



ADVANCED PROCESS MODELLING FORUM 2017

London 25–26 April

gPROMS ProcessBuilder 1.2.0

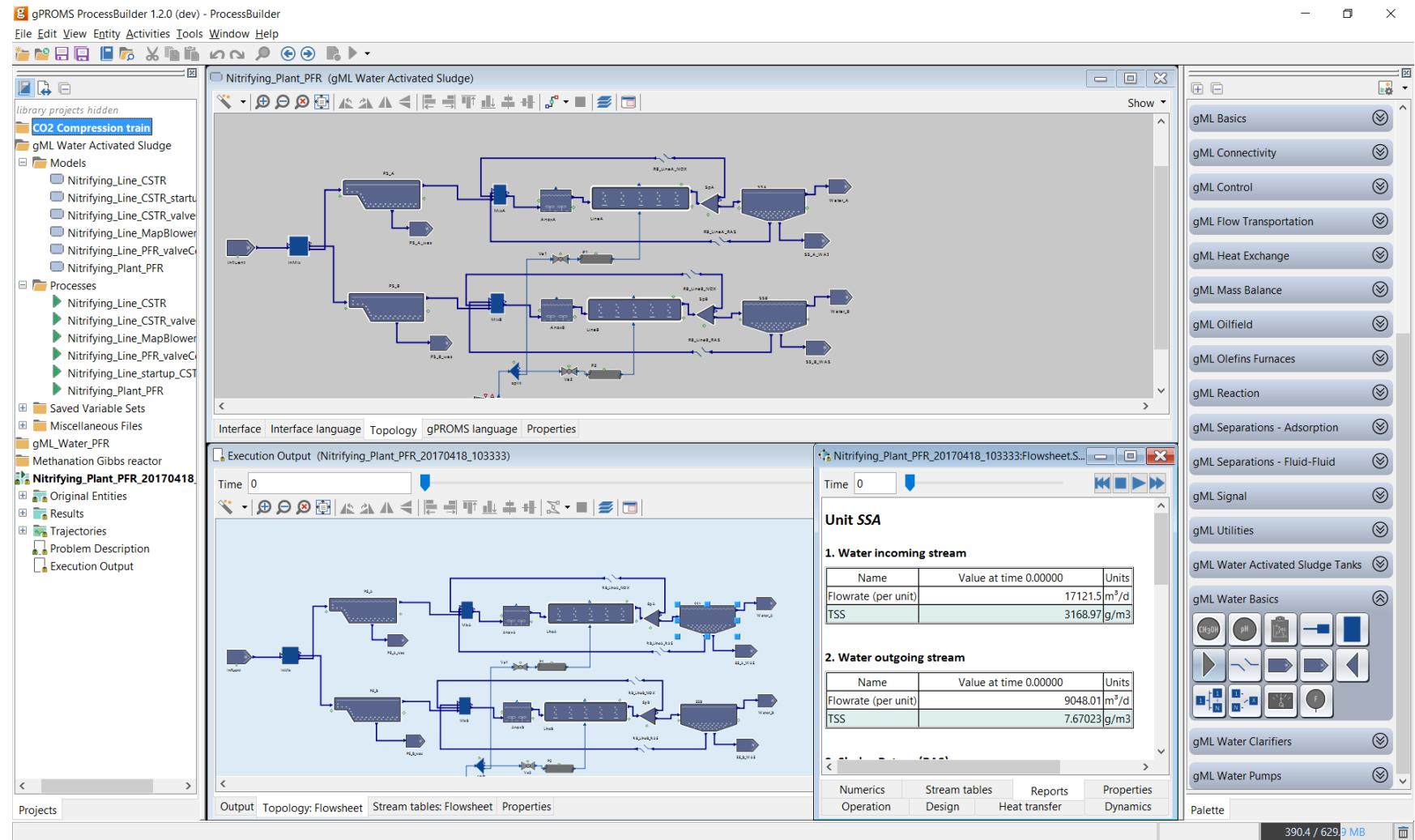
A unified environment for applications across the plant

Maarten Nauta – Principal Consultant



gPROMS ProcessBuilder 1.2.0

Integrated modelling and simulation environment for process industries



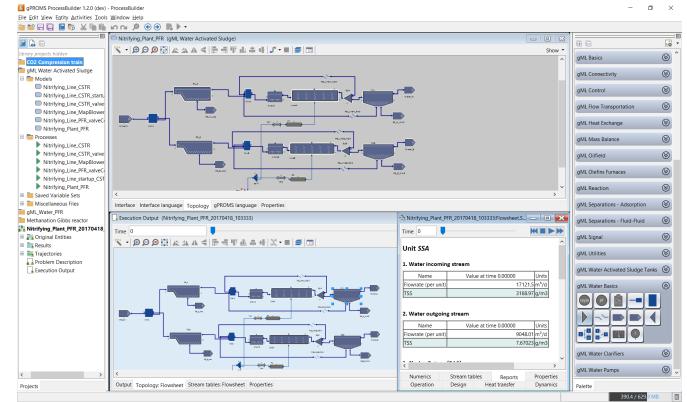
gPROMS ProcessBuilder 1.2.0

Product formulation



■ Key features

- Comprehensive set of model libraries
 - gML Process
 - gML Olefins (NEW in gPROMS ProcessBuilder 1.2.0)
 - gML Water (NEW in gPROMS ProcessBuilder 1.2.0)
 - gML Utilities (NEW in gPROMS ProcessBuilder 1.2.0)
 - AML:FBCR (UPGRADED in gPROMS ProcessBuilder 1.2.0)
 - AML:TBR (NEW in gPROMS ProcessBuilder 1.2.0)
 - AML:GLC (NEW in gPROMS ProcessBuilder 1.2.0)
 - gML Oilfield (Upcoming in ProcessBuilder 1.3.0)
 - gML Power (Upcoming in ProcessBuilder 1.3.0)
- Built on gPROMS platform 5.0.0
- Materials modelling
 - Multiflash + DIPPR
 - gSAFT
- online help, reference examples, workflow guides, training videos, training courses

