



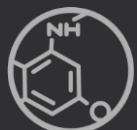
ADVANCED PROCESS MODELLING FORUM

22-23 APRIL 2015

gPROMS ProcessBuilder v1.0

What's in it?

Maarten Nauta – Principal Consultant

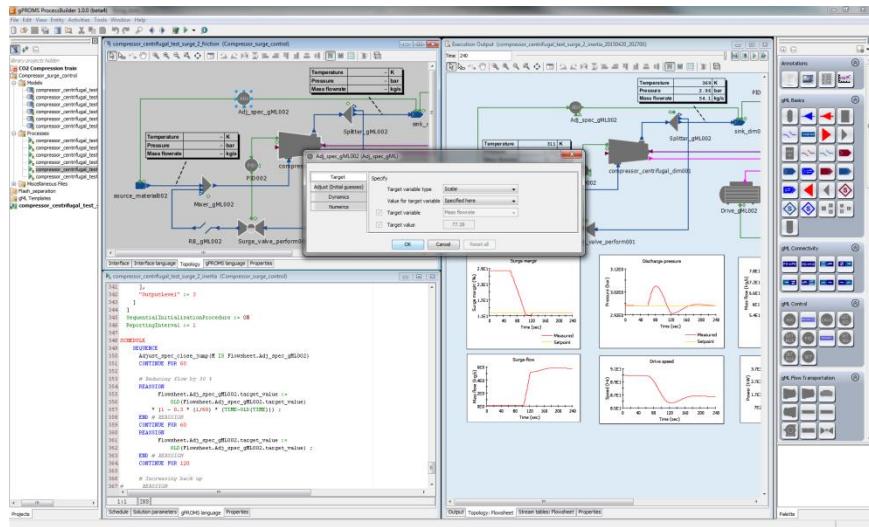


1. Model libraries

- unit operation MODELS
- associated TASKs, Foreign Objects,...
- documentation

2. Physical properties

- Multiflash + DIPPR databank
- gSAFT
 - SAFT-VR SW + SAFT- γ Mie databanks
 - Custom Databank Management



3. Workflow guides

4. Demonstration examples

5. Training courses

- I. Steady-state flowsheet modelling & optimisation in gPROMS ProcessBuilder (1-day)
- II. Developing custom unit operation models for gPROMS ProcessBuilder (3-day)
- III. Dynamic flowsheet modelling in gPROMS ProcessBuilder (1-day)

gPROMS ProcessBuilder v1.0

Demo #1: What does it look like?



The screenshot displays the gPROMS ProcessBuilder 1.0.0 (beta4) interface. On the left, the project tree shows a 'CO2 Compression train' with multiple 'compressor_centrifugal_test' models. The main workspace contains two windows: 'compressor_centrifugal_test_surge_2_friction (Compressor_surge_control)' and 'Execution Output (compressor_centrifugal_test_surge_2_inertia_20150420_202700)'. The flowsheet diagram in the first window illustrates a control loop for a compressor. It includes a source material node, a mixer, a PID controller (PID 002), a compressor, a splitter, and a sink. A dialog box titled 'Adj_spec_gML002 (Adj_spec_gML)' is open, showing settings for adjusting initial guesses, dynamics, or numerics. The second window shows the execution output with real-time data plots for surge margin, discharge pressure, surge flow, and drive speed over a 240-second period. The right side of the interface features toolbars for annotations, gML basics, connectivity, control, and flow transportation, along with a properties palette.



gPROMS ProcessBuilder v1.0

Model libraries



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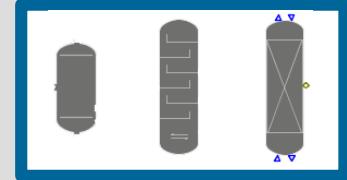
1. gML:Separations – Fluid-Fluid

- Flash drum
- Decanter
- 3-phase separator
- Distillation column (tray, equilibrium)
- Distillation column (packed-bed, HETP)
- Column section (tray, equilibrium)
- Absorption column (packed-bed, 1D/2D rate-based)

2. gML:Separations – Adsorption*

- Adsorption bed (axial+radial flow)
- Scheduler for periodic processes (PSA, TSA)
- Scheduler for self-interacting bed (SiB)

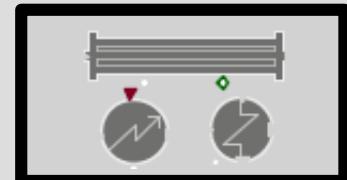
Separation



Reaction



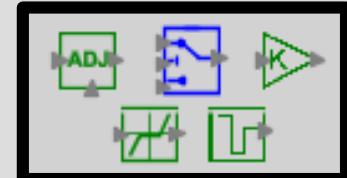
Heat exchange



Flow transportation



Instrumentation & control



* Unique in general process simulation tools

gPROMS ProcessBuilder v1.0

Model libraries – Reaction



3. gML:Reaction

Conversion reactor

Gibbs reactor

CSTR, single and two phase (kinetic & equilibrium reactions)

PFR (kinetic & equilibrium reactions)

Reaction mechanisms

- Power-law
- Langmuir-Hinshelwood
- User-specified

4. AML:Fixed-Bed Catalytic Reactor*

(axial & radial flow configurations)

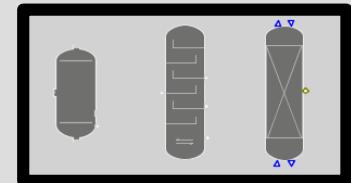
Fixed-bed catalytic reactor (1D)

Fixed-bed catalytic reactor (1D + intra-particle)

Fixed-bed catalytic reactor (2D)

Fixed-bed catalytic reactor (2D + intra-particle)

