ADVANCED PROCESS MODELLING FORUM
22–23 APRIL 2015

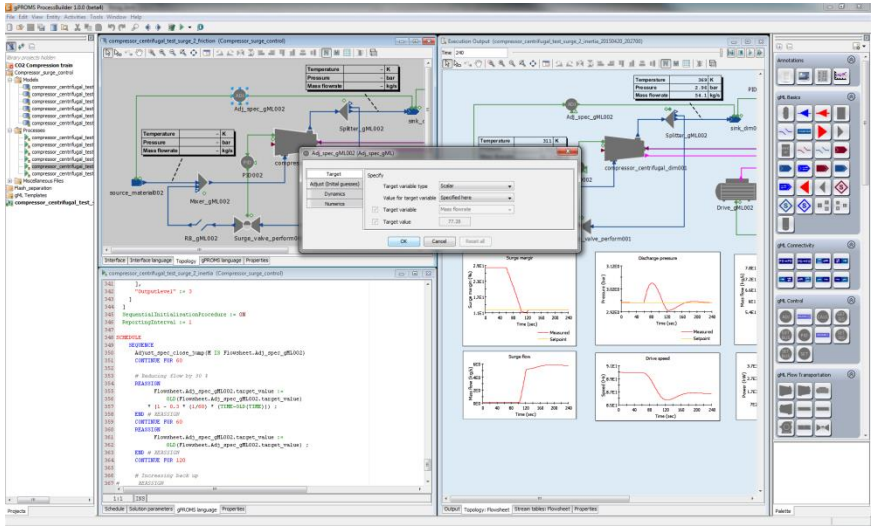
gPROMS ProcessBuilder v1.0

What's in it?

Maarten Nauta – Principal Consultant

gPROMS ProcessBuilder v1.0

Product formulation



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)

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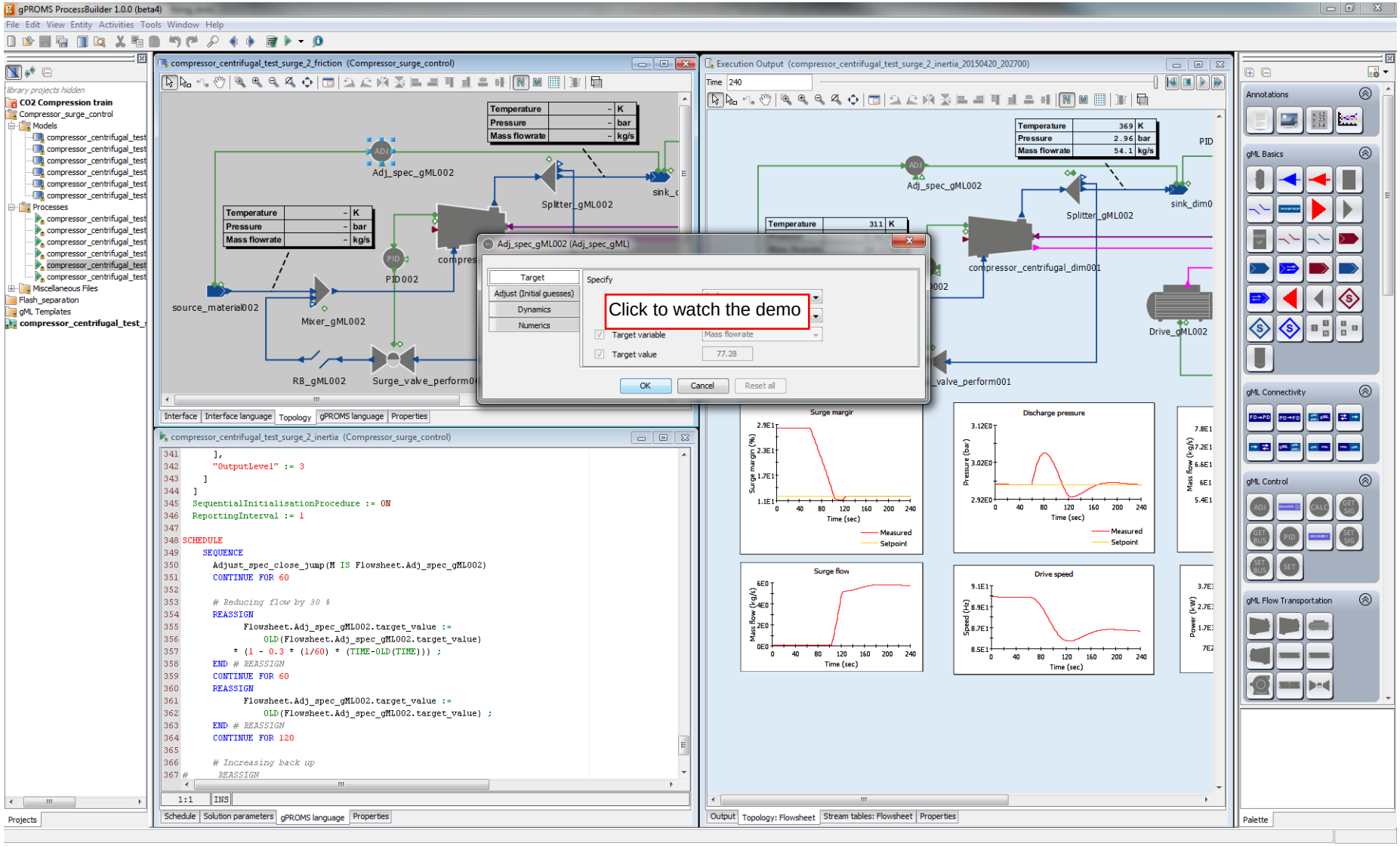
Demo #1: What does it look like?