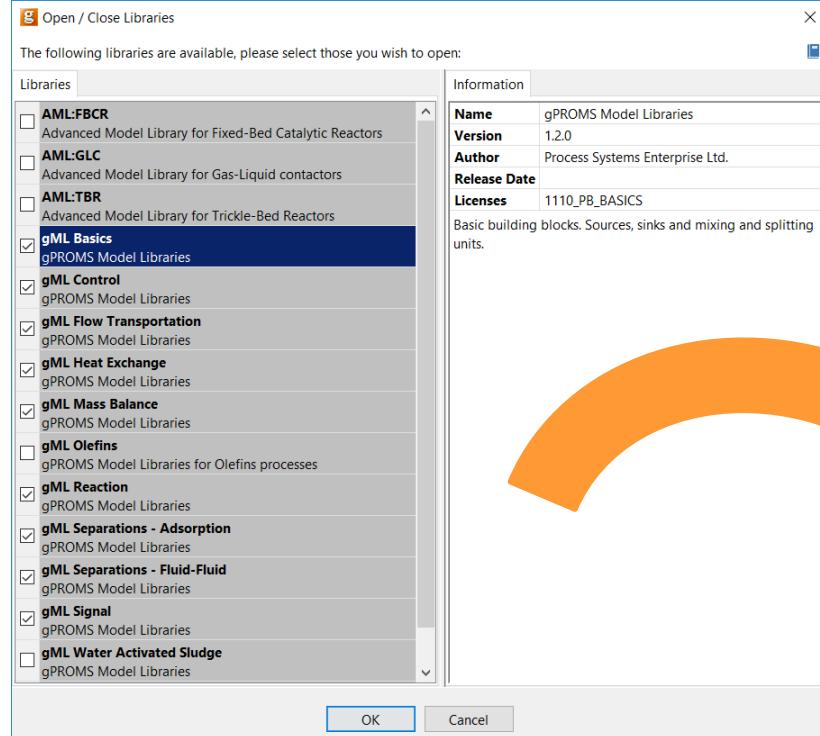


gPROMS ProcessBuilder 1.2.0

Product formulation



- Load and license the libraries required to model and optimise your process



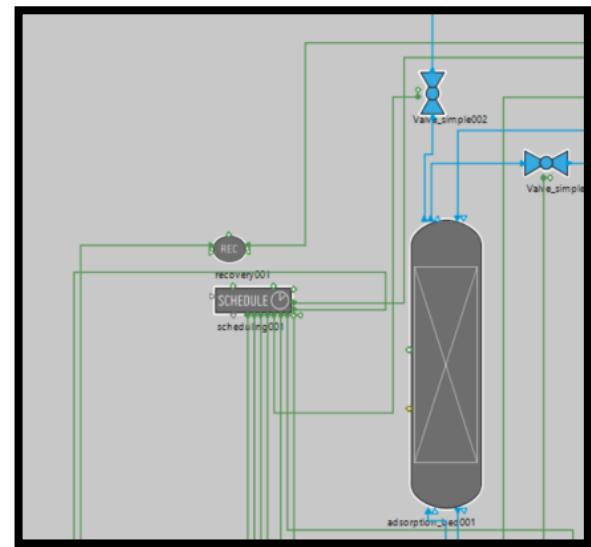
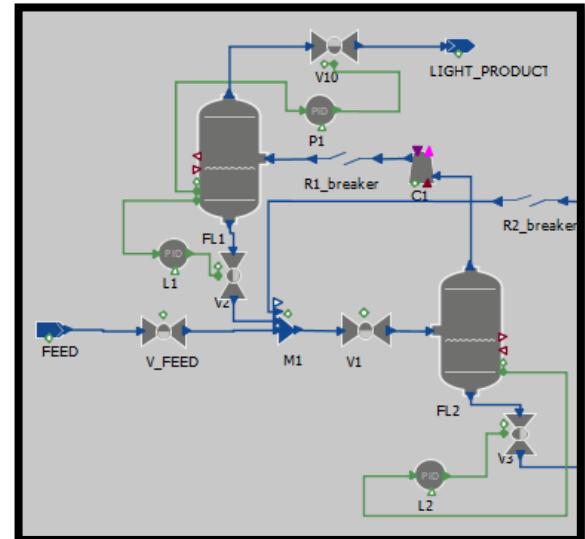
| | |
|--|-------------------------------------|
| AML-FBCR Basics | <input checked="" type="checkbox"/> |
| AML-FBCR Catalyst Bed - Axial Flow | <input checked="" type="checkbox"/> |
| AML-FBCR Catalyst Bed - Axial Flow - ... | <input checked="" type="checkbox"/> |
| AML-FBCR Catalyst Bed - Radial Flow | <input checked="" type="checkbox"/> |
| AML-FBCR Cooling System | <input checked="" type="checkbox"/> |
| AML-GLC Columns | <input checked="" type="checkbox"/> |
| AML-TBR Basics | <input checked="" type="checkbox"/> |
| AML-TBR Bed Sections | <input checked="" type="checkbox"/> |
| AML-TBR Heat Exchange | <input checked="" type="checkbox"/> |
| gML Basics | <input checked="" type="checkbox"/> |
| gML Connectivity | <input checked="" type="checkbox"/> |
| gML Control | <input checked="" type="checkbox"/> |
| gML Flow Transportation | <input checked="" type="checkbox"/> |
| gML Heat Exchange | <input checked="" type="checkbox"/> |
| gML Mass Balance | <input checked="" type="checkbox"/> |
| gML Oilfield | <input checked="" type="checkbox"/> |
| gML Olefins Furnaces | <input checked="" type="checkbox"/> |
| gML Reaction | <input checked="" type="checkbox"/> |
| gML Separations - Adsorption | <input checked="" type="checkbox"/> |
| gML Separations - Fluid-Fluid | <input checked="" type="checkbox"/> |
| gML Signal | <input checked="" type="checkbox"/> |
| gML Water Activated Sludge | <input checked="" type="checkbox"/> |
| gML Water Basics | <input checked="" type="checkbox"/> |
| gML Water Clarifiers | <input checked="" type="checkbox"/> |

New and updated libraries in gPROMS ProcessBuilder 1.2.0



- Libraries for general process modelling
 - Reaction, separation, heat-exchange, fluid flows
- Applications
 - Modelling and optimisation of a broad range of base and speciality chemical manufacturing processes
 - High-level network modelling and optimisation
 - Dynamic simulation of chemical plants
 - Dynamic adsorption processes (PSA, TSA, ..)

- NEW in gPROMS ProcessBuilder 1.2.0
 - Consistent with all other gML and AML libraries
 - Molar fractions and vapour fractions reported in connections
 - Fired heater model
 - Packed column sizing
 - Better handling of pure component streams
 - Robustness improvements

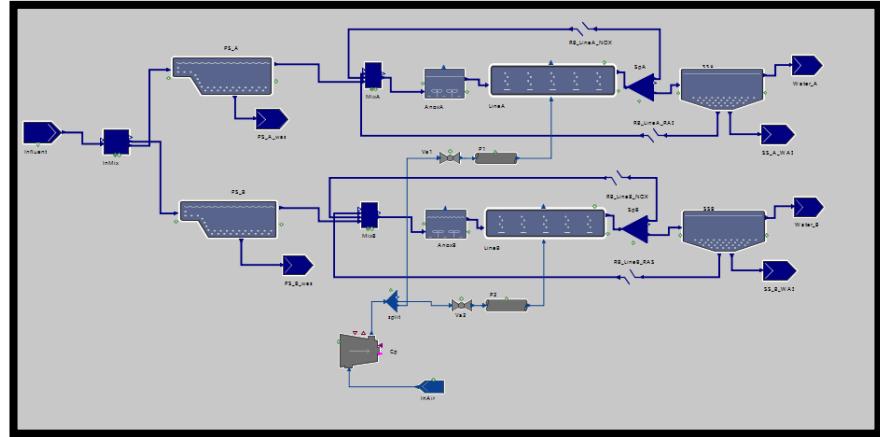


gPROMS ProcessBuilder 1.2.0

gML Water (NEW in gPROMS ProcessBuilder 1.2.0)



- Library for urban and industrial wastewater treatment processes
 - Main applications
 - Scenario simulation for an existing plant: varying loads, control strategy, equipment parameters, etc.
 - Optimisation of efficiency with key control variables: blowers operation point, nitrate recycles, sludge recycles and extraction, etc.
 - New process concept design.
 - Key features
 - Predict performance and energy use of water treatment plant
 - Detailed modelling of biochemistry of activated sludge processes ASM
 - Upcoming release will include comprehensive array of treatment processes



- Current release includes:
 - Activated Sludge Process units
 - Upcoming in ProcessBuilder 1.3.0
 - Adsorption
 - Ion exchange
 - Filter separation
 - Membrane separation

■ Library for olefins processes

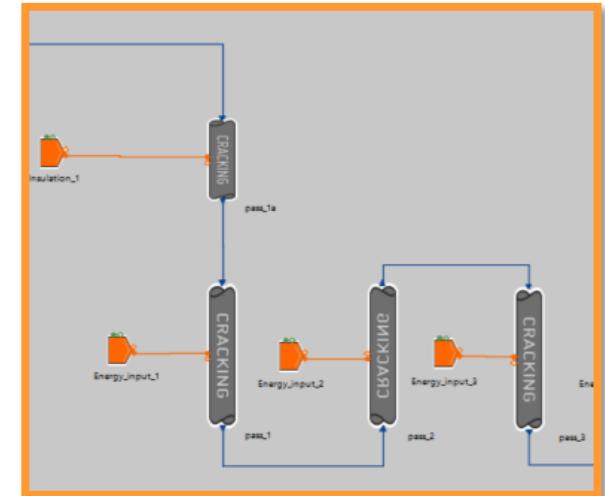
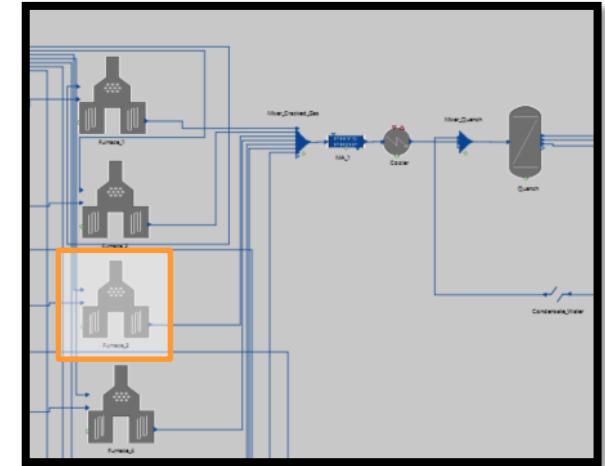
- Simulate the cracking of hydrocarbons in the radiant section of a steam cracking furnace to produce olefins

■ Applications

- Furnace performance modelling and optimisation
- Olefins plant modelling

■ Key features

- Kinetics for ethane, propane and Naphta cracking
- Predicts the cracking products and temperature and pressure profiles in the furnace
- Takes into account the effect of coking accumulation
- Ability to model different coil types and configurations