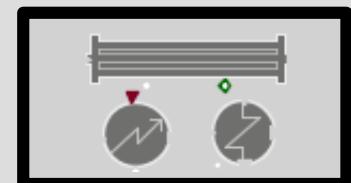
Separation



Reaction



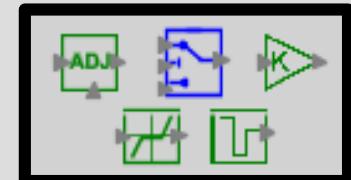
Heat exchange



Flow
transportation



Instrumentation
& control



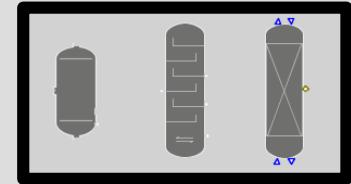
5. gML:Heat Exchange

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

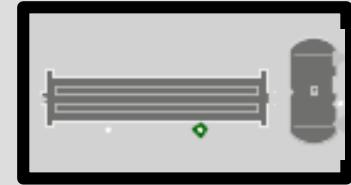
6. gML:Flow Transportation

- Pipe (single phase)
- Pump
- Valve
- Compressor - Centrifugal
- Compressor - Reciprocating
- Expander
- Shaft
- Electric drive

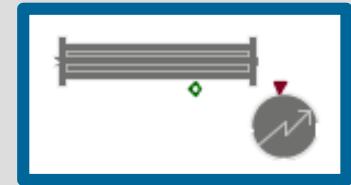
Separation



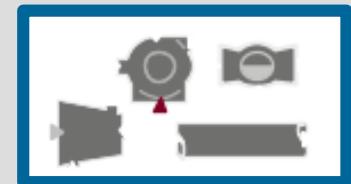
Reaction



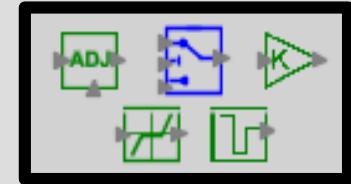
Heat exchange



Flow
transportation



Instrumentation
& control



7. gML:Signal

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

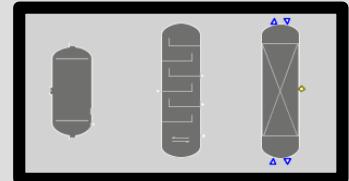
Data

- Lookup table

Logic programming

- Special Ordered Set (SOS1)

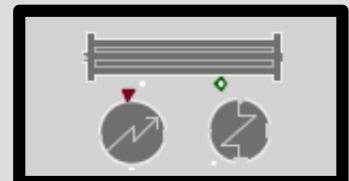
Separation



Reaction



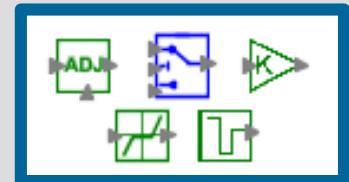
Heat exchange



Flow transportation



Instrumentation & control





gPROMS ProcessBuilder v1.0 Workflow

■ How to...

- ...specify process materials
- ...build flowsheets
- ...trade off degrees of freedom
- ...close recycles
- ...switch from design to rating mode
- ...switch from steady-state to dynamic mode
- ...troubleshoot problems
- ...build your own models
- ...configure cyclic processes

Switch from steady-state to dynamic mode

gML Library Documentation v1.0

Troubleshooting

gML Library Documentation v1.0

Custom modeling

gML Library Documentation v1.0

Trading off specifications

gML Library Documentation v1.0

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gML Library Documentation v1.0

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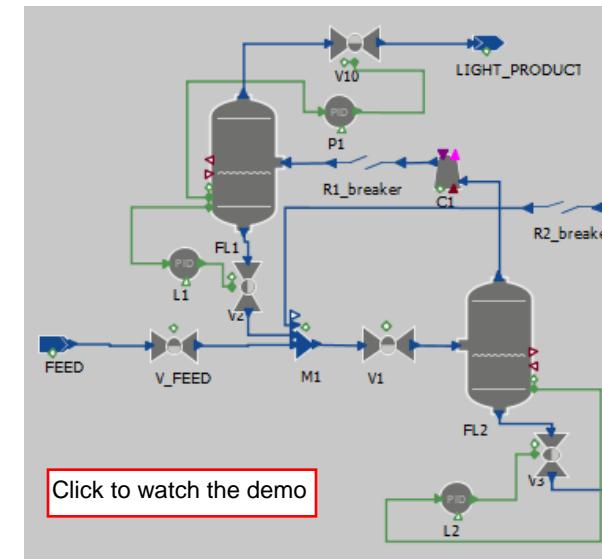
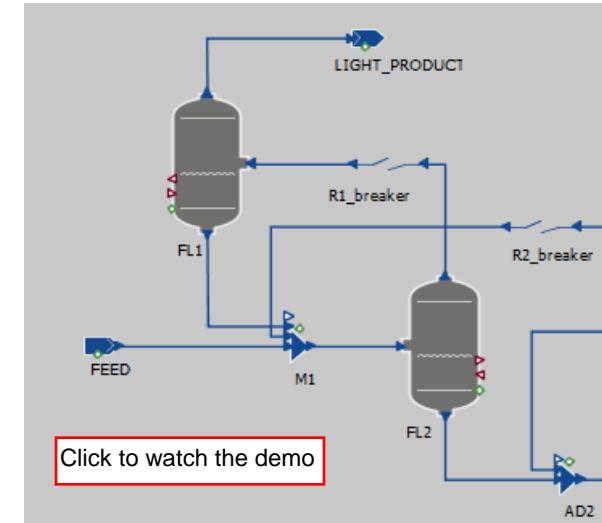
Switching