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Model libraries

Model libraries – Separation

1. gML:Separations – Fluid-Fluid

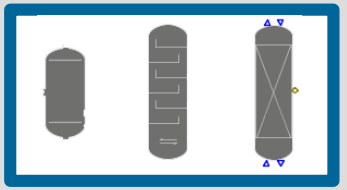
Flash drum
Decanter
3-phase separator
Distillation column (tray, equilibrium)
Distillation column (packed-bed, HETP)
Column section (tray, equilibrium)
Absorption column (packed-bed, 1D/2D rate-based)

2. gML:Separations – Adsorption*

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

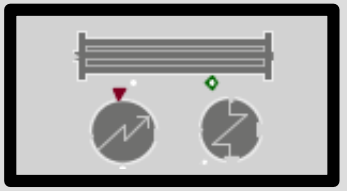
** Unique in general process simulation tools*

Separation



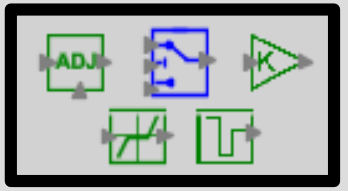
Reaction

Heat exchange



Flow transportation

Instrumentation & control



Model libraries – Reaction

3. gML:Reaction

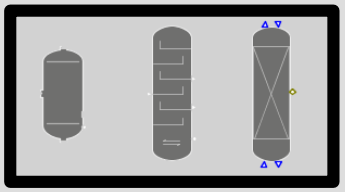
Conversion reactor
Gibbs reactor
CSTR, single and two phase (kinetic & equilibrium reactions)
PFR (kinetic & equilibrium reactions)
Reaction mechanisms ▪ Power-law ▪ Langmuir-Hinshelwood ▪ User-specified

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)

** Unique in general process simulation tools*

Separation



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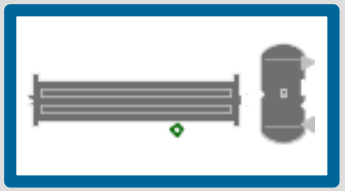

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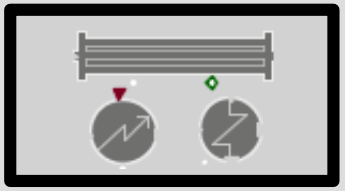
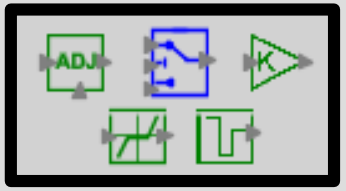


Flow transportation

Instrumentation & control



Model libraries – Heat exchange, flow transportation

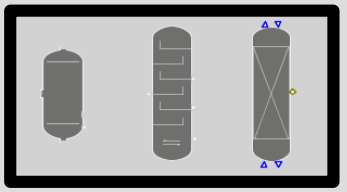
5. gML:Heat Exchange

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

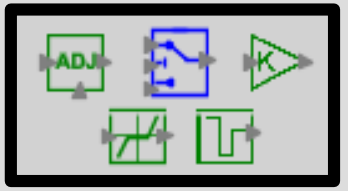


Reaction

Heat exchange

Flow transportation

Instrumentation & control



Model libraries – 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

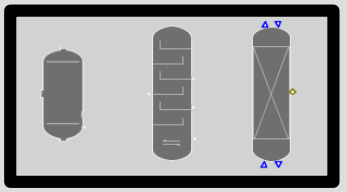
Signal Sources
- Constant, ramp, step signal, function generator, time signal

Signal Sinks
- Display, plot, X-Y plot

Data
- Lookup table

Logic programming
- Special Ordered Set (SOS1)

Separation



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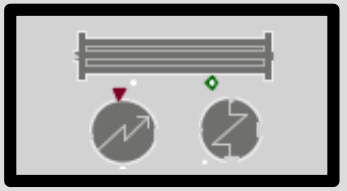
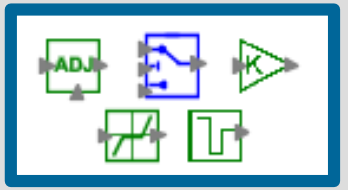