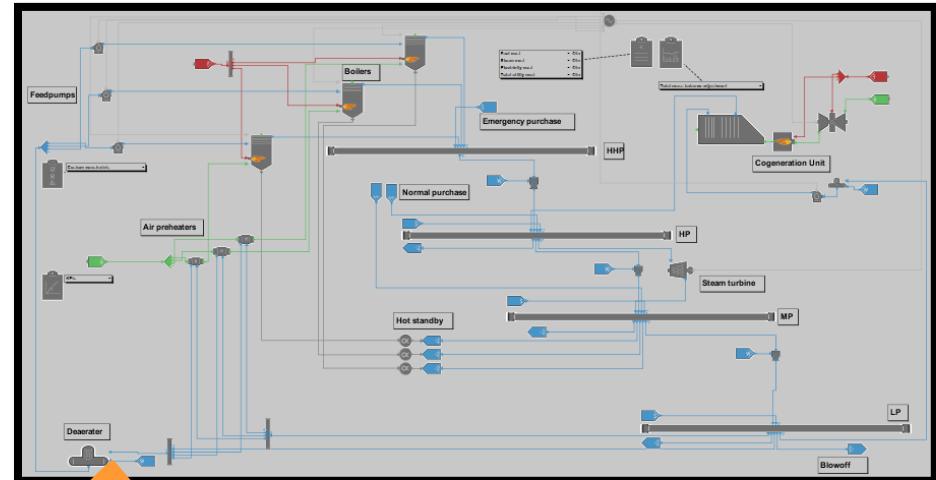


gPROMS ProcessBuilder 1.2.0

gML Utilities (NEW in gPROMS ProcessBuilder 1.2.0)



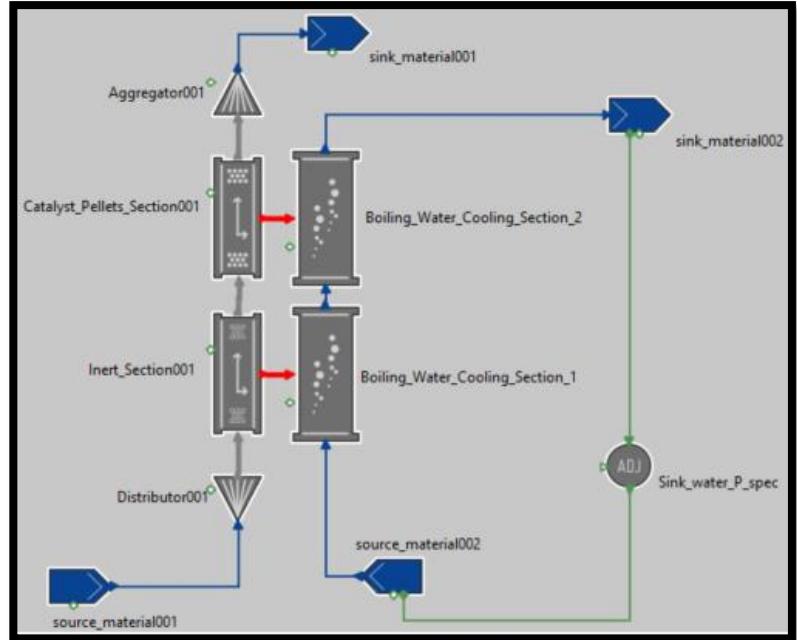
- Library for utility plant modelling
 - Optimise utility plants
- Applications
 - Plant and site-wide utilities optimisation (chemical parks, refineries, ...)
- Key capabilities
 - Predict and minimise fuel, steam and electricity use of complex utility plants
 - Deploy to operations for planning (gPROMS Utilities Planner) and online optimisation (gPROMS Utilities Advisor)
 - Rapid solutions to optimisation problems, in the order of seconds for typical processes
 - Handle 10s of optimisation decision variables in a complex process



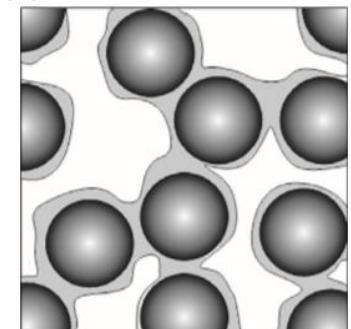
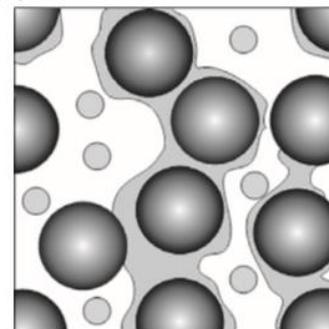
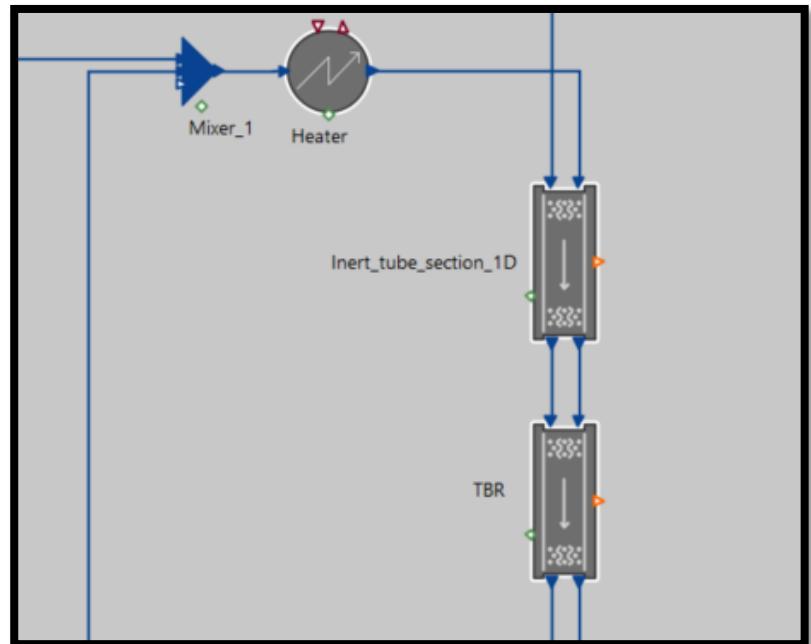
gPROMS Utilities Advisor

gPROMS Utilities Planner

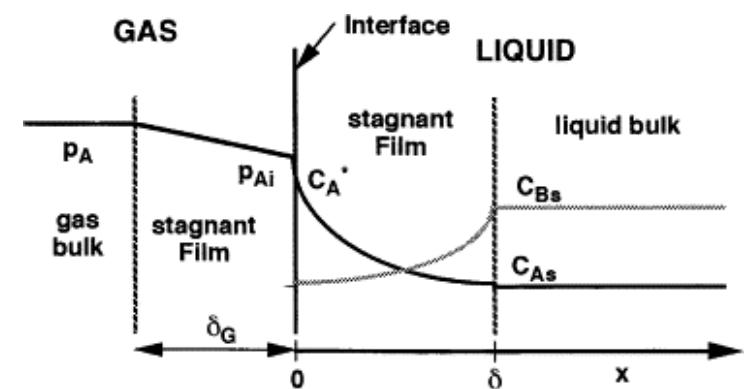
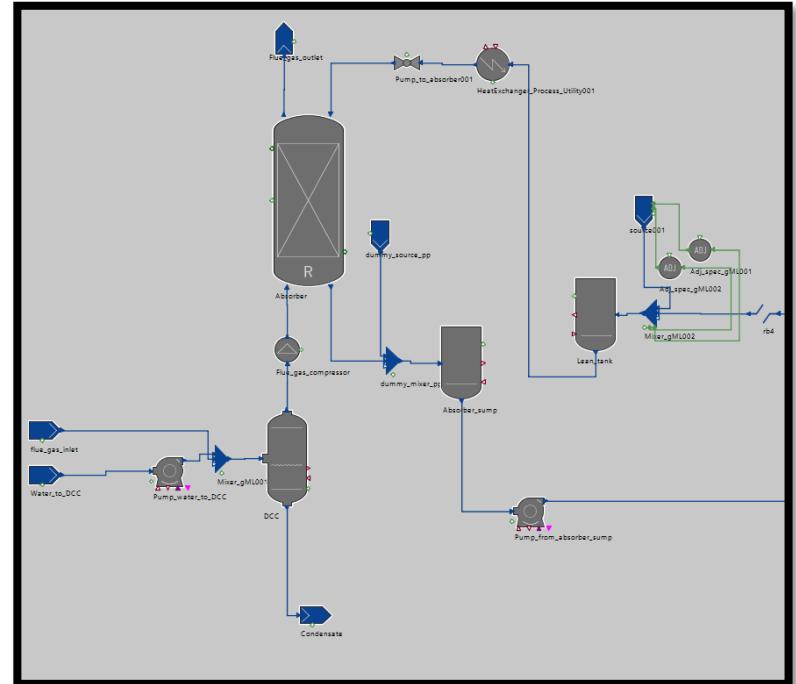
- High fidelity models for
 - Fixed bed catalytic reactors
 - Single phase systems
- Applications
 - Gas or liquid phase reactions
 - Styrene, Methanol, Reforming, ...
- Key improvements
 - Liquid phase (**NEW in gPROMS ProcessBuilder 1.2.0**)
- Modular library
 - Configure model with preferred complexity and detail
 - Multiple configurations available