- ...from design to rating
- ...from steady-state to dynamics

STEPS

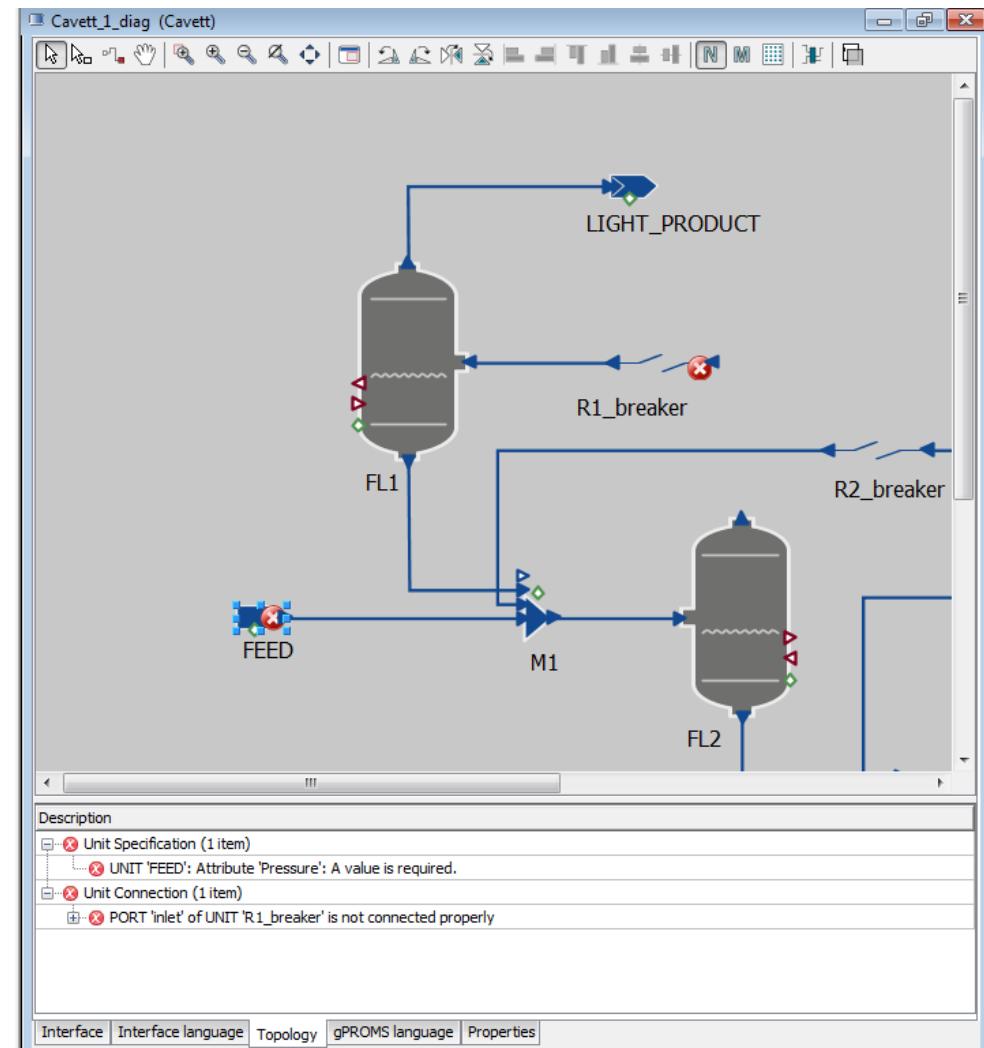
1. Heat and material balance
2. Equipment sizing
3. Dynamic simulation

Dynamic simulation can be started from the original steady-state of the heat and material balance



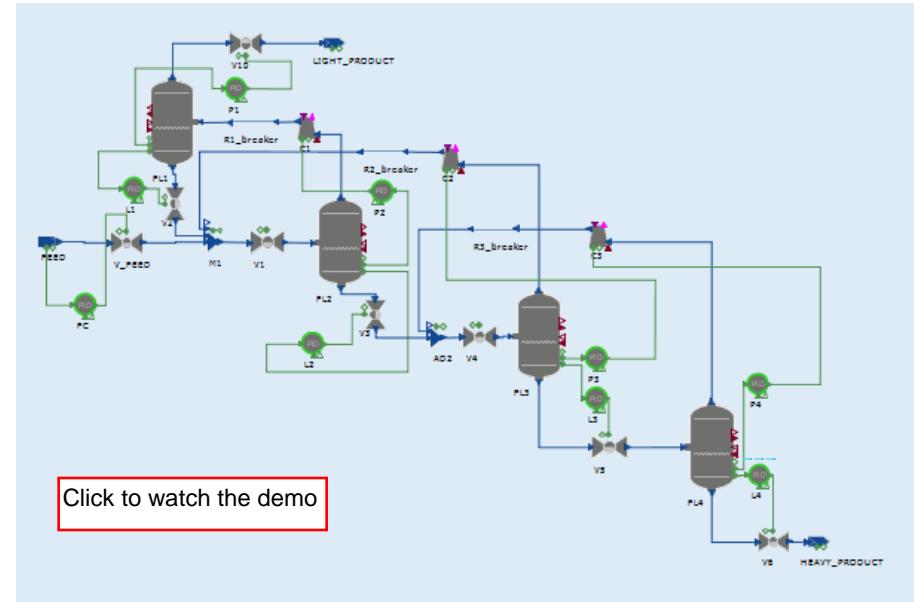
■ During flowsheet construction

- Preventing common flowsheeting mistakes
- Ensuring that essential input information is entered and valid



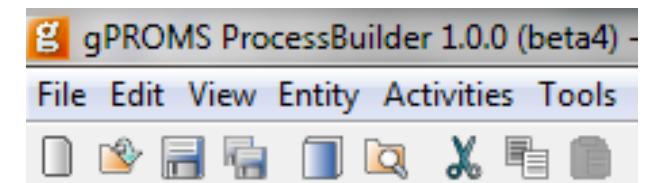
■ During simulation

- Notify user of operation outside of normal equipment operating range
- Vessels running empty, wrong phase in equipment, actuators running into saturation, compressors running into surge, flow-reversal etc.



