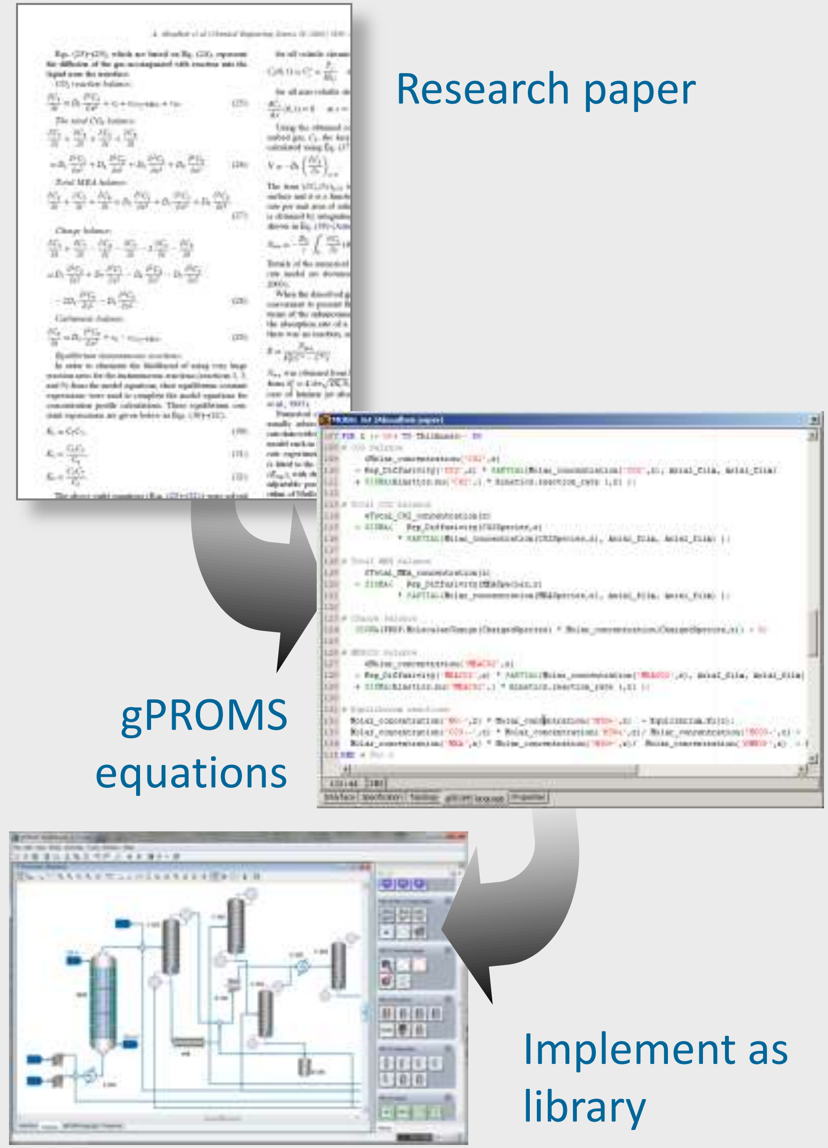
Instrumentation & control



gPROMS ProcessBuilder – the difference

2. Powerful custom modeling

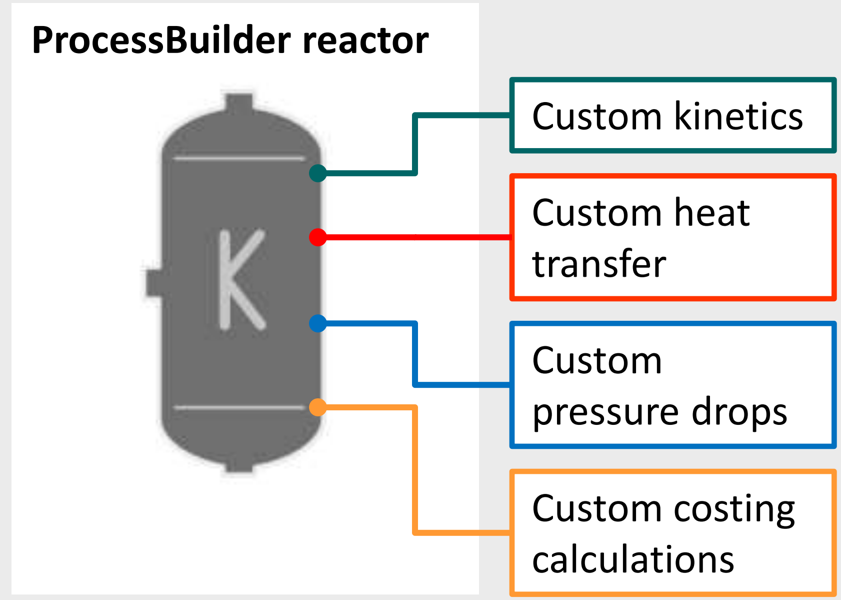
- Full power of gPROMS platform
  - Distributed systems, dynamics, discontinuity handling, etc.
- Advantages & benefits
  - Augment with own models
    - e.g. reactor, multi-stream heat exchanger
  - Capture competitive advantage
    - not using off-the-shelf black-box models like every body else
  - Validate against experimental data
    - capture corporate knowledge
- Add as ProcessBuilder library
  - Leverage knowledge across the organization
  - Multiple ROI

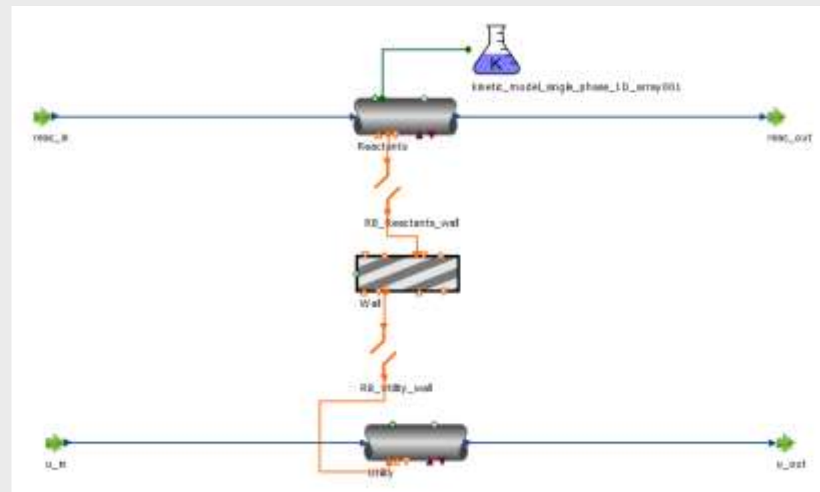


2. Powerful custom modeling

Accelerate development and reduce maintenance

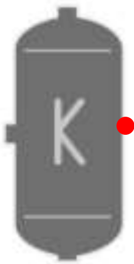
- ProcessBuilder models have custom model interfaces for common types of customization
  - Augment/modify only the parts that need modification
  - Benefit from automatic initialization of ProcessBuilder models
  - Reduce maintenance of custom models and potential for error
- Use ProcessBuilder "component" models to build complex unit operations using a flowsheeting approach
  - Rapid development
  - Reduced potential for error





Example – Changing heat transfer correlation

ProcessBuilder reactor model



Custom heat transfer sub-model

```
PARAMETER
components              AS ORDERED_SET
number_of_tubes         AS REAL

use_viscosity           AS INTEGER
use_lambda              AS INTEGER
use_heat_capacity       AS INTEGER
use_two_phase           AS INTEGER

# Declare custom parameters here
design_htc              AS REAL

DISTRIBUTION_DOMAIN
axial AS [0:1]

VARIABLE
# Input
T                       AS DISTRIBUTION(axial)                        OF temperature_gML                  # Temperature (K)
P                       AS DISTRIBUTION(axial)                        OF pressure_gML                     # Pressure (bar)
w                       AS DISTRIBUTION(components,axial)             OF mass_fraction_gML                # Mass fraction (-)
F                       AS DISTRIBUTION(axial)                        OF mass_flowrate_gML                # Mass flowrate (kg/s)
d                       AS                                               length_gML                       # Channel diameter (m)
M_T                     AS DISTRIBUTION(axial)                        OF mass_density_gML                 # Mass density (kg/m3)
u                       AS DISTRIBUTION(axial)                        OF velocity_gML                     # Velocity (m/s)

# Optional input
viscosity               AS DISTRIBUTION(use_viscosity,axial)          OF dynamic_viscosity_gML            # Fluid viscosity (kg/(m·s))
lambda                  AS DISTRIBUTION(use_lambda,axial)             OF thermal_conductivity_gML         # Fluid thermal conductivity (W/(m·K))
c_P                     AS DISTRIBUTION(use_heat_capacity,axial)      OF mass_specific_heat_capacity_gML  # Mass specific heat capacity kJ/(kg.K)

# Output
htc                     AS DISTRIBUTION(axial)                        OF heat_transfer_coefficient_gML    # Heat transfer coefficient W/(kg.K)

# Declare custom variables here

SET
use_viscosity := 0;
use_lambda := 0;
use_heat_capacity := 0;
use_two_phase:=0;

EQUATION
#---------------------------------------------------------------------------------------------
# Enter custom heat transfer correlation here
HTC() = design_htc * ABS(F(0) / (165))^0.78;
```