- High fidelity models for
 - Trickle bed catalytic reactors
- Applications
 - Refining
 - Petrochemicals
 - Fine chemicals
 - Biochemicals
- Processes
 - Petrochemicals – hydrogenation
 - Refinery – Hydrotreating
 - Fischer-Tropsch synthesis
- Modular library
 - Different reactor configurations
 - Different level of detail (1-D, 2-D)

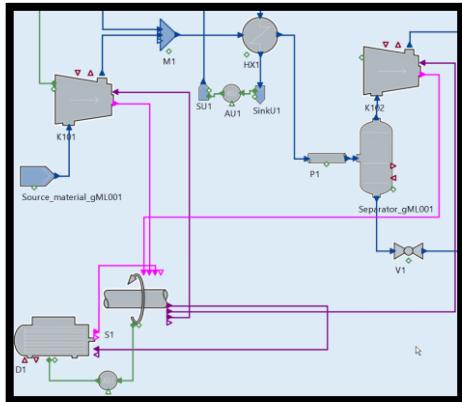


- Library for rate-based distillation
 - Predict mass and heat transfer for columns that do not reach equilibrium between gas and liquid
- Applications:
 - CO₂ capture using amine processes
 - Natural gas sweetening
 - Reactive distillation
- Key capabilities:
 - Detailed representation of non-equilibrium heat and mass transfer
 - Custom modelling option to introduce custom correlations for heat and mass transfer
 - Integration with gSAFT

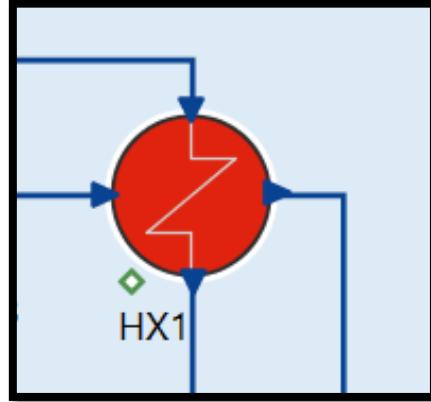


gPROMS ProcessBuilder 1.2.0

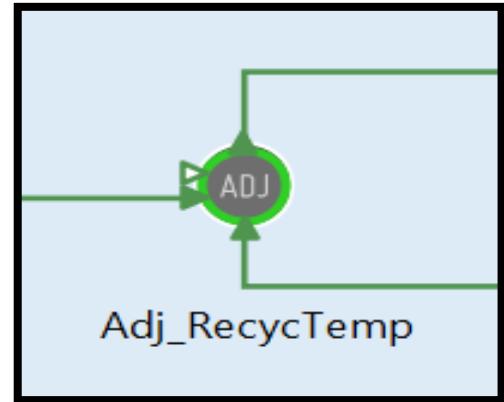
Consistent way of building and simulating flowsheets



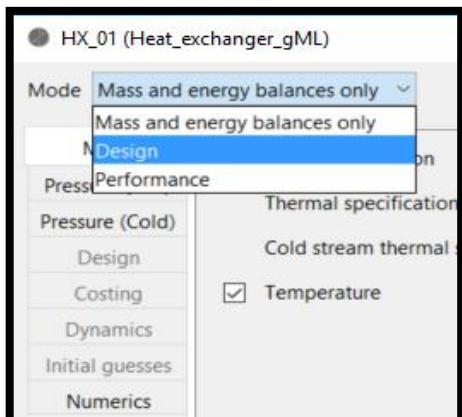
Visual indication for
flowsheet convergence



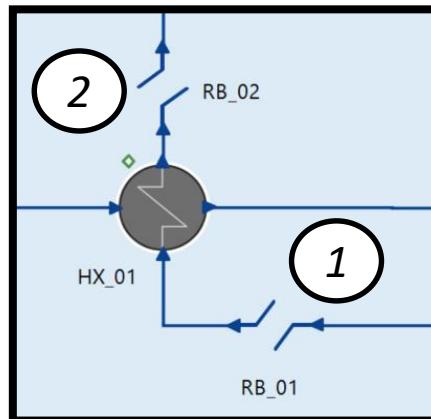
Warnings for inconsistent
specifications



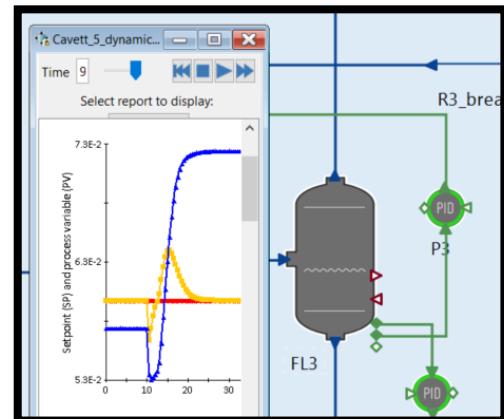
Specification trade-offs



Simulation modes



Automatic flowsheet initialisation
**(NEW in gPROMS ProcessBuilder
1.2.0)**

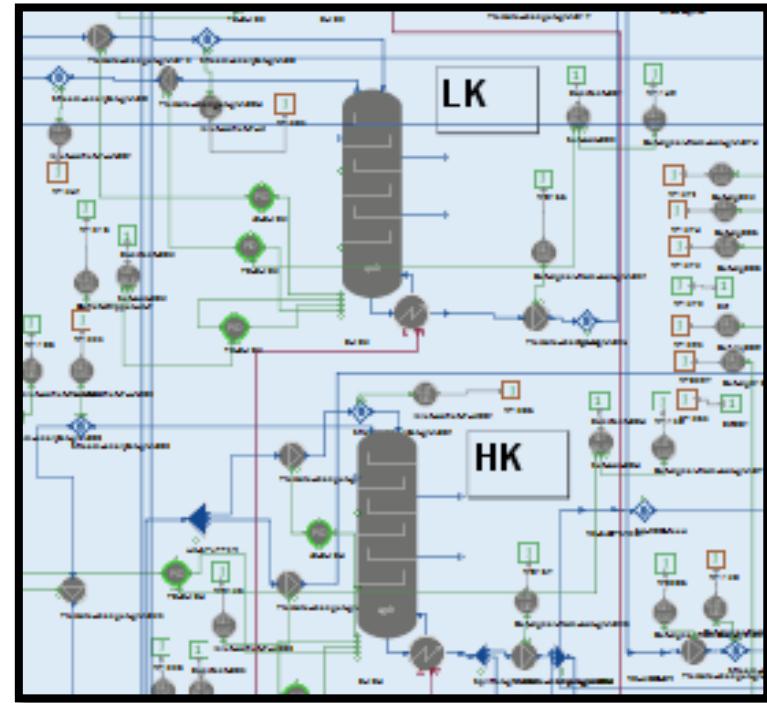


Dynamic simulation



■ Complex flowsheets

| Application | System size (variables) | Convergence time (from previous solution, indicative) |
|-----------------------|-------------------------|---|
| Refinery | 300K | 2 – 3 mins |
| Gas network | 320K | 1 mins |
| Olefins plant | 220K | 2 mins |
| Propylene-Oxide plant | 500K | 1-2 mins |

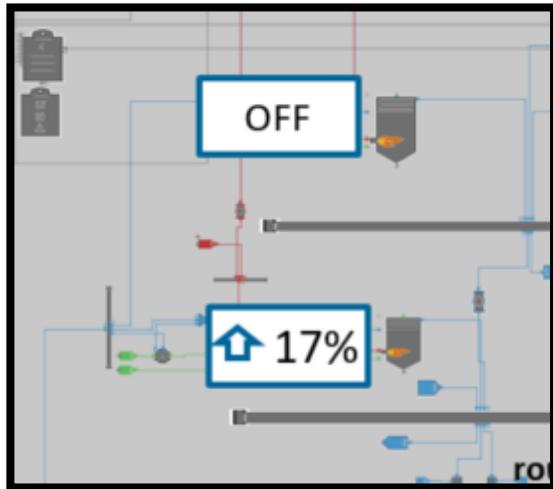


■ Improvements in gPROMS ProcessBuilder 1.2.0

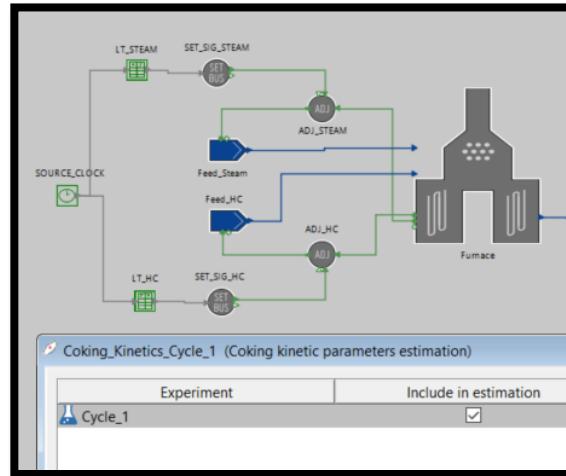
- Model pruning during initialisation (**NEW in gPROMS ProcessBuilder 1.2.0**)
- DAEBDF integration solver now default solver for new projects (**NEW in gPROMS ProcessBuilder 1.2.0**)