gPROMS ProcessBuilder v1.0

Demonstration examples



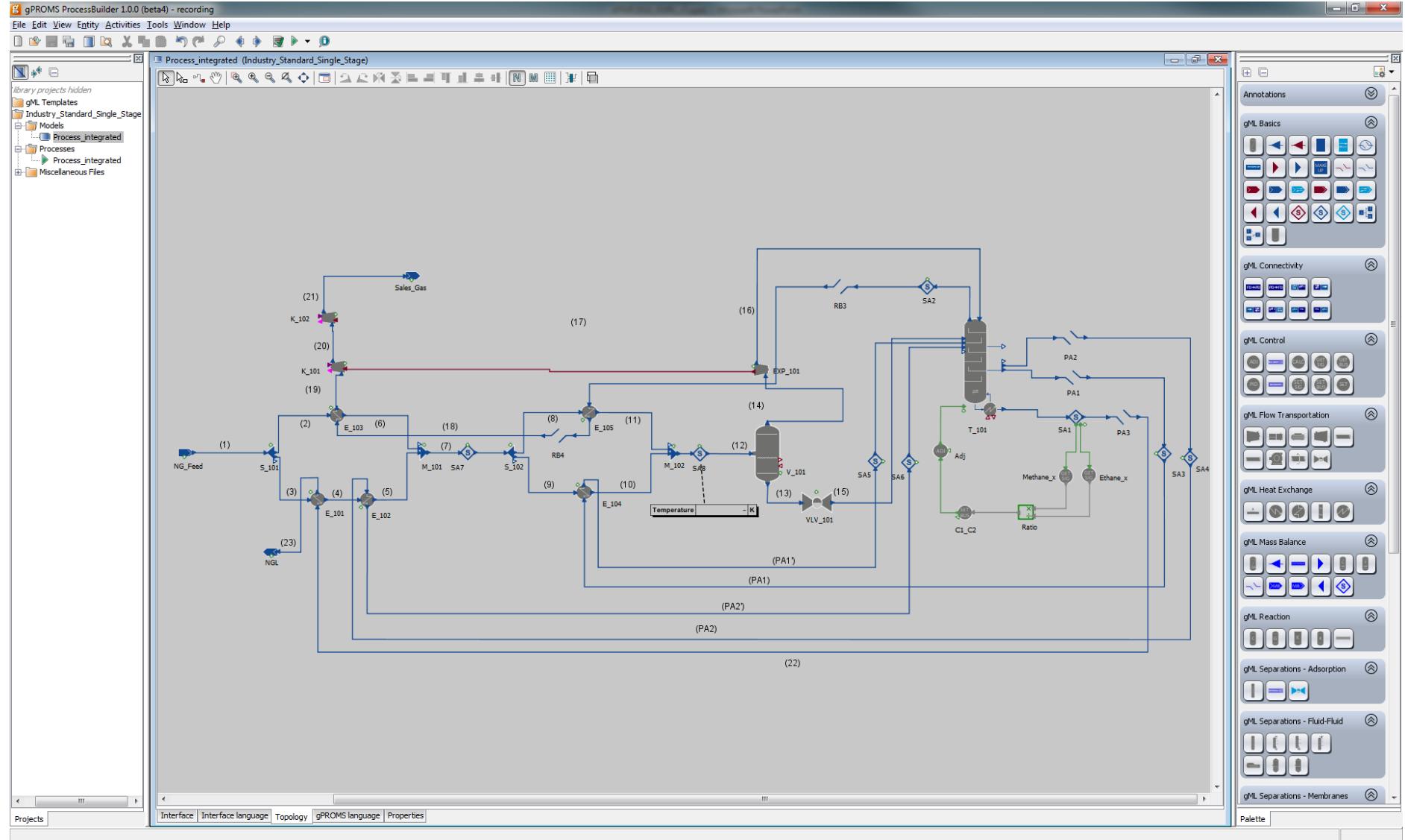
Demonstration examples

Example*	Process
CO2_compression_train	CO2 compression train for
Compressor_surge_control	Compressor surge control using a surge valve for CO2 compression
MP2_MDP_plant	Polymerisation plant
ASU	Air separation unit producing nitrogen, oxygen and argon
Industry_standard_single_stage	Natural Gas Liquids (NGL) recovery using the industry standard single stage process
LNG_plant_APX	APX process for natural gas liquefaction
LNG_plant_C3_MR	C3MR process for natural gas liquefaction
Acrylic_acid_reactor	Acrylic acid reactor for the production for propylene
Methanation_Gibbs_reactor	Gibbs reactor for methanation process
Cavett	Classic test problem for convergence with recycles
HF_H2O_gSAFT	Distillation column seperating hydrogen fluoride and water
PSA_4_4_1	Four-bed PSA process for hydrogen purification