Flow transportation

Instrumentation & control



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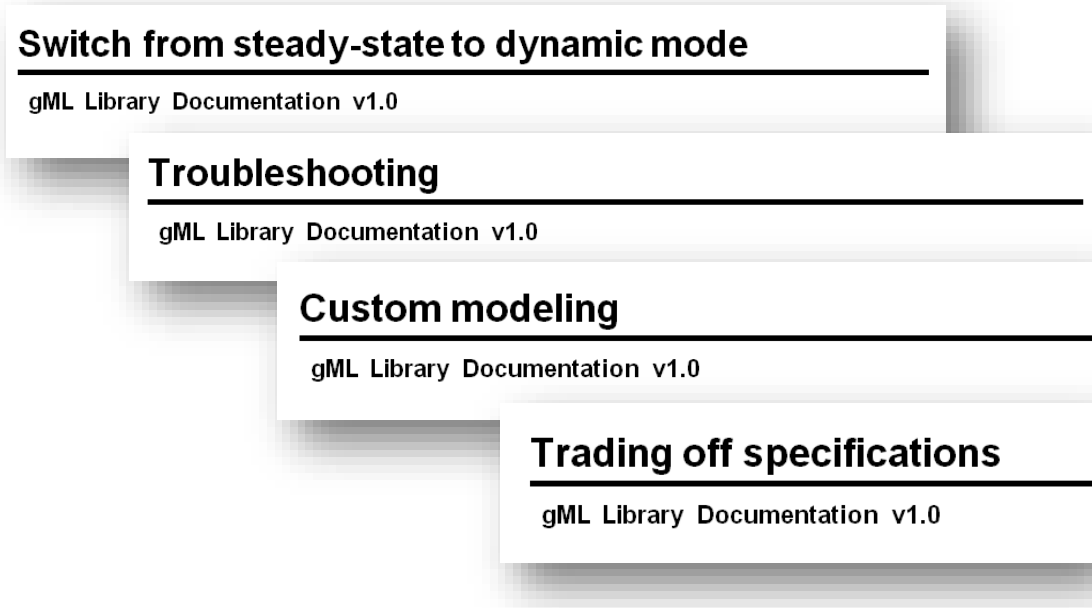
Workflow

Workflow guides

- 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



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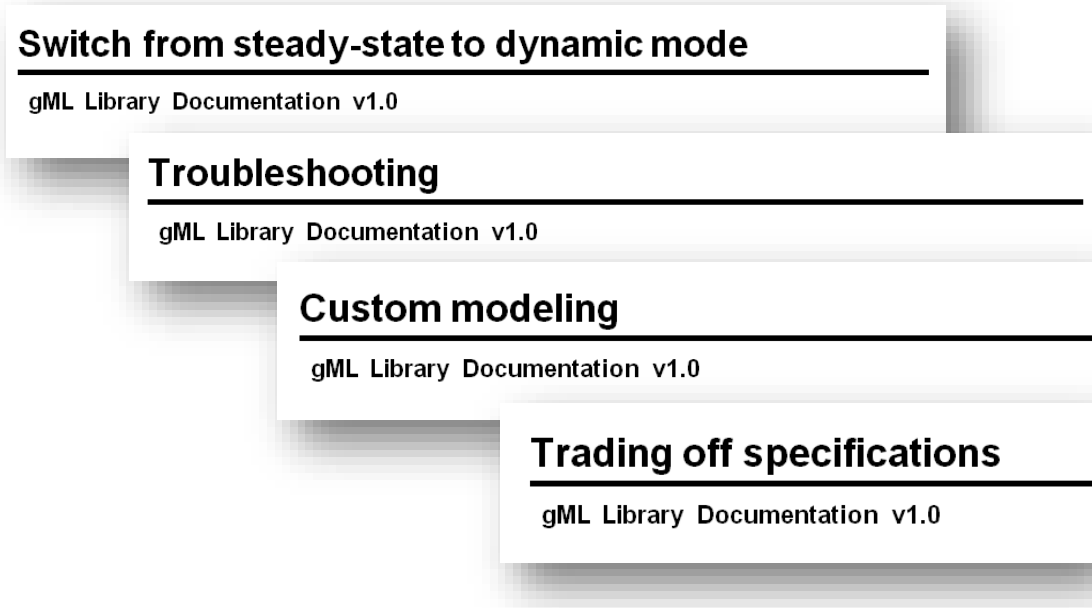


Workflow

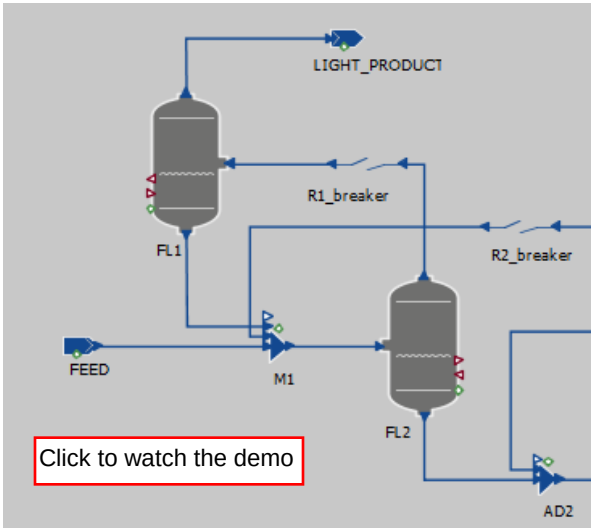
Switching

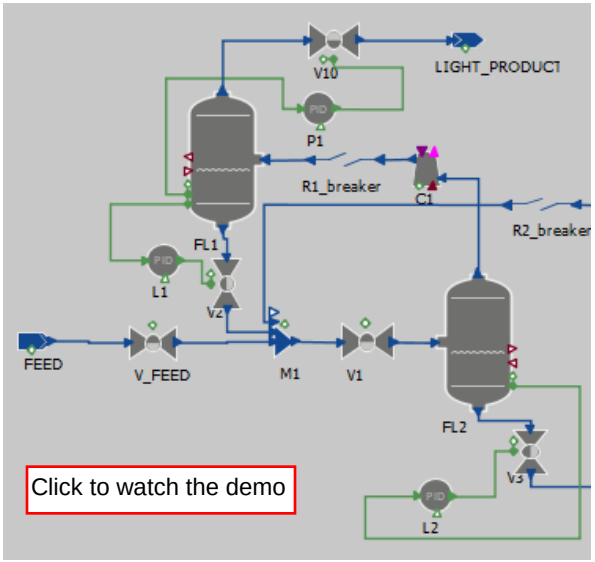
- …from design to rating
- …from steady-state to dynamics