Inputs

Fluid conditions in the reactor

Outputs

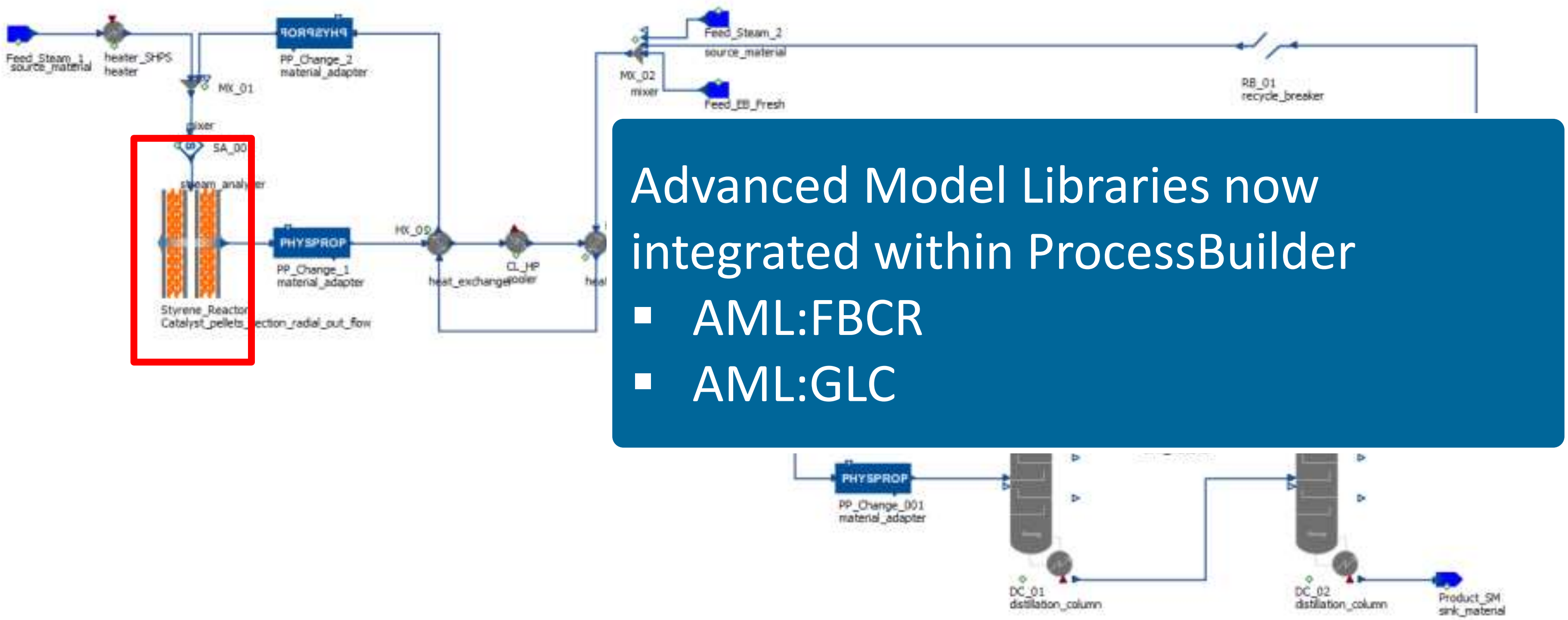
Heat transfer coefficient

Custom correlation

Single equation!

3. Complex reaction models with standard units

- Example: styrene monomer production
  - Radial-flow multitubular reactors
    - 2D fixed-bed catalytic reactor models
  - standard "flowsheeting" models for flash, heat exchanger, distillation

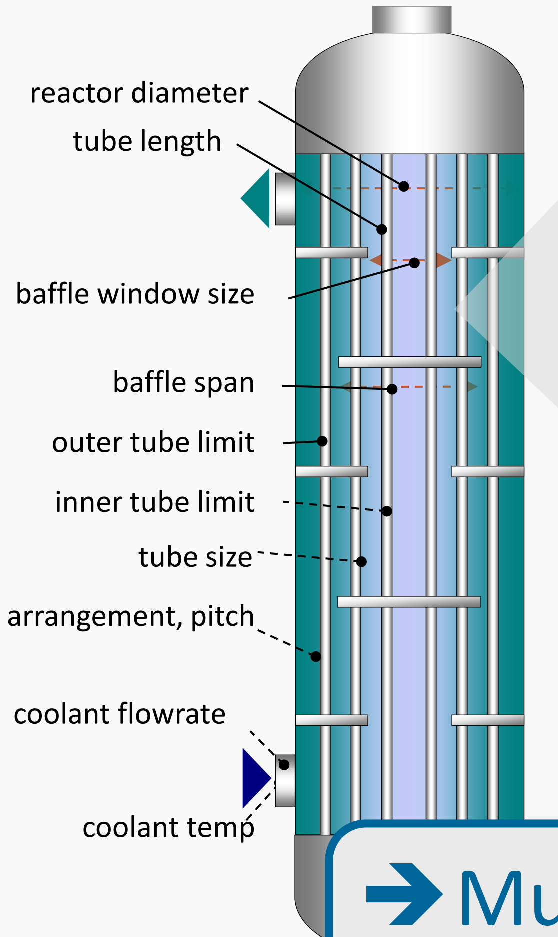


Advanced Model Libraries now integrated within ProcessBuilder
- AML:FBCR
- AML:GLC