gPROMS ProcessBuilder 1.2.0

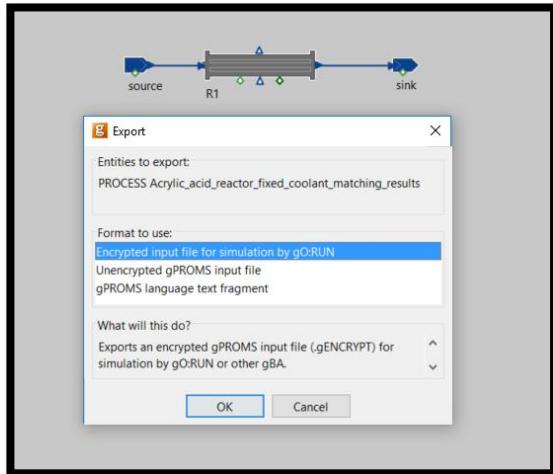
Applications



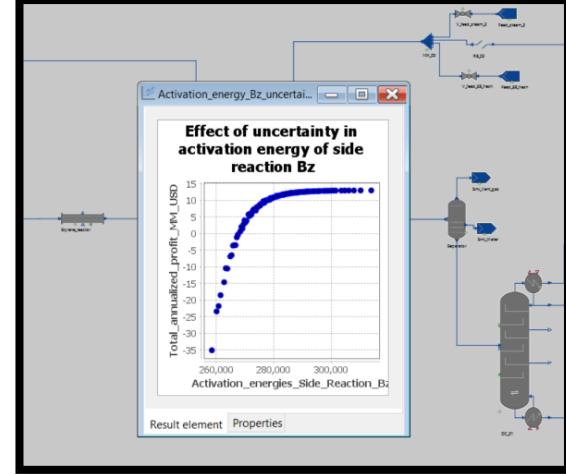
Optimisation



Parameter estimation



Deployment (increased functionality
in gPROMS ProcessBuilder 1.2.0)



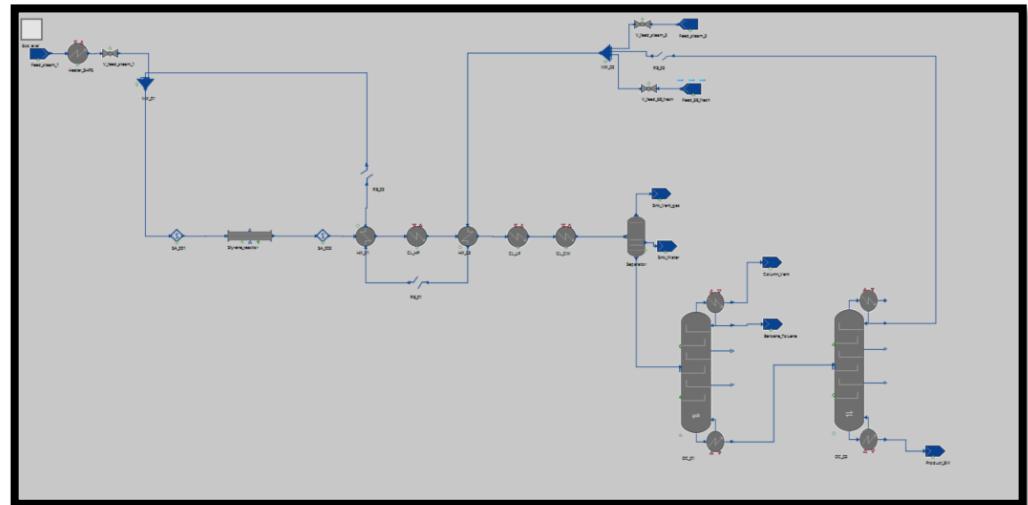
Global System Analysis
(NEW in gPROMS ProcessBuilder 1.2.0)



ADVANCED PROCESS MODELLING FORUM 2017

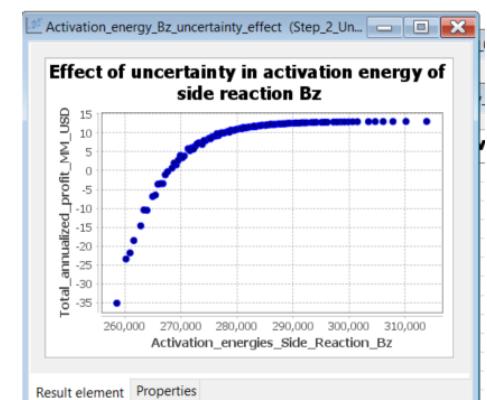
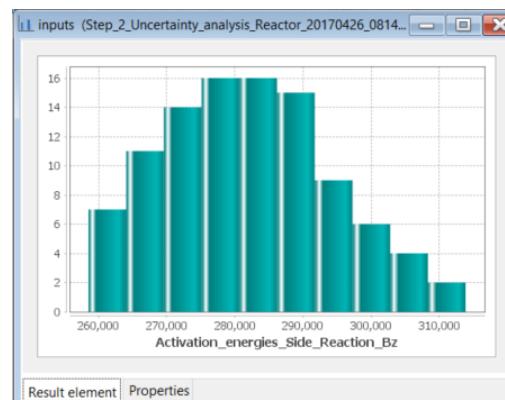
■ Styrene Process

- Tubular reactor, two distillation columns, recycle with heat integration
 - System size: medium size



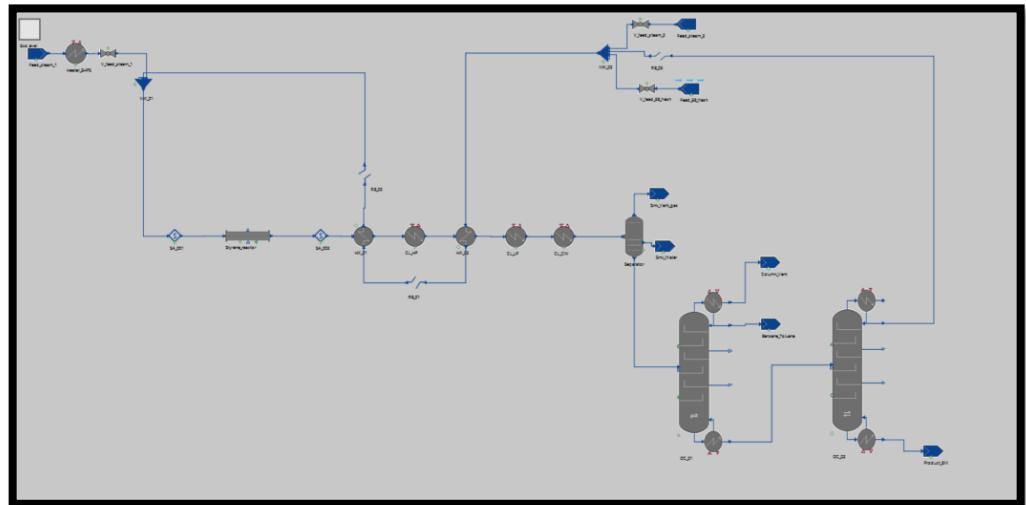
■ Typical applications:

- Risk analysis (uncertainty in market conditions, feed properties, kinetic parameters,...)
 - Explore the design (and operation) space