STEPS

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

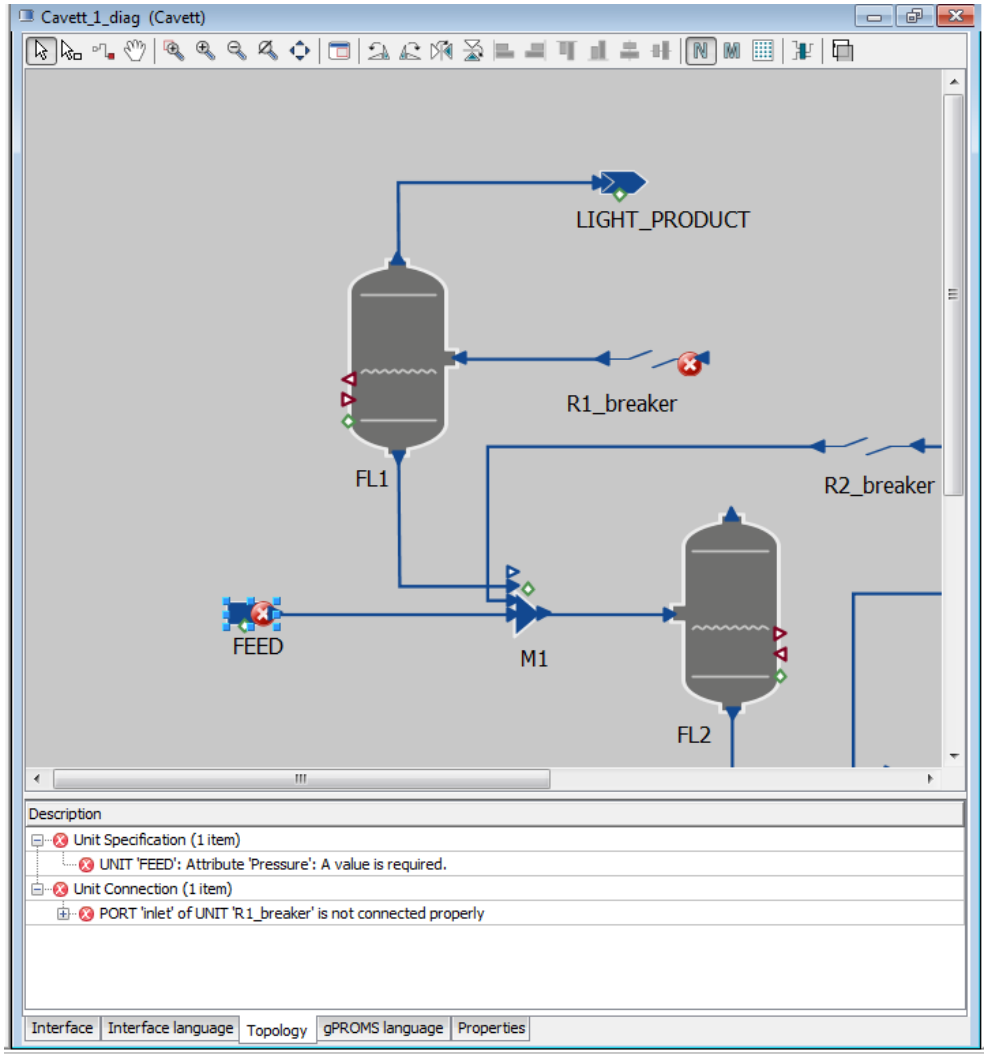
Dynamic simulation can be started from the original steady-state of the heat and material balance





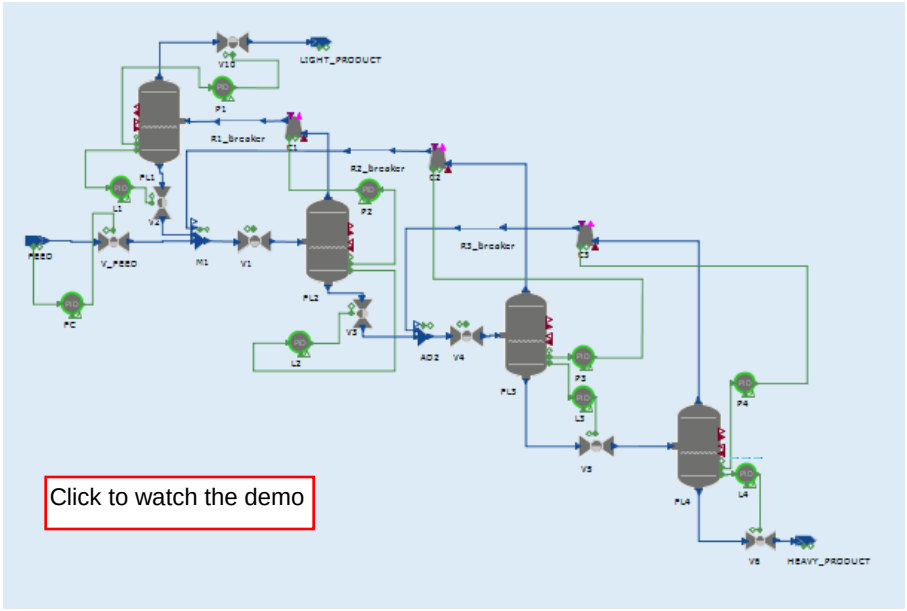
Workflow - Troubleshooting

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



Workflow - Troubleshooting

- 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.