AML:FBCR – multiscale modeling

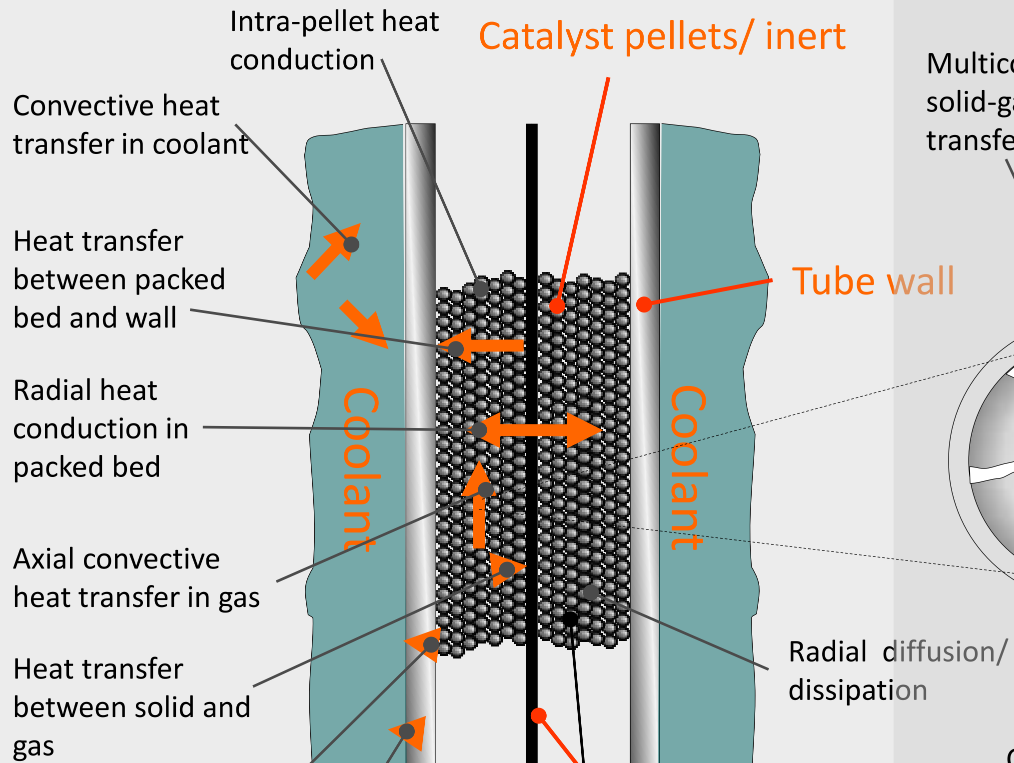
Reactor unit

Design variables



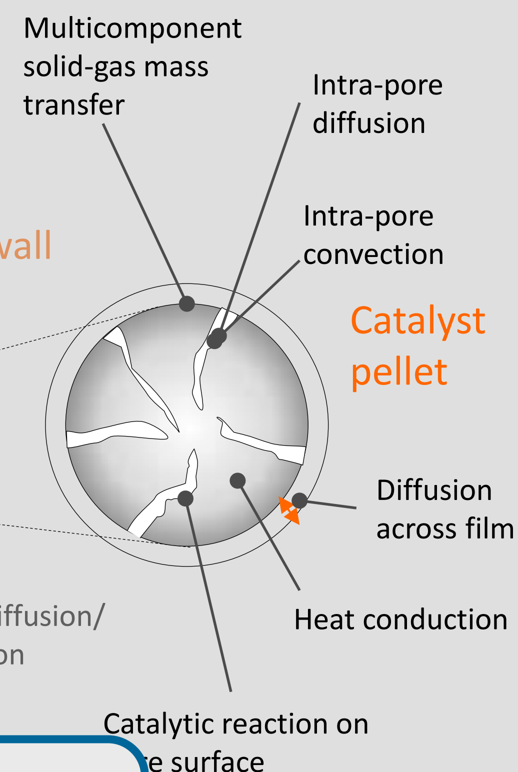
Tube

Bed heat and mass transfer phenomena



Catalyst pellet

Heat and mass transfer phenomena



→ Multiscale modeling approach

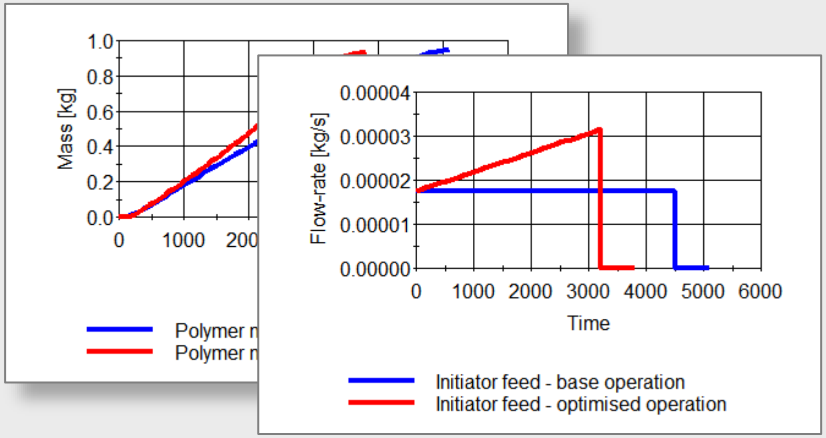
- microns to meters

4. Optimization

- Full power of gPROMS optimization
  - steady-state & dynamic
  - mixed-integer/continuous
- Objective function and constraints
  - arbitrary objective function – economic or technical
  - any constraints
- Decision variables
  - equipment dimensions
  - operating conditions
    - values or time trajectories
  - equipment configuration
    - e.g. feed tray location, no stages
  - process routing options