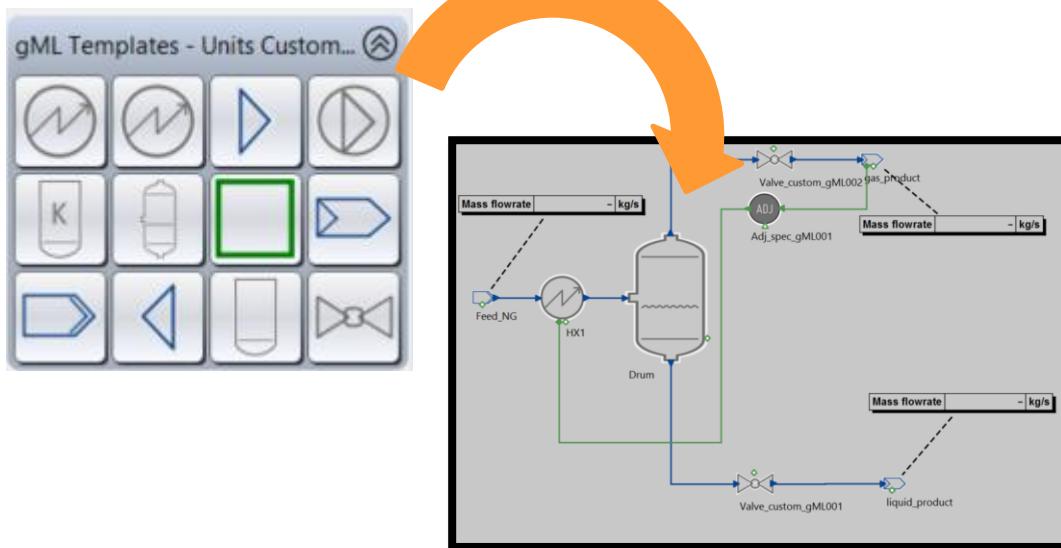
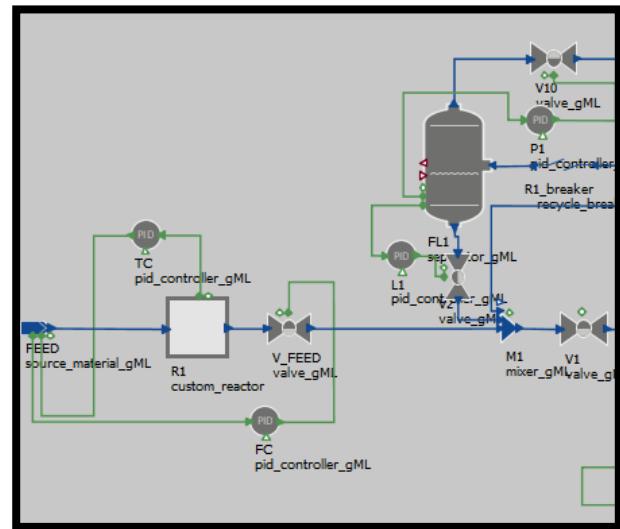
■ Styrene Process

- Tubular reactor, two distillation columns, recycle with heat integration
- System size: medium size



| Applications | Complexity | Time |
|--|-------------------------------------|-------------------------------------|
| Single simulation | 26K variables | 30 sec (8 sec re-initialisation) |
| Optimisation | Mixed-integer, 5 decision variables | 6 mins |
| Global System Analysis (NEW in gPROMS ProcessBuilder 1.2.0) | Uncertainty analysis, 106 samples | 6m47sec (2 processors) |

- Code the model in the gPROMS language
 - use standard ProcessBuilder variable & connection types
- Template models for common unit operations available to start from



```

custom_reactor (Cavett_6_dynamic_with_control_out)
1 PARAMETER
2 nset AS INTEGER
3
4 UNIT
5   BVS AS ARRAY (nset) OF bus_variable_selector_gML
6
7 PORT
8   inlet AS gMLMaterial DIRECTION_INLET
9   outlet AS gMLMaterial DIRECTION_OUTLET
10  setport AS ARRAY (nset) OF Bus
11
12 SET
13 BVS().bus_types := ['My hotspot temperature'];
14
15 TOPOLOGY
16 setport(1:nset) = BVS(1:nset).setPort;
17
18 EQUATION
19 Outlet.w("HYDROGEN") = (Inlet.T-300)^1.2 * Inlet.w("WATER");

```

19:41 INS

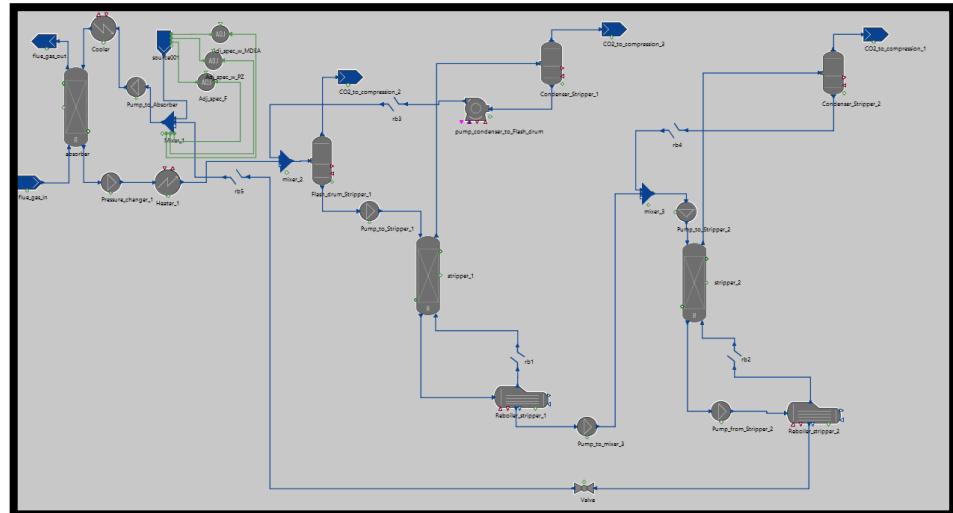
Interface Interface language Topology gPROMS language Properties

gPROMS ProcessBuilder 1.2.0

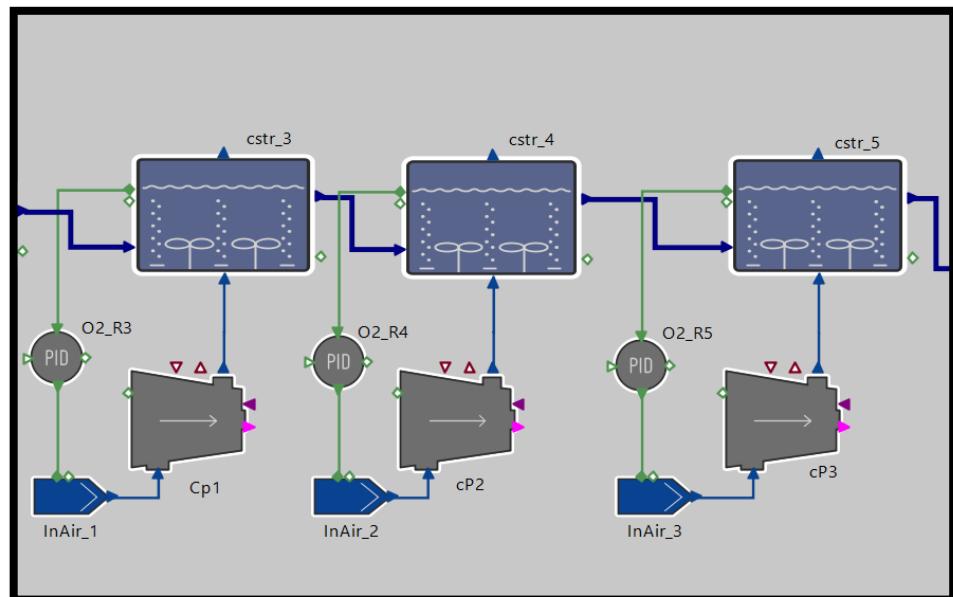
A unified environment for applications across the plant



gML Process + AML:GLC
CO₂ capture using amine
process (MEA)