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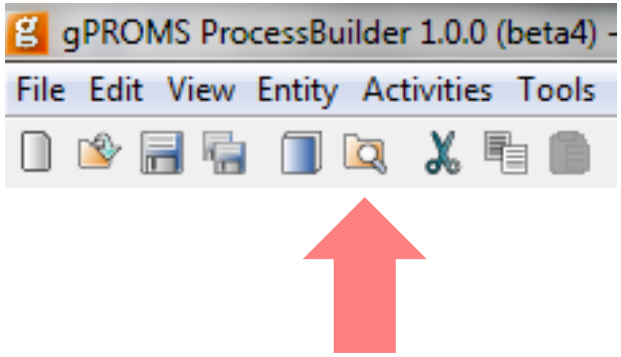
Demonstration examples



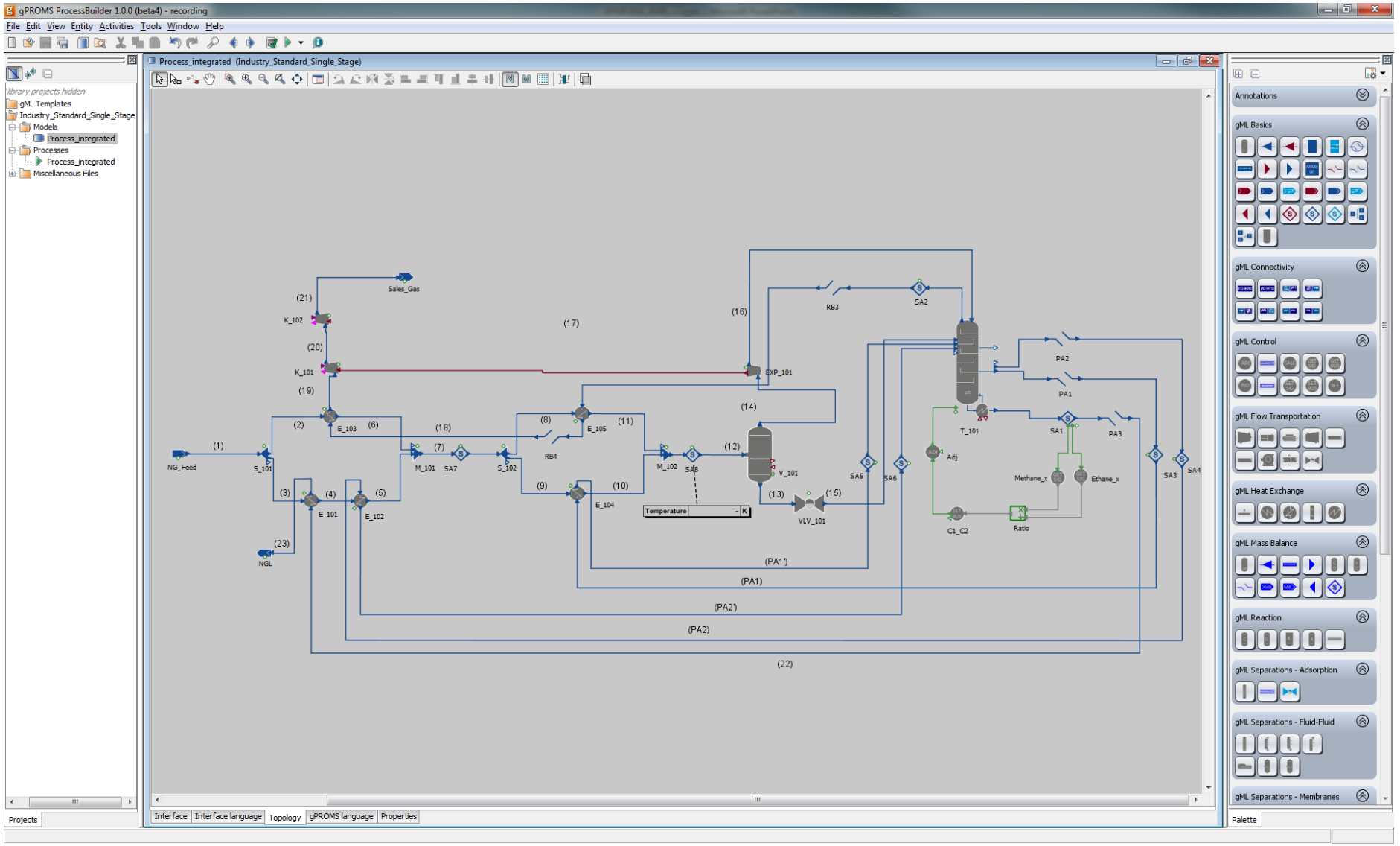
Demonstration examples

Example*	Process
CO2_compression_train	CO2 compression train for
Compressor_surge_control	Compressor surge control using a surge valve for C02 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_H20_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