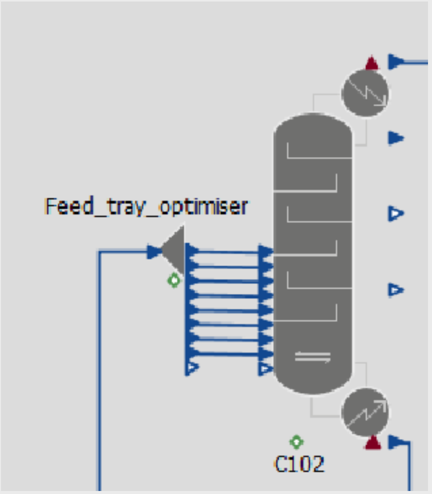
Dynamic optimization

Minimize batch time



Integer optimization

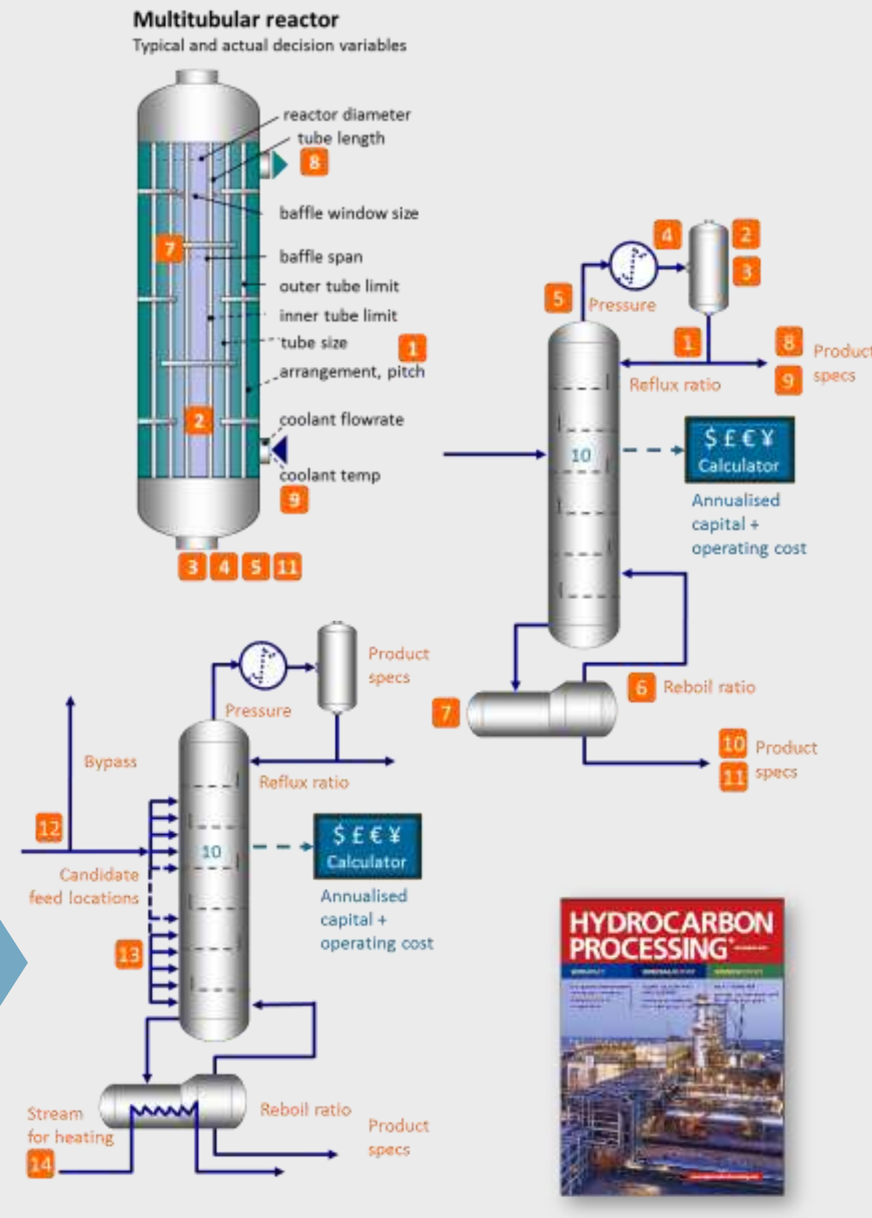
Choose optimal feed tray location



New ways to create or add value

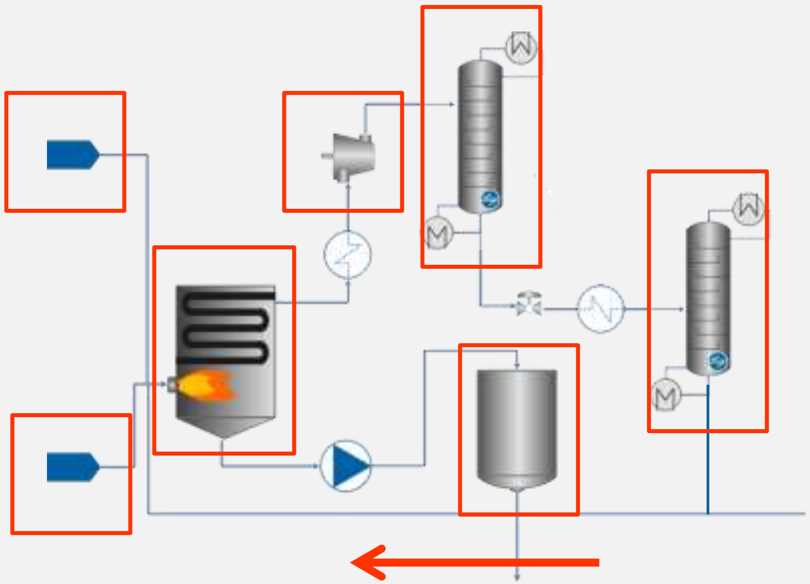
- Many new classes of application
  - Whole-plant steady-state optimization
    - many (typically 20-50) equipment design & operating decisions
  - Optimize start-up, grade-change
  - Batch recipe optimization
  - Process synthesis

- e.g. Repsol whole-plant optimization
  - multitubular reactor, full separation section → 50 decision variables
  - equipment, operational, routing decisions
  - improved process economics by $10s of millions per annum



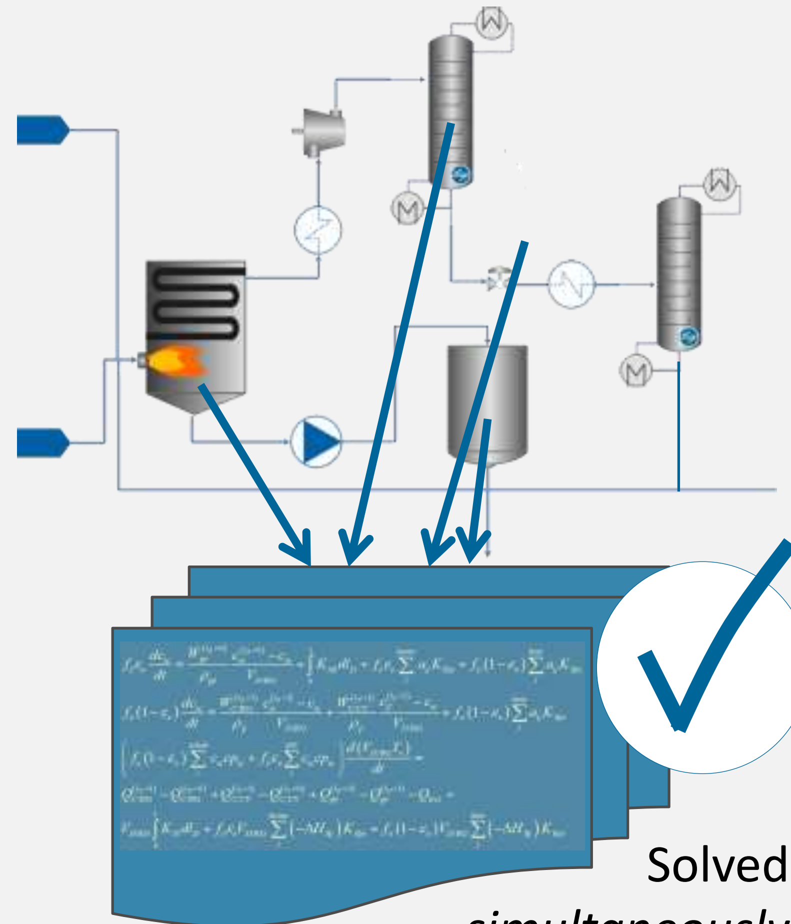
5. Equation-oriented power

Traditional sequential-modular



- Solve in sequence
- Iterate around recycle loops until converged

Equation-oriented approach



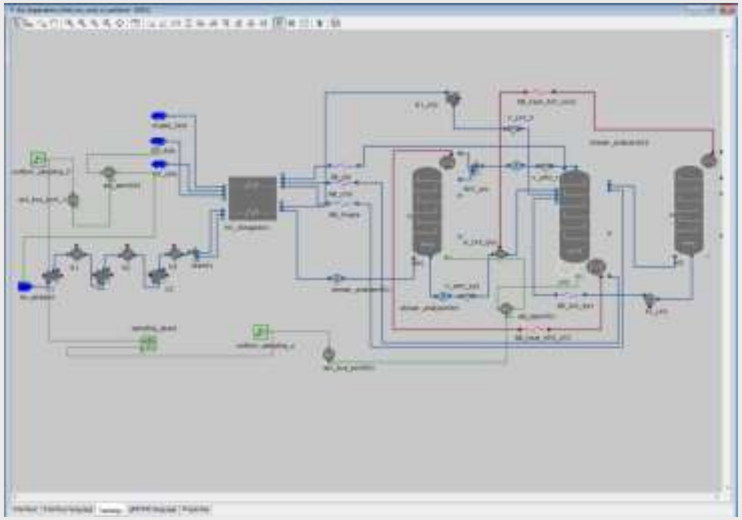
Advantages of EO – 1

- Multiple calculation types based on same model
  - steady-state & dynamic simulation
  - steady-state & dynamic optimization
  - parameter estimation
  - linearized model generation, …

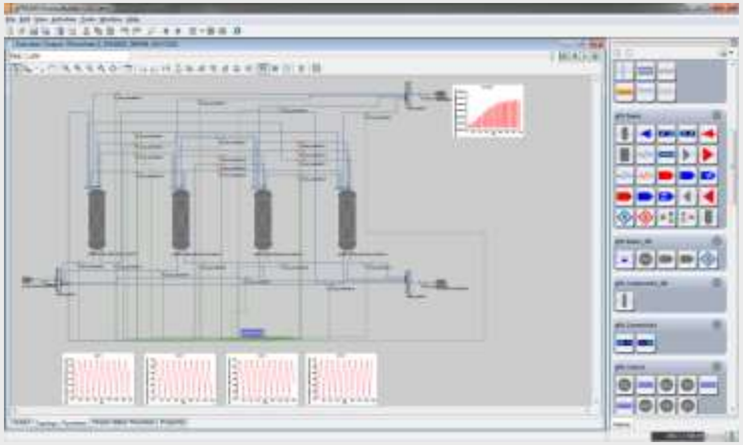
- ‘Back-to-front’ solution easy
  - given downstream values (e.g. throughput, conversion)
    calculate upstream conditions (e.g. feed flow)
    and/or equipment design parameters (e.g. reactor size)

Advantages of EO – 2

- Solve **new classes of problem**
  - Flowsheets with **complex recycles**
  - **Large-scale optimization** – complex reaction and separation section
  - **Mixed-integer optimization** problems – process synthesis, equipment configuration
  - Rigorous **sensitivity analysis**
  - **Online model-based applications** with **rigorous** models
  - **Complex dynamic processes – e.g. pressure-swing adsorption**