* file included in gPROMS ProcessBuilder installer

Demonstration example #1: Industry_Standard_Single_Stage.gPJ-PB

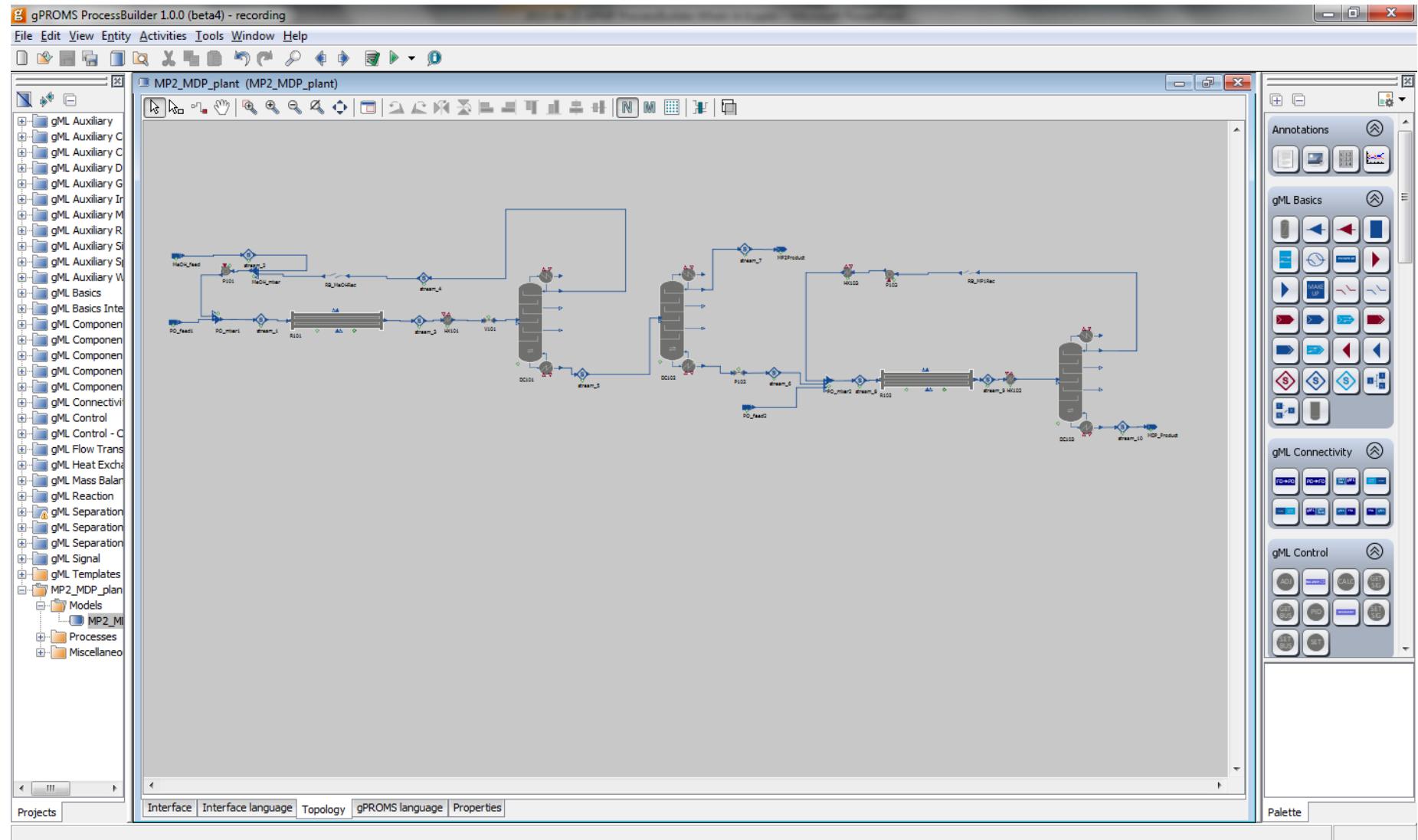
NGL Recovery



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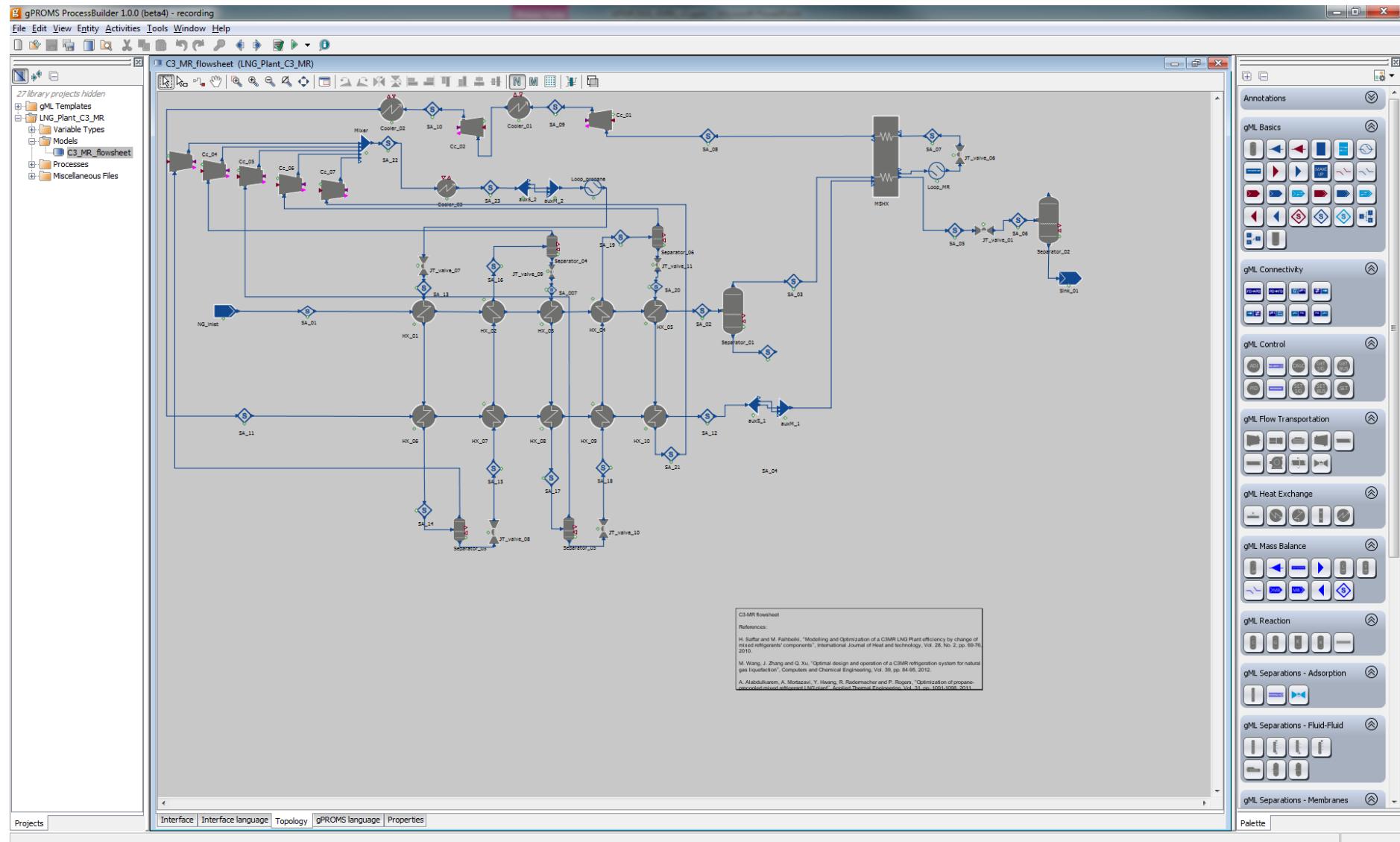
Demonstration example #2: MP2_MDP_plant.gPJ-PB