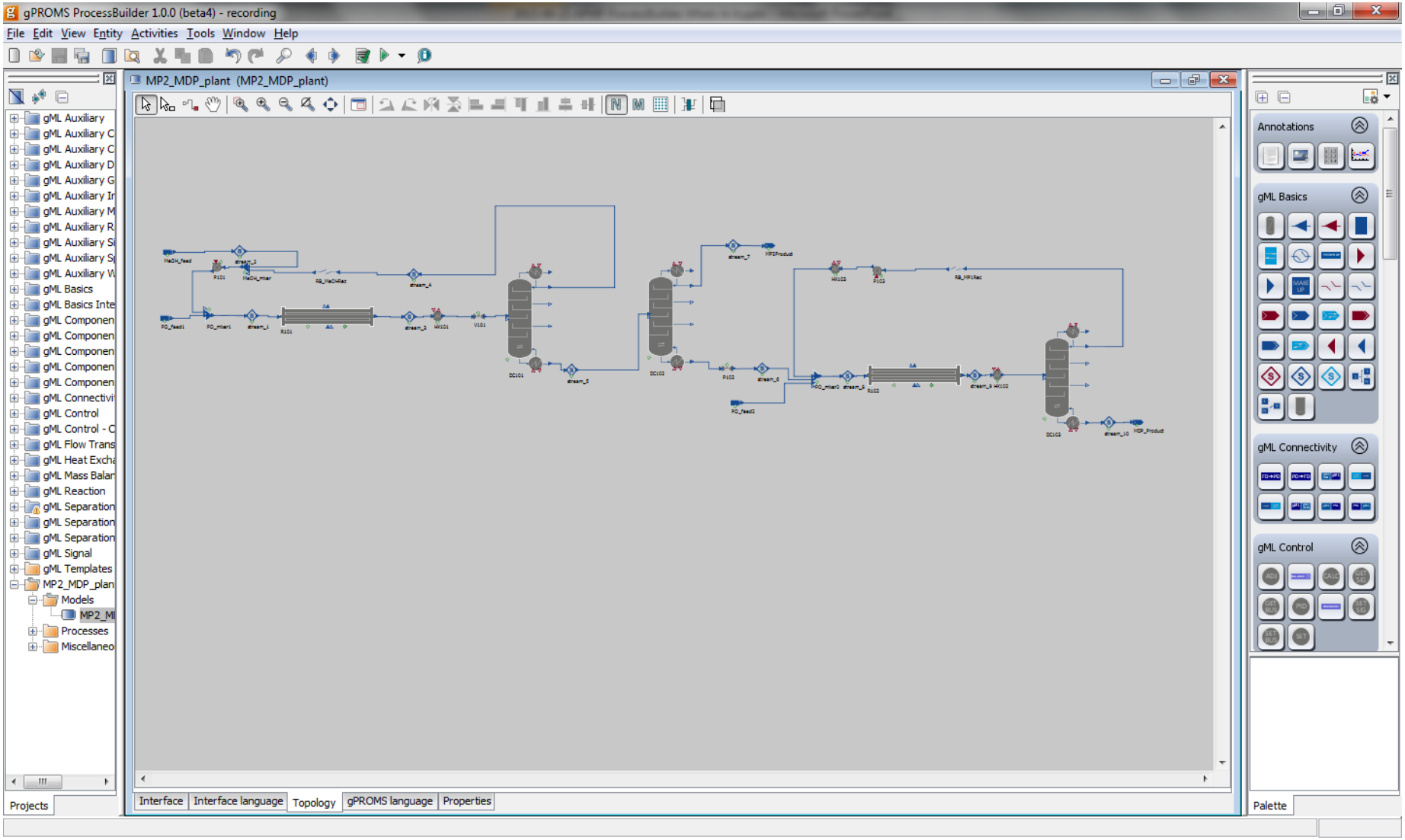
Demonstration example #1: Industry_Standard_Single_Stage.gPJ-PB