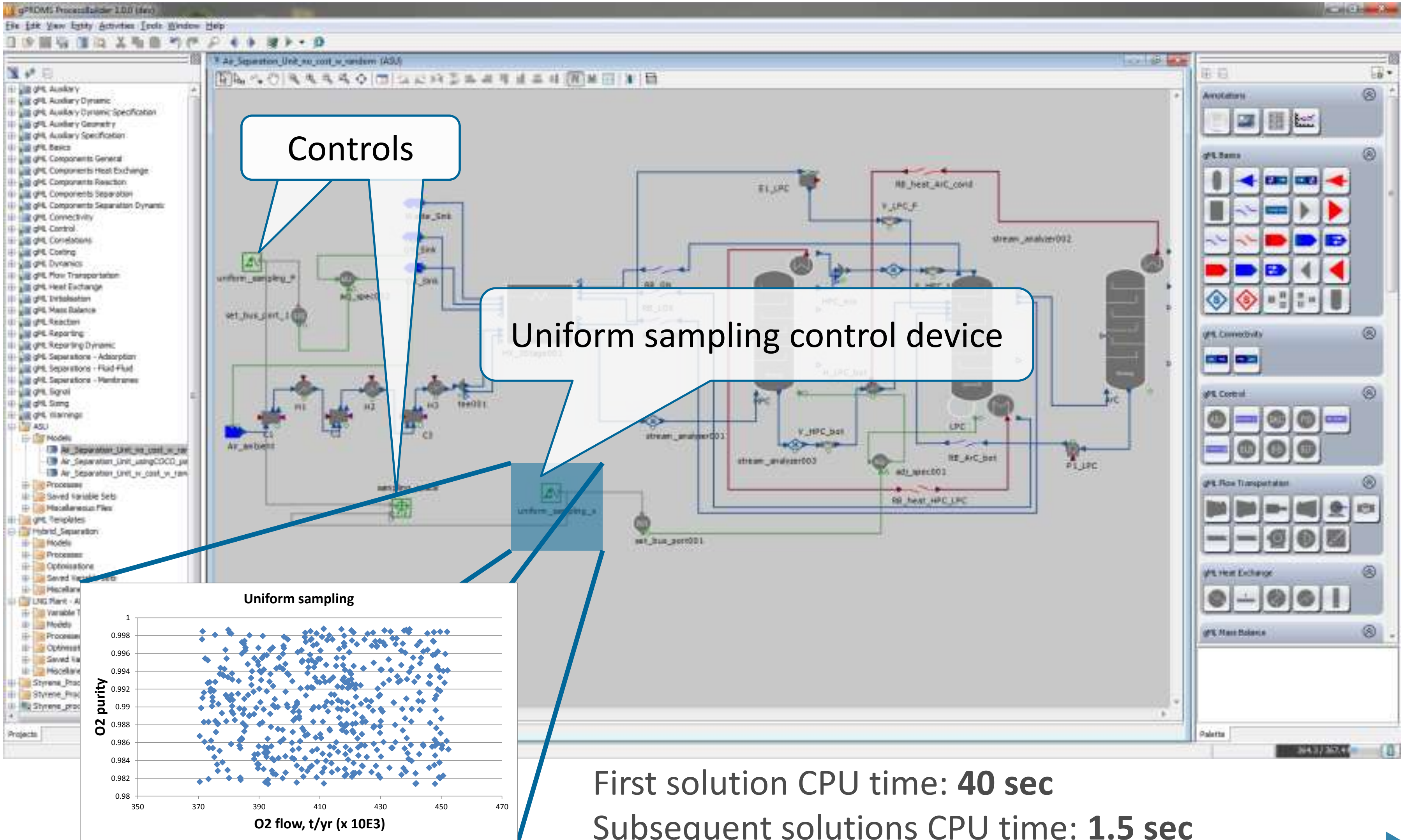


Complex recycles
Air Separation Unit (ASU)



Complex dynamics
Pressure-Swing Adsorption (PSA)

Advantages of EO - Example



First solution CPU time: **40 sec**

Subsequent solutions CPU time: **1.5 sec**

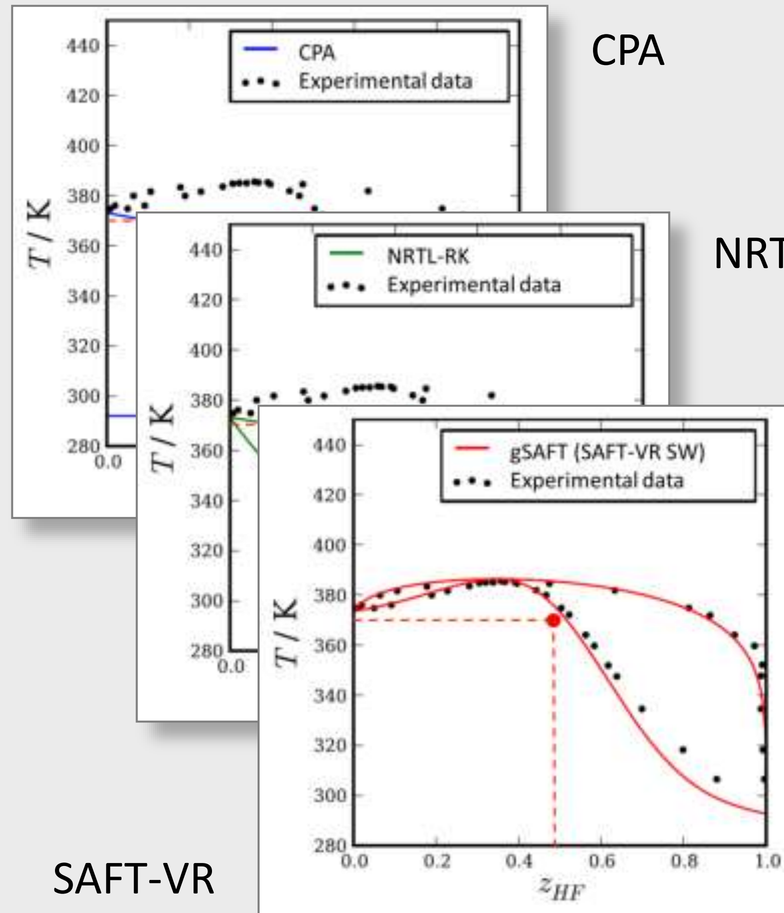
Demo

6. State-of-the art physical properties

- **gPROMS Properties**
  - KBC Multiflash®
  - DIPPR database – 2000+ components
  - All standard thermodynamic models
- **gSAFT Advanced thermodynamics**
  - New-generation equations of state
  - SAFT-VR Square Well & SAFT-γ Mie
  - High-accuracy prediction

- **Other options**
  - **Proprietary physprops pachage**
    - New streamlined interface
  - **CAPE-OPEN physprops**
    - Aspen Properties™, etc.

HF – H_2O system [INEOS]