Pressure-swing adsorption process for H₂ recovery



Demonstration example #3: LNT_Plant_C3_MR.gPJ-PB

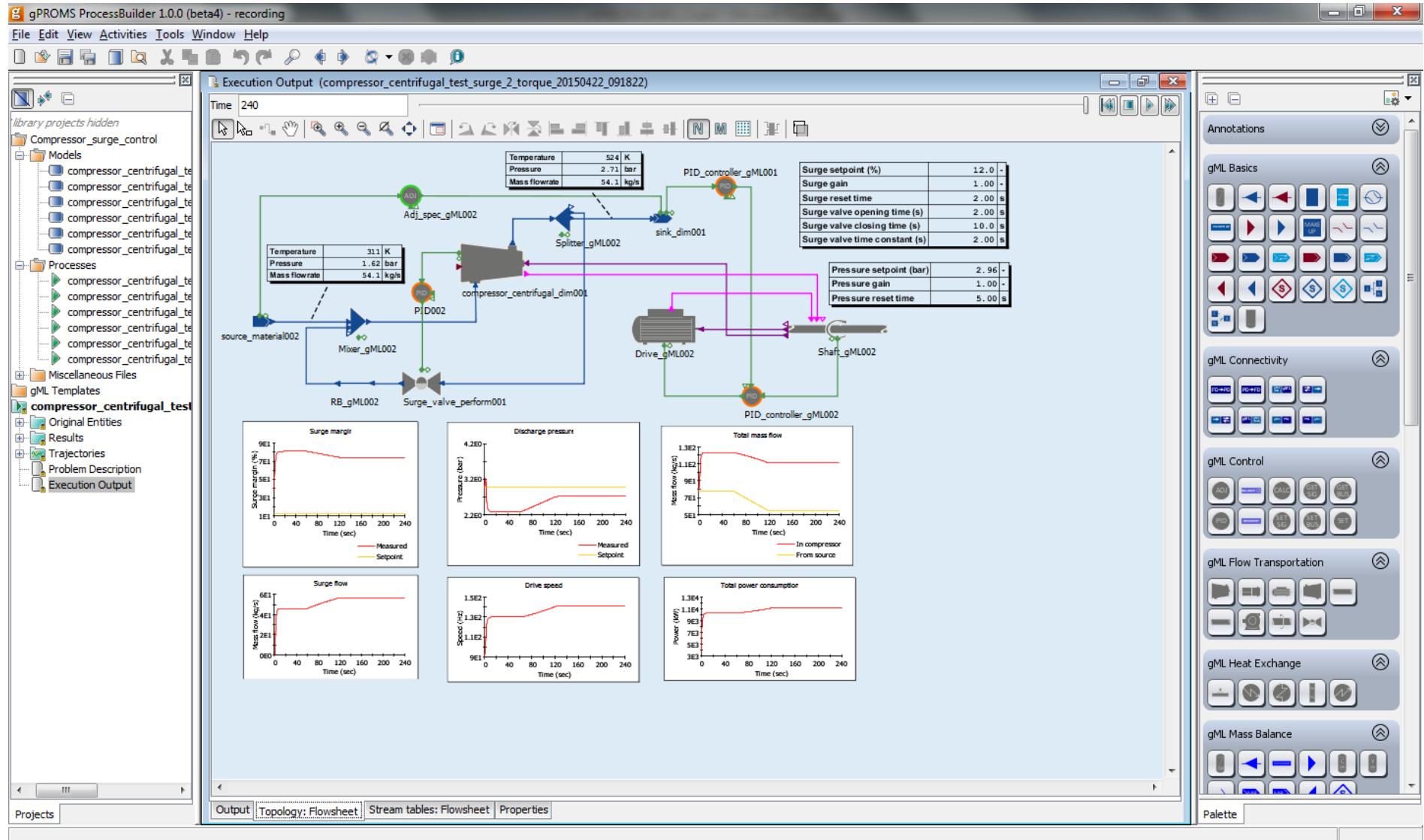
LNG liquefaction



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Demonstration example #4: Compressor_surge_control.gPJ-PB