NGL Recovery



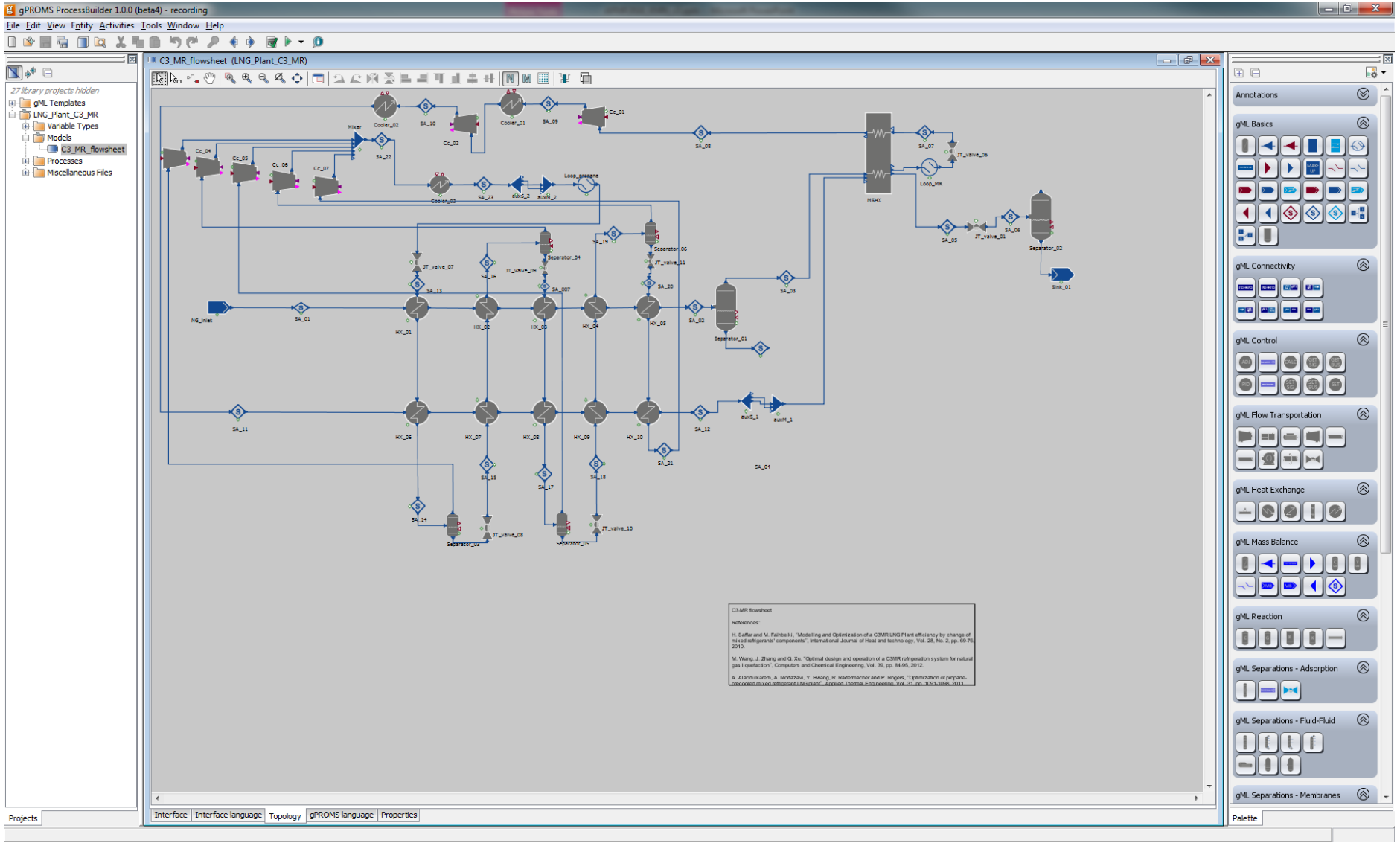
Demonstration example #2: MP2_MDP_plant.gPJ-PB

Pressure-swing adsorption process for H_2 recovery



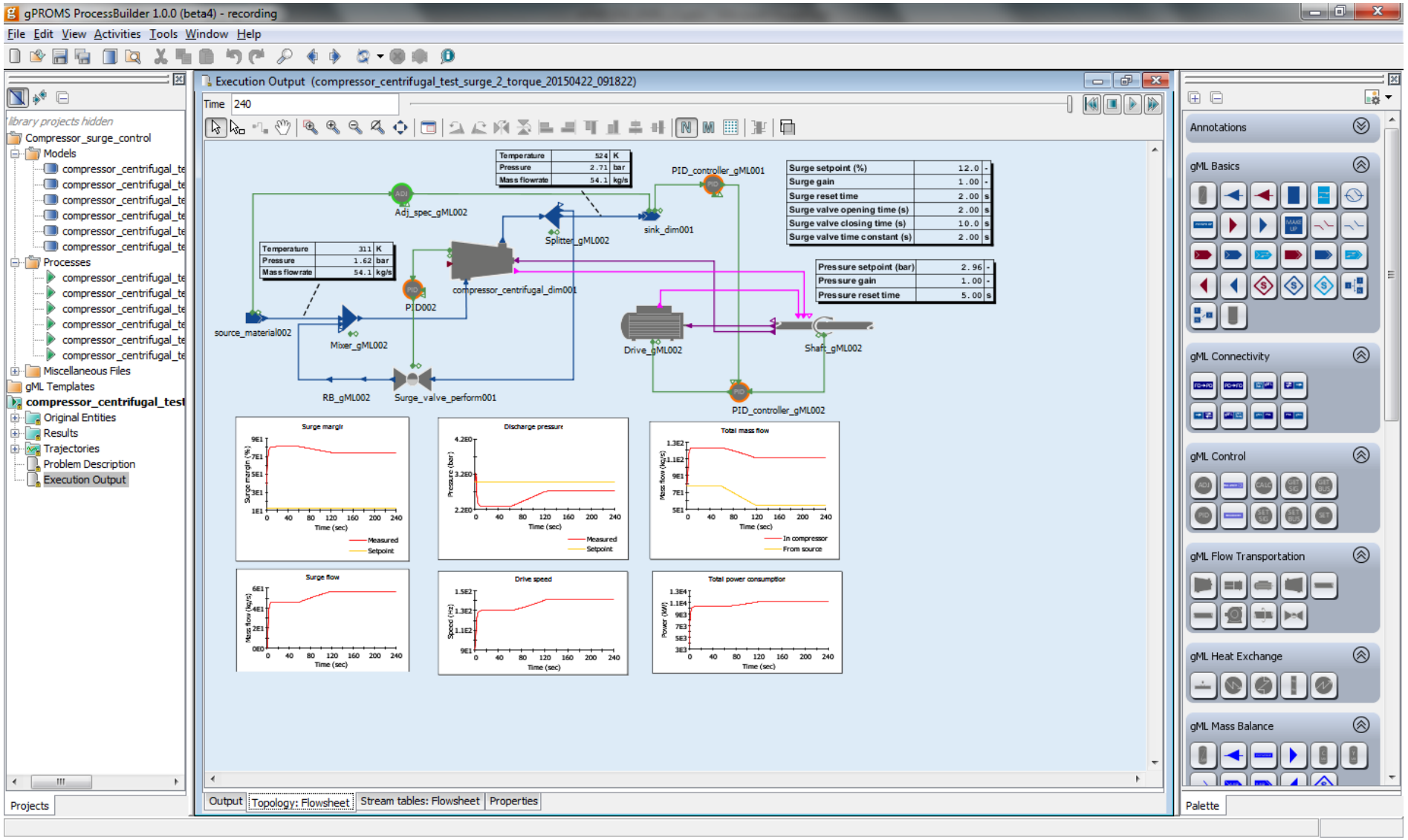
Demonstration example #3: LNT_Plant_C3_MR.gPJ-PB