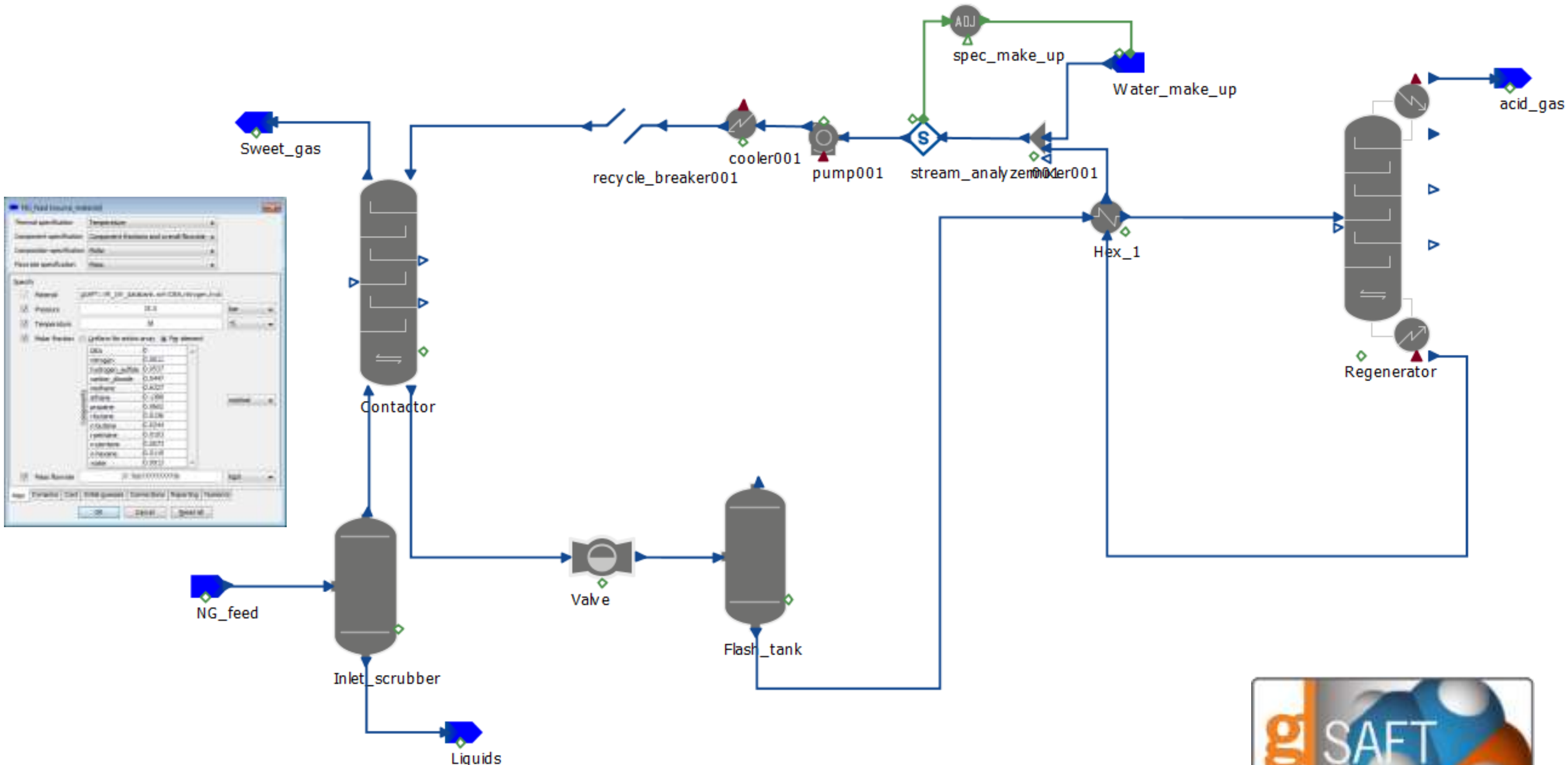
CPA

NRTL

SAFT-VR

Example: Acid gas removal from LNG using DEA

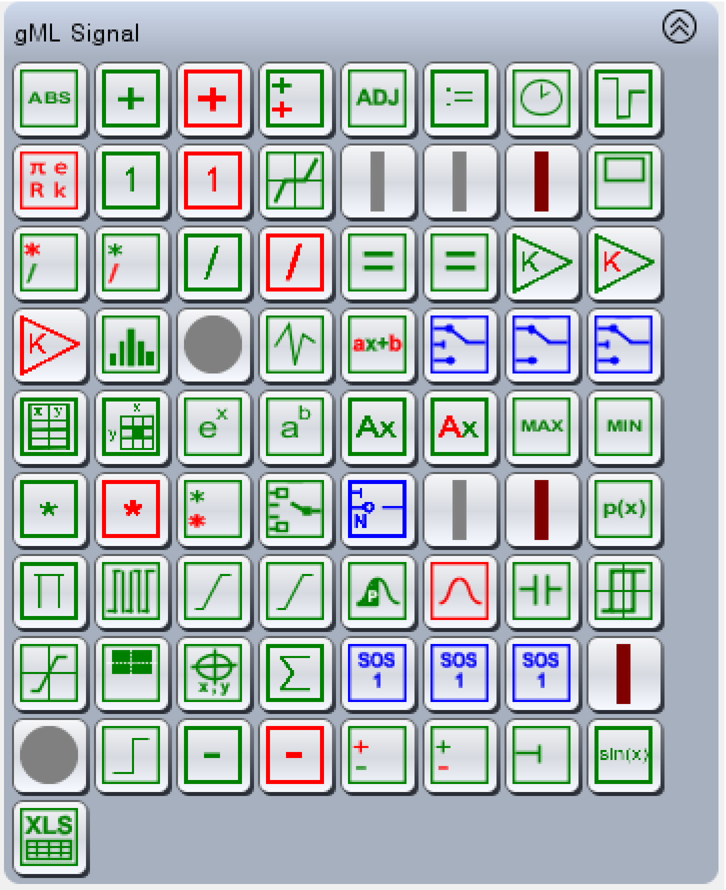
- <literature reference>



gPROMS ProcessBuilder – the difference

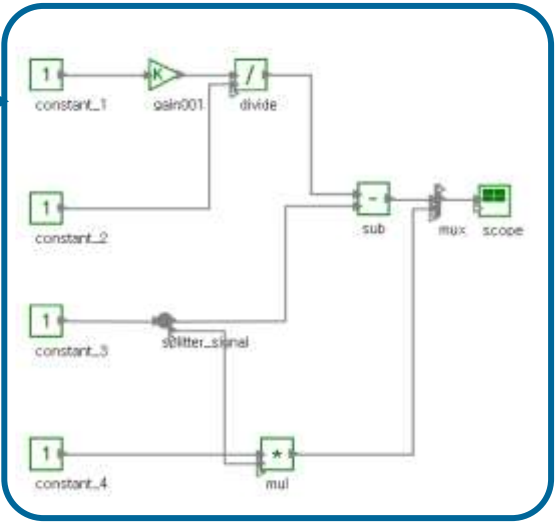
7. Instrumentation & control

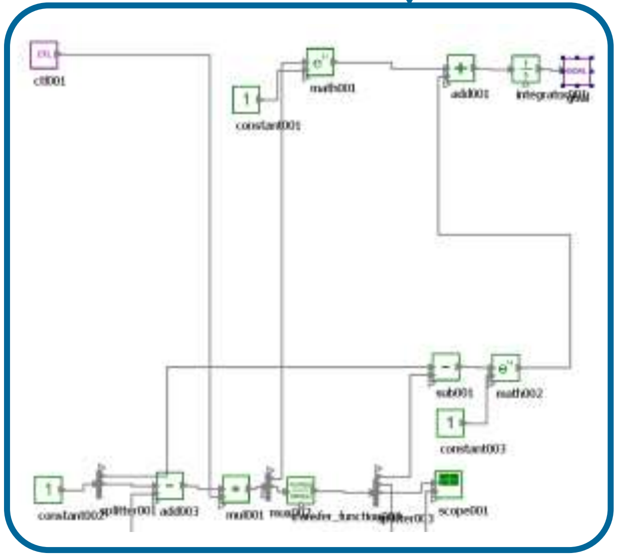
- Library contains models that operate on signals
  - In gPROMS: arrays of non-dimensional numbers
- Library can be used to
  - add signalling & control logic to flowsheets
  - add basic post-processing calculations to flowsheets in a graphical manner
  - Create custom models as “flowsheets” of signals
- Interfaces to ProcessBuilder unit operation models
  - bus connection is used to select and apply signals from quantities in unit operation models (e.g. flowrates, concentrations, temperatures, etc.)

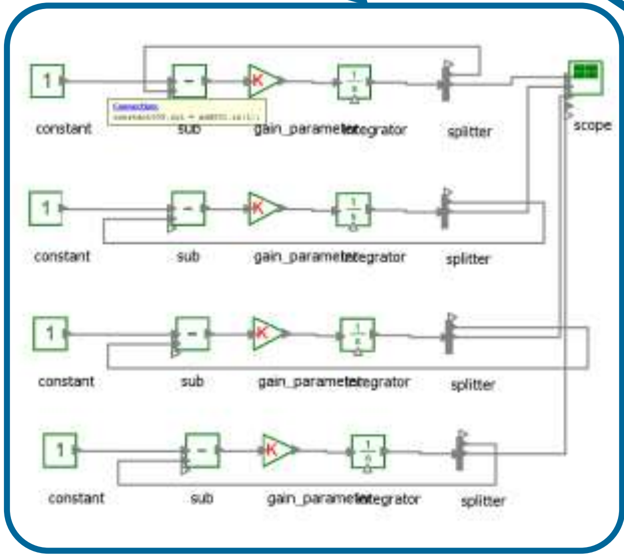


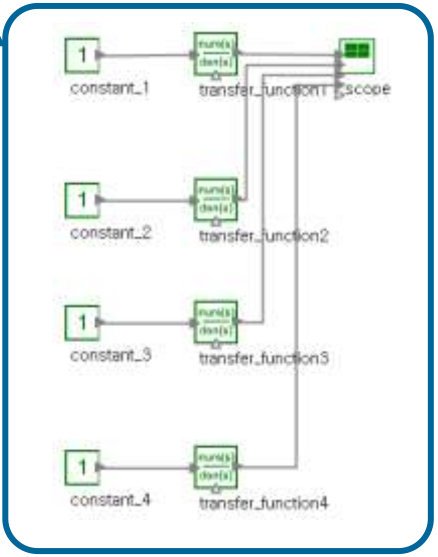
Enhanced steady-state and dynamic analysis

- Basic calculation
- Linear dynamic system
- Nonlinear dynamic system
- Control loop optimization