gML Process + gML Water
Model nitrifying line with
aeration control

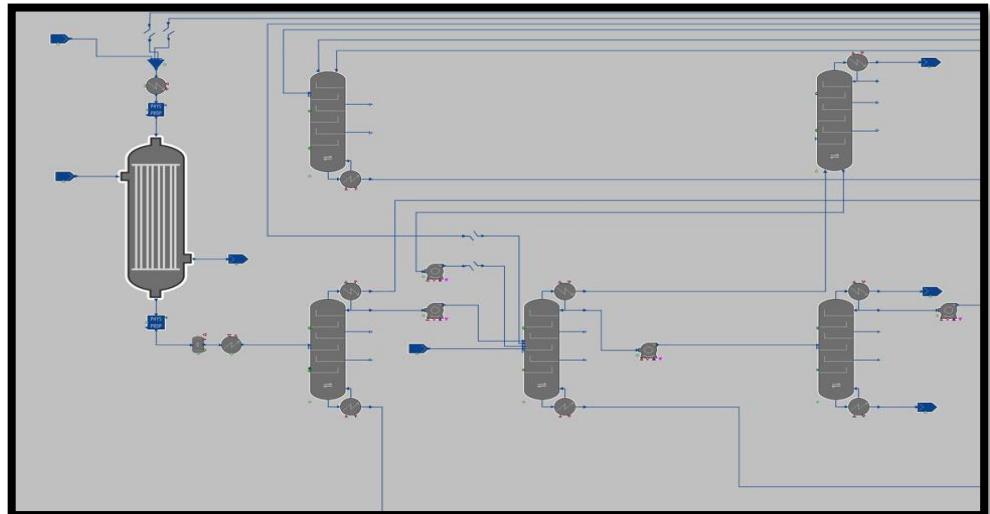


gPROMS ProcessBuilder 1.2.0

A unified environment for applications across the plant

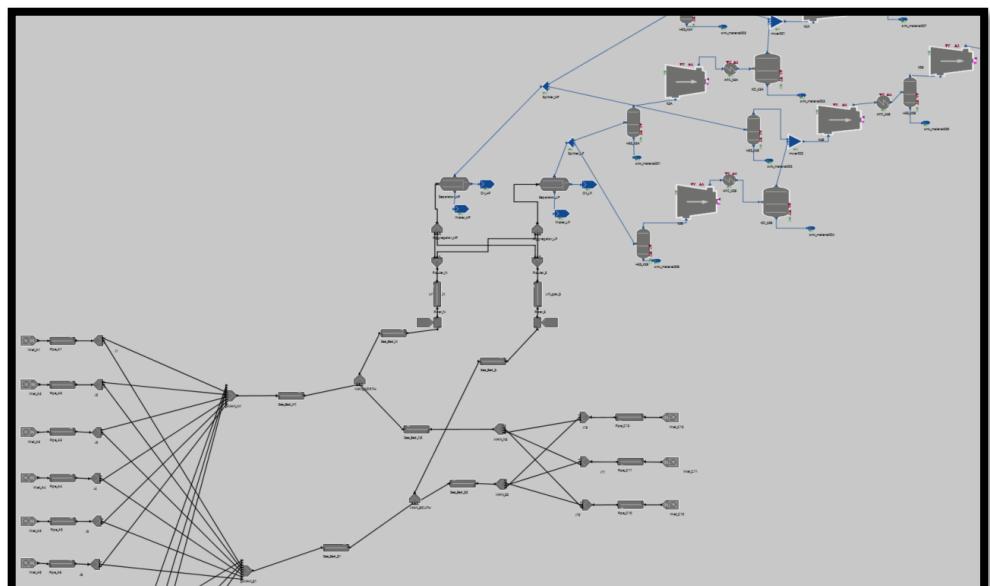
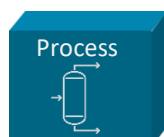


gML Process + AML:FBCR
Optimise a Propylene Oxidation process including reaction and separation section with detailed reactor model



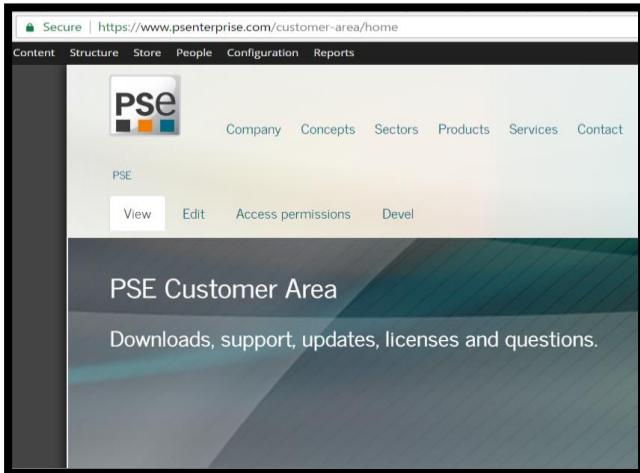
gML Process + gML Oilfield
Optimise well settings taking into account effects on top-side equipment

(Upcoming in ProcessBuilder 1.3.0)

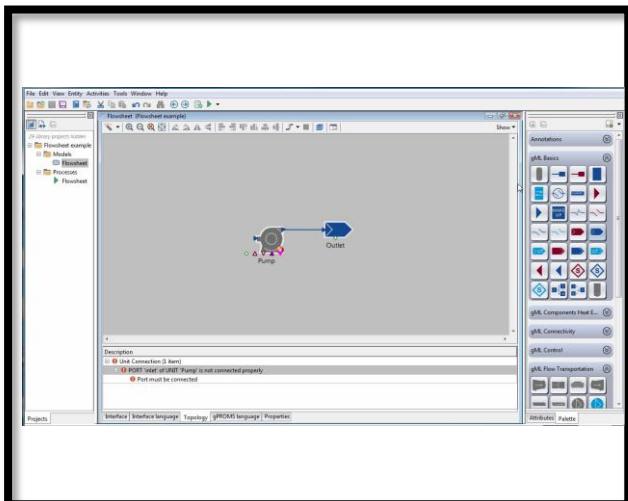


gPROMS ProcessBuilder 1.2.0

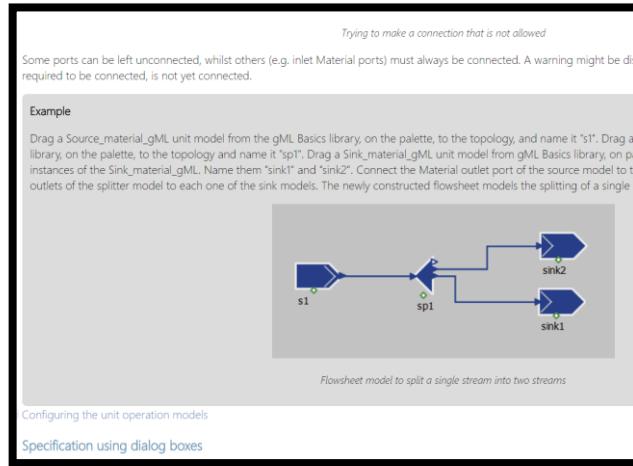
Customer support



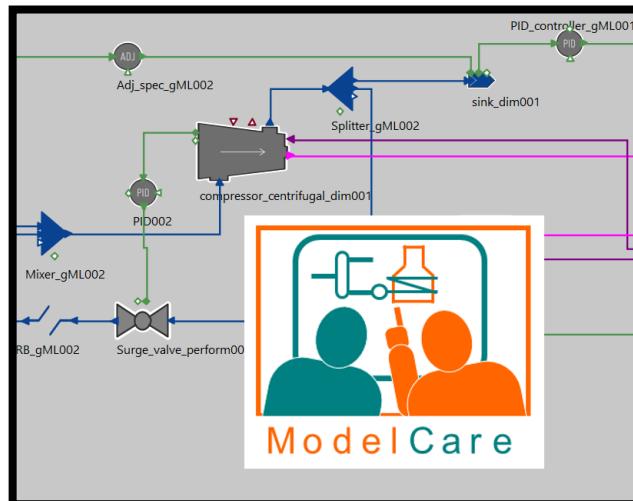
MyPSE Customer Area



Training videos and training courses



Product documentation and workflow guides

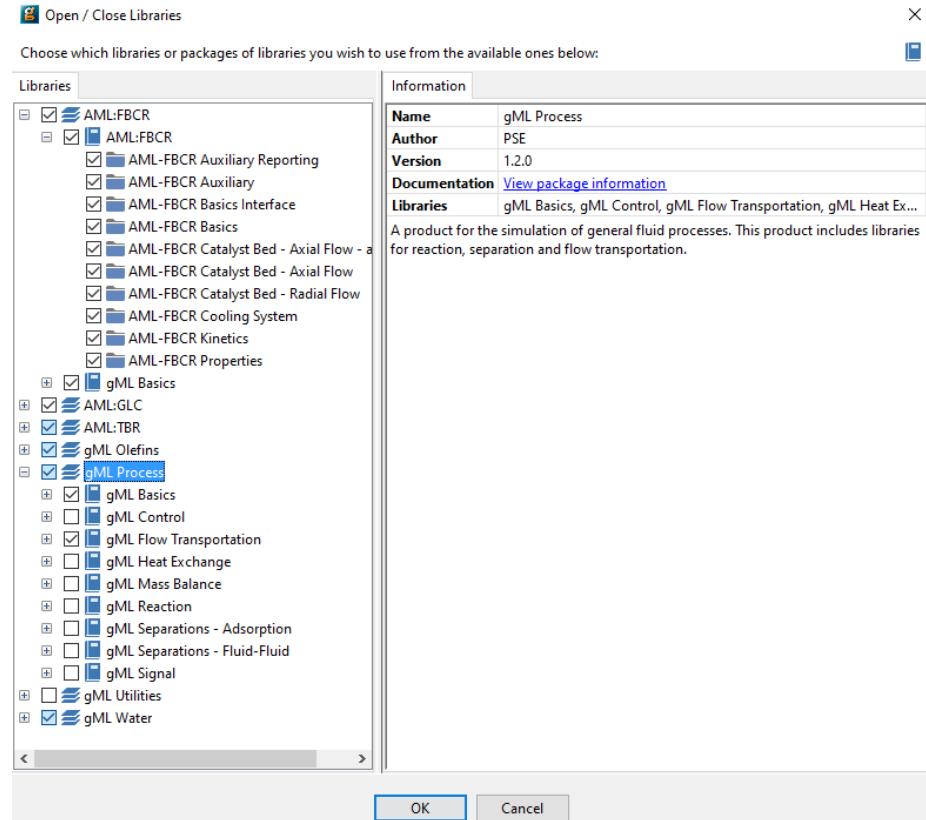


PSE Consulting Group



ADVANCED PROCESS MODELLING FORUM 2017

- Diagnostics improvements
 - Extend unit-specific warning and error messages
- New functionality for existing gML and AML libraries
- Extend application range to new sectors
 - gML Power
 - gML Oilfield