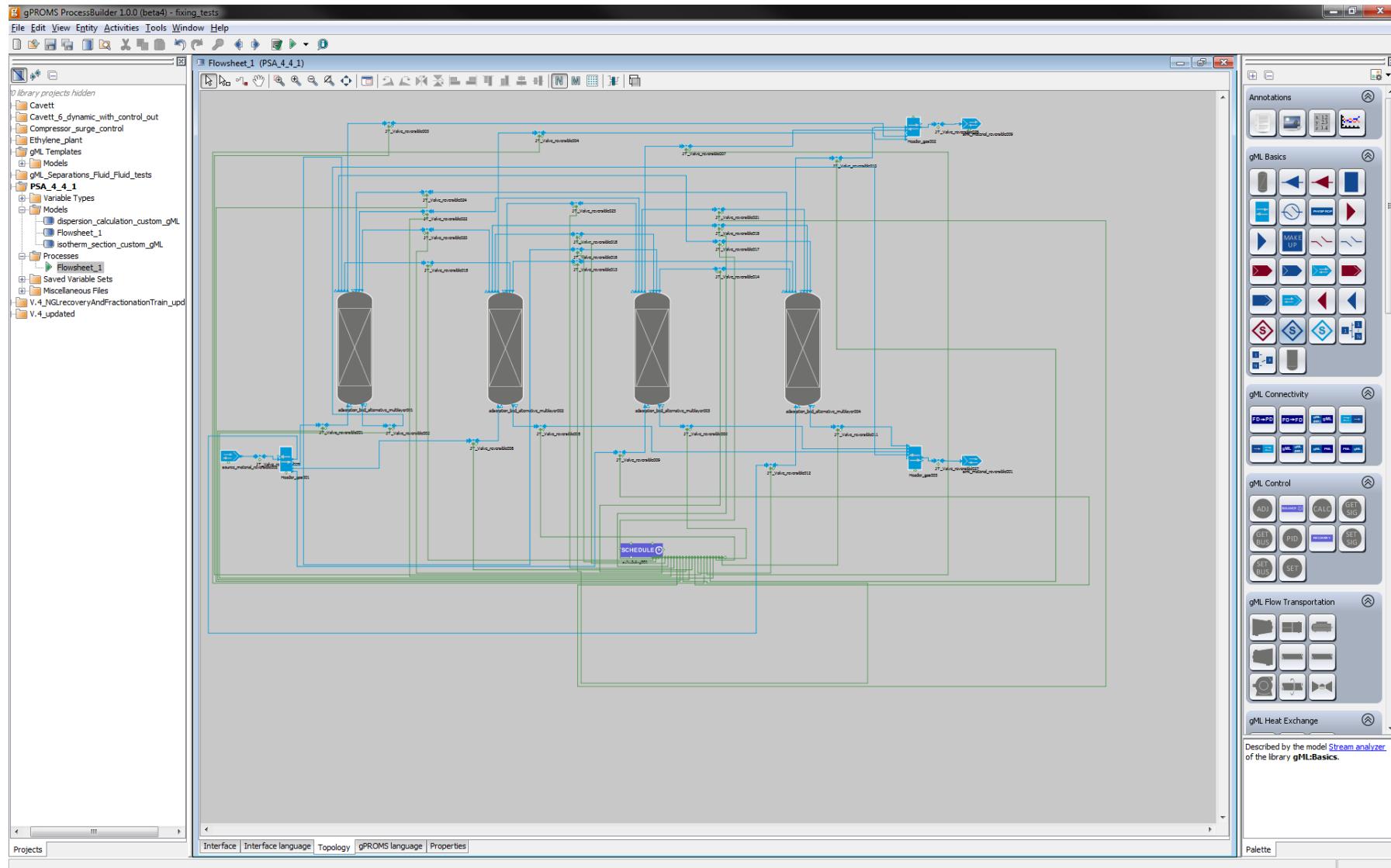
Compressor dynamics



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Demonstration example #5: PSA_4_4_1.gPJ-PB

Pressure-swing adsorption process for H₂ recovery



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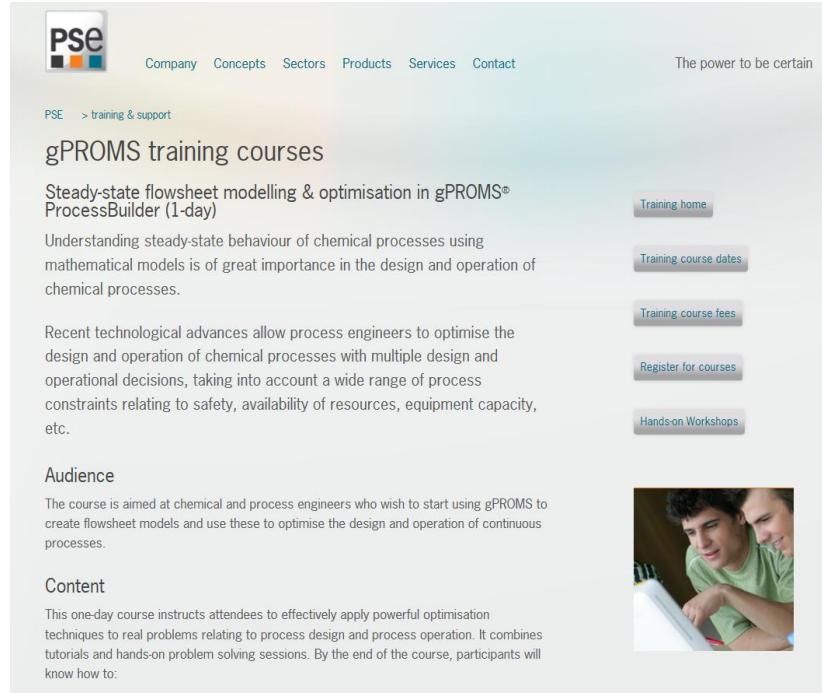


gPROMS ProcessBuilder v1.0 Training courses

I. Steady-state flowsheet modelling & optimisation in gPROMS ProcessBuilder (1-day)

II. Developing custom unit operation models for gPROMS ProcessBuilder (3-day)

III. Dynamic flowsheet modelling in gPROMS ProcessBuilder (1-day)



The screenshot shows the PSE website with the following details:

- PSE Company Concepts Sectors Products Services Contact**
- The power to be certain**
- PSE > training & support**
- gPROMS training courses**
- Steady-state flowsheet modelling & optimisation in gPROMS® ProcessBuilder (1-day)**
- Description:** Understanding steady-state behaviour of chemical processes using mathematical models is of great importance in the design and operation of chemical processes.
- Benefits:** Recent technological advances allow process engineers to optimise the design and operation of chemical processes with multiple design and operational decisions, taking into account a wide range of process constraints relating to safety, availability of resources, equipment capacity, etc.
- Audience:** The course is aimed at chemical and process engineers who wish to start using gPROMS to create flowsheet models and use these to optimise the design and operation of continuous processes.
- Content:** This one-day course instructs attendees to effectively apply powerful optimisation techniques to real problems relating to process design and process operation. It combines tutorials and hands-on problem solving sessions. By the end of the course, participants will know how to:



See PSE website for course schedule

Conclusions

1. Model libraries

- unit operation MODELS
- associated TASKs, Foreign Objects,...
- documentation

2. Physical properties

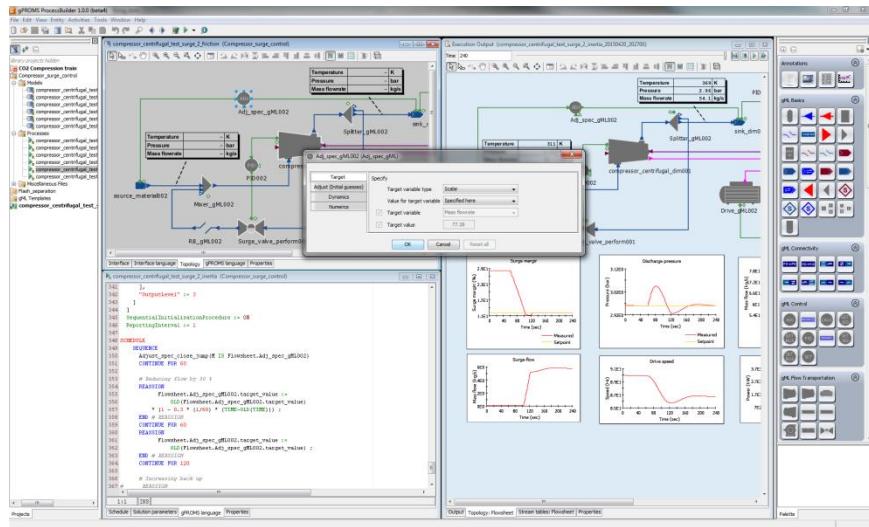
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3. Workflow guides

4. Demonstration examples

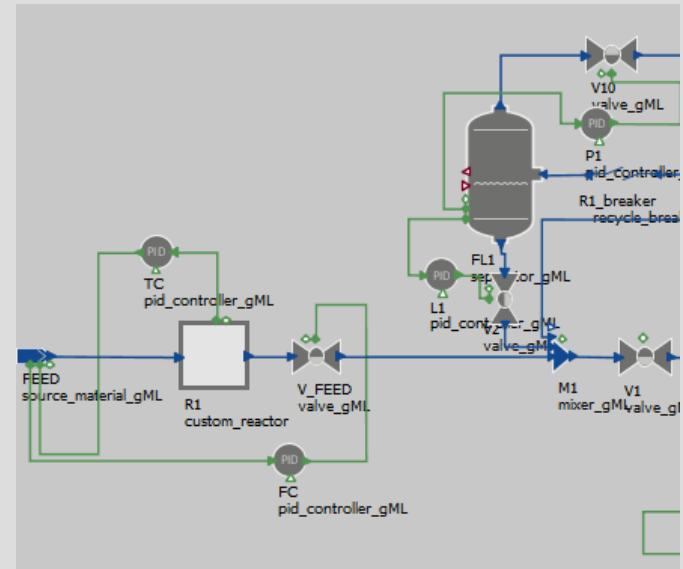
5. Training courses

- I. Steady-state modelling & optimisation in the gPROMS ProcessBuilder
- II. Developing custom unit operation models for the gPROMS ProcessBuilder
- III. Dynamic flowsheet modelling in the gPROMS ProcessBuilder



Planned official release date
15 May 2015

- Code the model in the gPROMS language
 - use standard ProcessBuilder variable & connection types
- Add specification dialogs and initialisation procedures
- For more information, see
 - workflow guide “*Developing custom models for use with gPROMS ProcessBuilder*”
 - Training course



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

■ Introduce custom correlations within standard ProcessBuilder equipment models

- Growing range of custom correlation plugins for standard models
- Start from template for the particular correlation
- Add implemented correlation model to project and select “Custom”

- Kinetic models
- Adsorption isotherm models
- Equipment cost models
- Heat transfer coefficient
- Mass transfer coefficient
- Dispersion coefficient
- Pressure drop relations
- Interfacial area
- Custom physical properties relations

Acknowledgements

- ProcessBuilder team
 - Charles Brand
 - Luis Domingues
 - Maria Viseu
 - Vasco Manacas
 - Nouri Samsatli
 - Christian Schulz
 - Mario Calado
 - Costas Pantelides
- Interns
 - Sara Astilleros
 - Joana Alves
 - Frederico Montes
 - Yera Seok
 -and all previous ones ☺
- Application Engineering
- PSE Consulting group
- Software Technology Group (STG)
- ProcessBuilder advance customers

Thank you