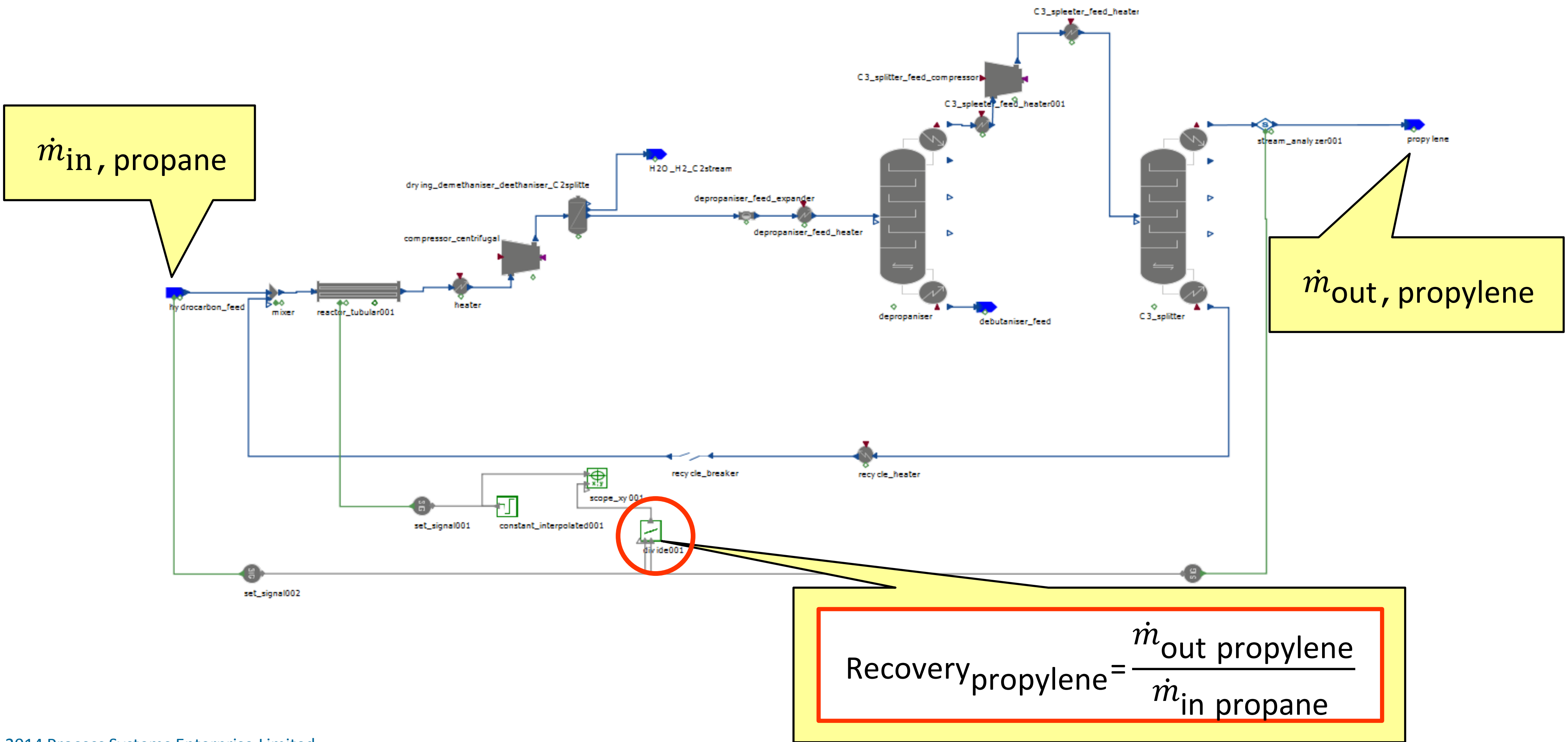






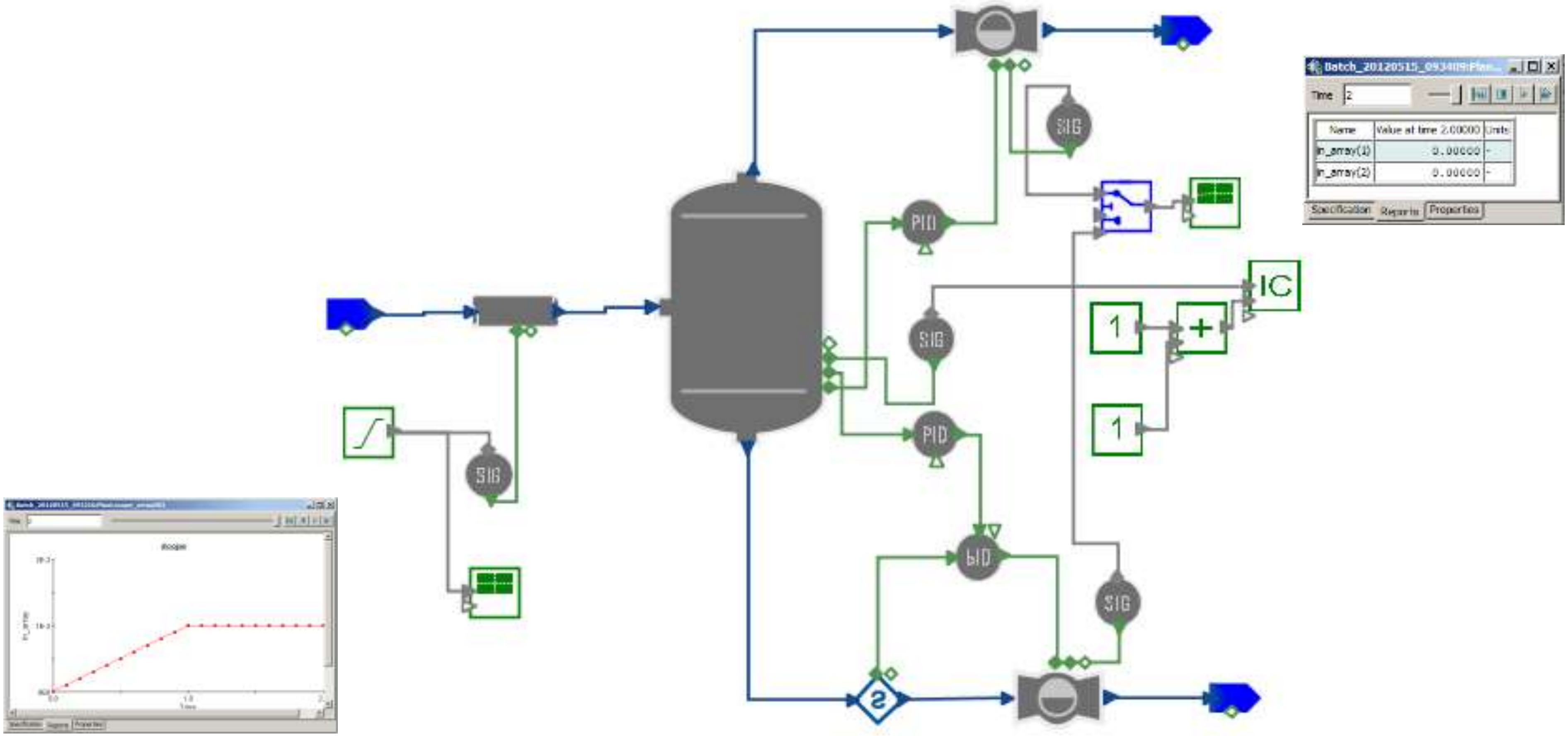
Enhanced steady-state and dynamic analysis

- Use gML Signal and gML Control model libraries to plot recovery of propylene against energy rate



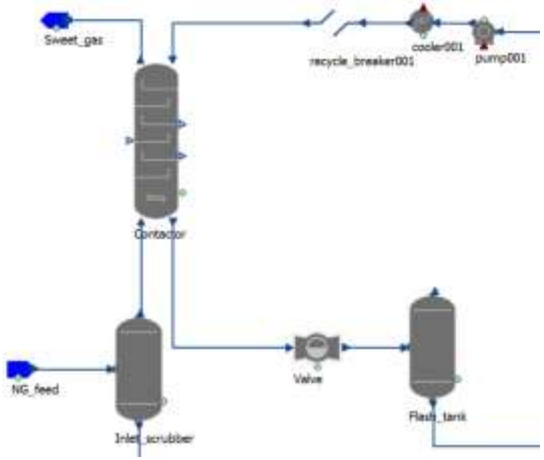
Enhanced steady-state and dynamic analysis