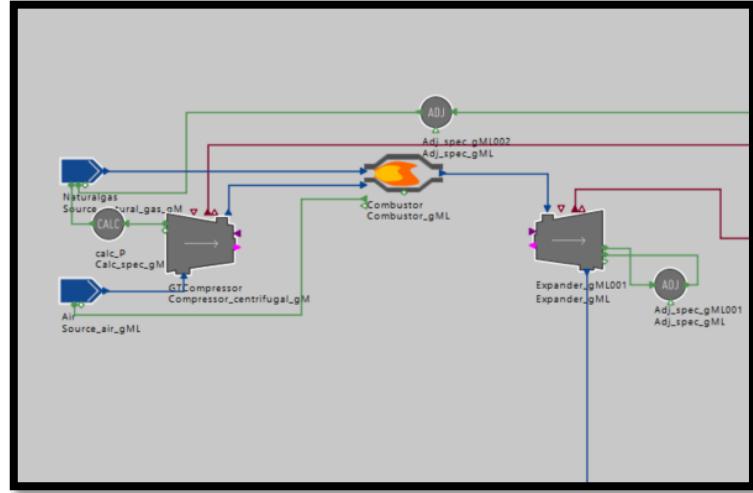
Roadmap

gML Oilfield and gML Power (Upcoming in ProcessBuilder 1.3.0)



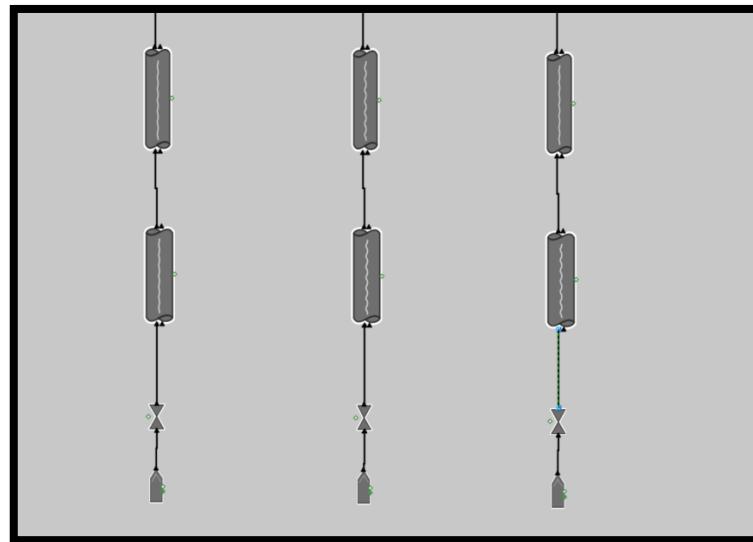
■ gML Power

- Conventional (coal and gas-fired) and oxyfuel powerplant modelling
- Boilers, combustion, steam-cycles
- Evaluate powerplant designs at nominal points and dynamic responses.



■ gML Oilfield

- Optimisation of oilfield operation
- Different types of wells, multiphase flow, choke valves
- Black-oil and compositional modelling of oil and gas flows.



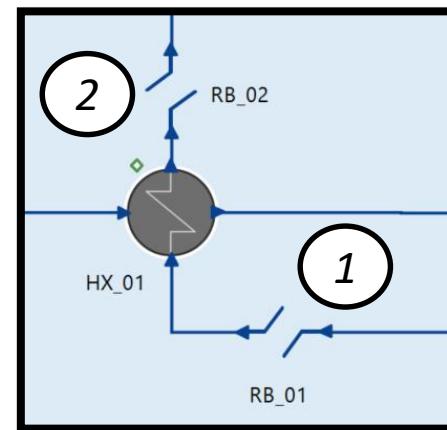
- gPROMS ProcessBuilder 1.2.0 release date
 - Target date: 15th May 2017
- gPROMS ProcessBuilder 1.2.0 beta can already be downloaded by existing customers
 - Contact your account manager for a download link
- Many of the examples and applications shown in this presentation can be accessed on APMF demo pods
- Online resources on MyPSE:
 - ProcessBuilder download page
 - Training videos

- Acknowledgements:
 - Thanks to our ProcessBuilder beta customers, everyone in the PSE Software, Process Model and Materials Technology Groups and to PSE interns.

Thank you



- Automated determination of flowsheet initialisation procedure
 - Determines automatically optimal order of closing recycle breakers on the flowsheet (**NEW in gPROMS ProcessBuilder 1.2.0**)
 - In general, no need to write initialisation procedures, even for complex flowsheets



Section



■ Text

- bullet
- bullet

■ Now

- bullet

■ Level 1

- Level 2

- Level 3

■ Level 1

- Level 2

- Level 3

| | Heading | Heading |
|-----|---------|---------|
| Row | x | y |
| Row | x | y |

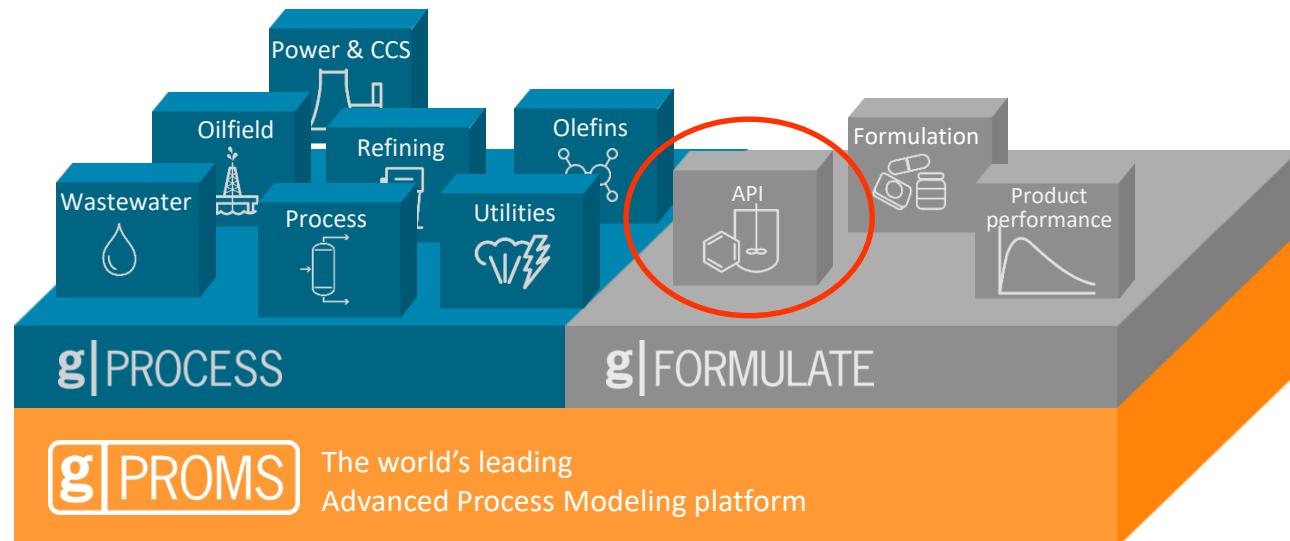
Thank you



The gPROMS software suite – 2017



Platform Environments Libraries



Efficient software development & maintenance

A single powerful software platform
serving diverse sectors
via high-value applications

Platform functionality

Process modelling

- Equation-oriented solution power
- Custom model construction
- Steady-state and dynamic simulation and optimisation
- Advanced parameter estimation
- Powerful dynamic and mixed-integer optimisation
- Global system analysis
- High-performance computing

Materials modelling

- Molecular & ionic species
- Complex species & mixtures
- Gas, liquid, solid phases
- Phase & reaction equilibrium



Logos and product names



Corporate



gPROMS environments

g|PROCESS

gPROMS ProcessBuilder

g|PROCESS

gPROMS ProcessBuilder

g|FORMULATE

gPROMS FormulatedProducts

g|FORMULATE

gPROMS FormulatedProducts

g|MODEL

gPROMS ModelBuilder

g|MODEL

gPROMS ModelBuilder

g|SAFT

gPROMS SAFT

g|SAFT

gPROMS SAFT



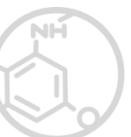
Internal or specialist products

g|FUELCELL

g|FUELCELL

g|FLARE

g|FLARE



MISSION

“define, develop and drive the adoption of next-generation modelling technology, methodologies and workflows throughout the process industries”



Royal Academy MacRobert Award for Engineering Innovation
UK's highest engineering award
Previous winners include: Microsoft, IBM, Johnson Matthey, Rolls-Royce, BP



Oil & Gas

Upstream, Midstream, LNG



Chemicals, Petrochem & Refining

Refining, GTL, Olefins, Intermediates & Derivatives, Polymers, Bulk, Metals



Formulated Products

Pharmaceuticals, Food, Personal & Home Care, Speciality Chemicals



Energy & Environment

Power, Water, CCS



Fuel Cells & Batteries

High-fidelity component and system models