- Full integration with “process simulation” flowsheets

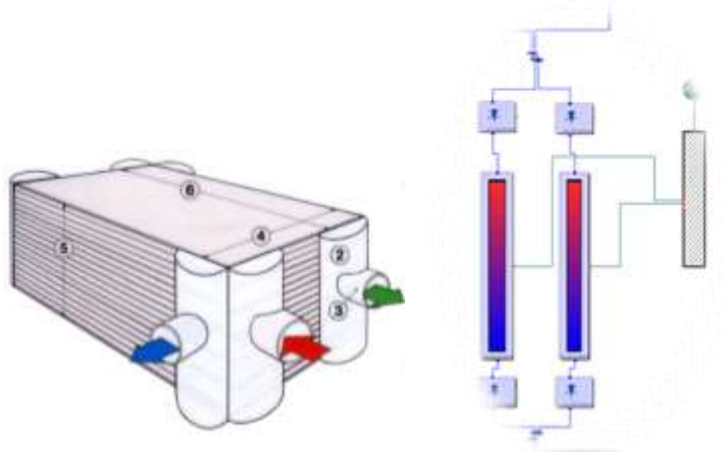


Example: LNG production

Dehydration and sweetening (amines, glycol, …)



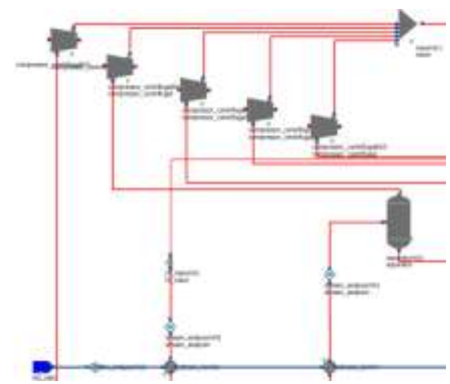
Detailed Multi-Stream Heat Exchanger design (PFHX & CWHX)



Fractionation

TO ADD screenshot…..

Liquefaction (C3MR, AP-X…)



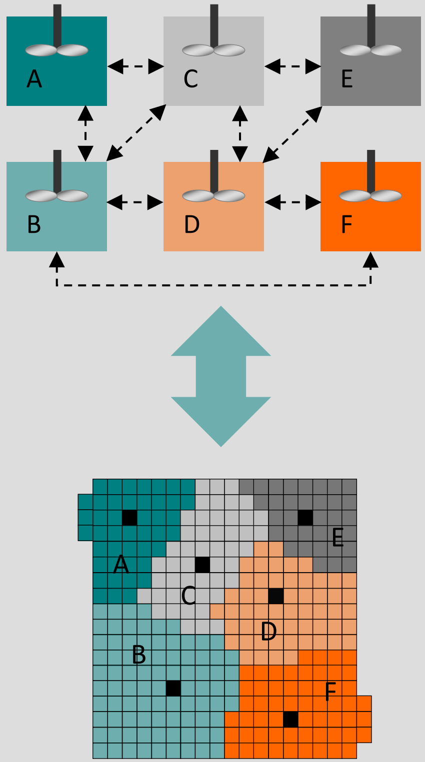
9. … and more

1. Link models to CFD
   - couple hydrodynamics (mixing) and physics/chemistry
2. Fit process behavior to plant, pilot-plant & lab data
3. Create libraries for other users in or outside the organization
   - Encrypted if necessary, to protect IP
4. Export process models for execution in other environments
   - Behind custom interfaces
   - CAPE-OPEN simulators – e.g. Aspen Plus
   - MATLAB®
5. …

Hybrid Multizonal/CFD approach

Multizonal gPROMS model

Zone population balance
Growth, nucleation kinetics
Network mass/energy balances



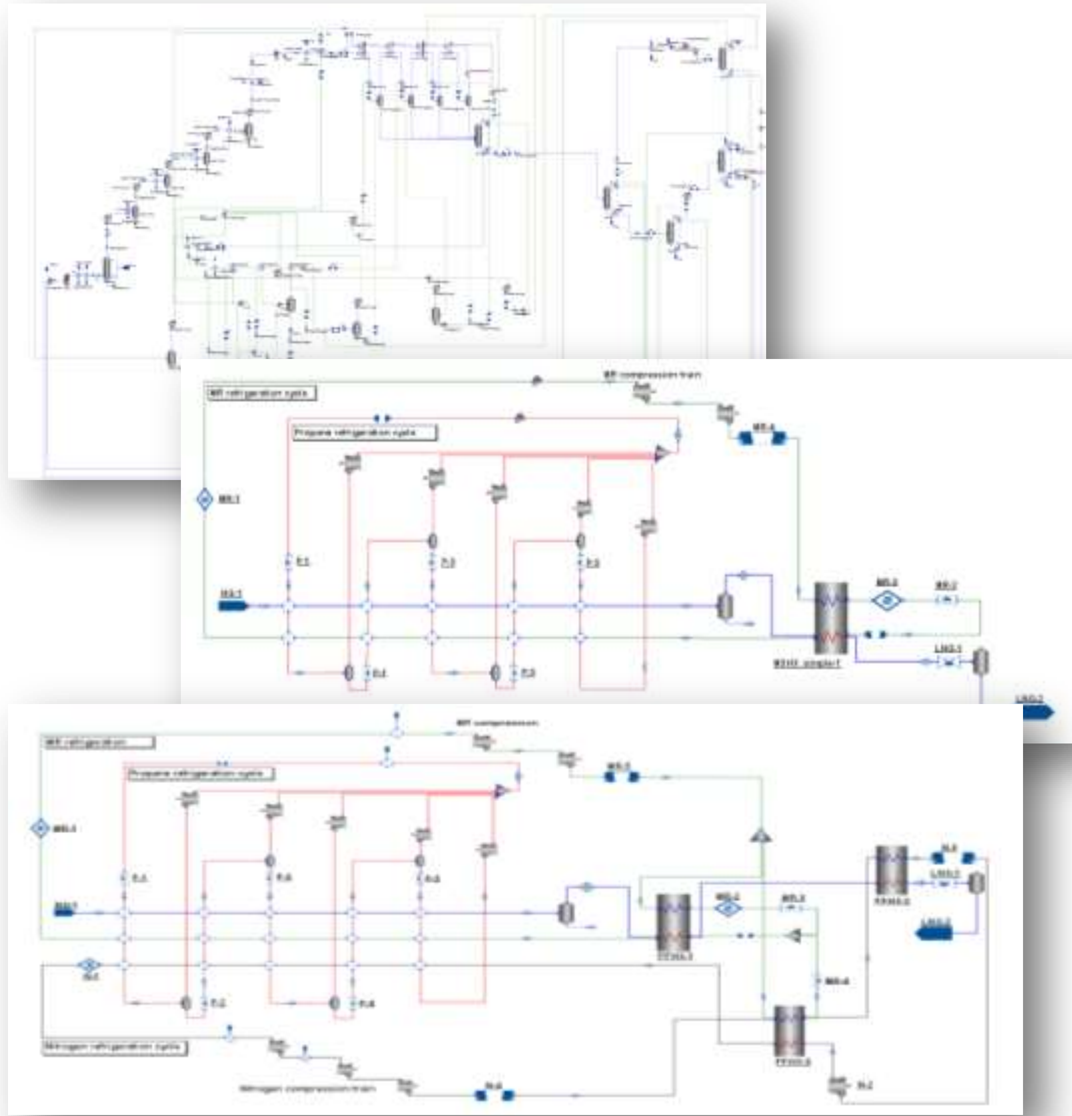
CFD model of unit

Total mass conservation
Momentum conservation

In conclusion…

gPROMS ProcessBuilder
Advanced Process Simulation

- **First "true equation-oriented" process flowsheeting tool**
  - modeling power
    with usability & robustness
- Current status
  - Model libraries complete
  - Application/testing
    on key processes
    - Olefins
    - Gas processing (NG/LNG)
    - Industrial gases
    - Syngas / hydrogen
    - Batch/reactive distillation
  - Ongoing evaluations by
    selected lead users
- Expected release date for v1.0:
  December 2014
  - based on gPROMS v4.1 platform



Thank you