LNG liquefaction



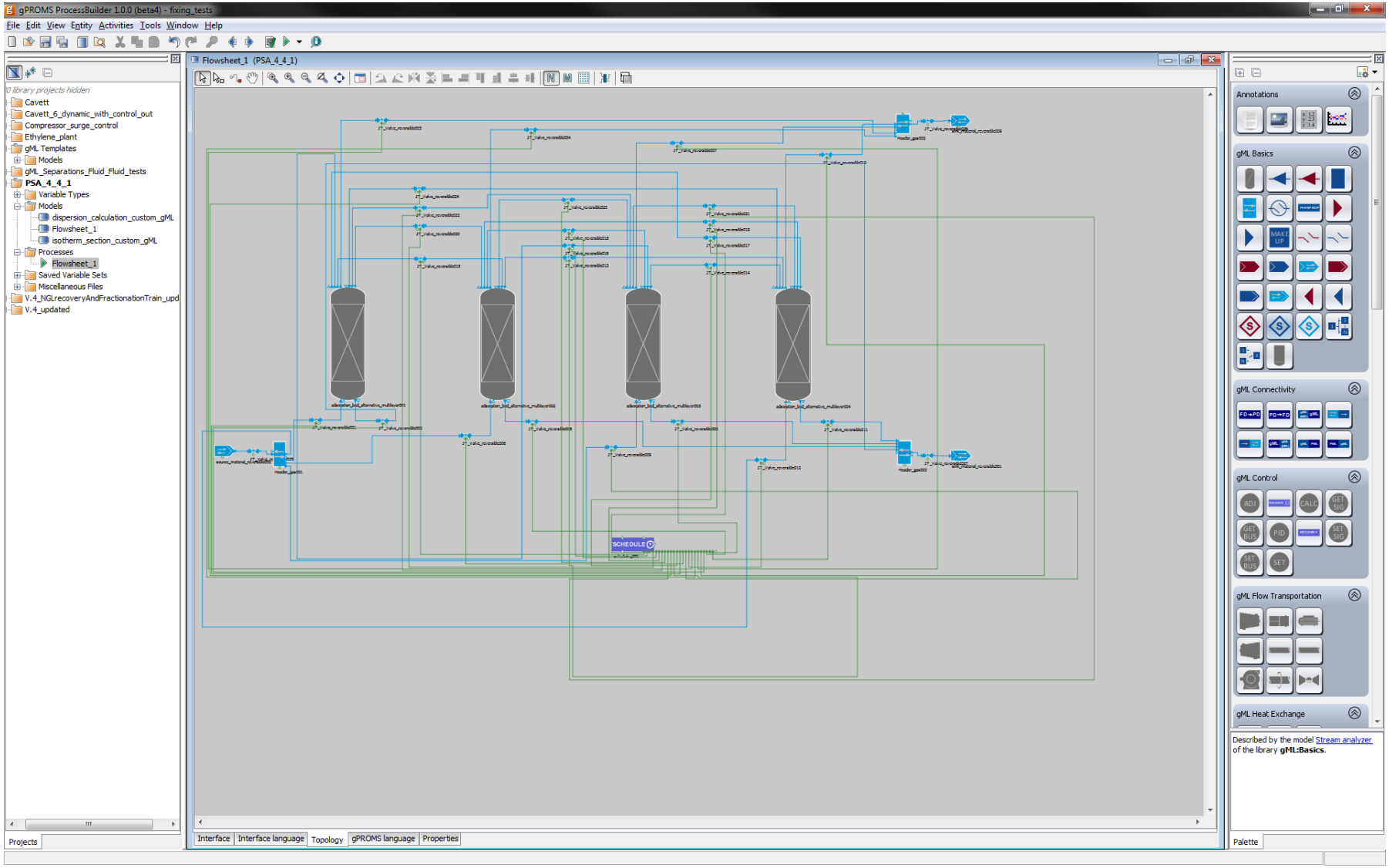
Demonstration example #4: Compressor_surge_control.gPJ-PB

Compressor dynamics



Demonstration example #5: PSA_4_4_1.gPJ-PB

Pressure-swing adsorption process for H_2 recovery



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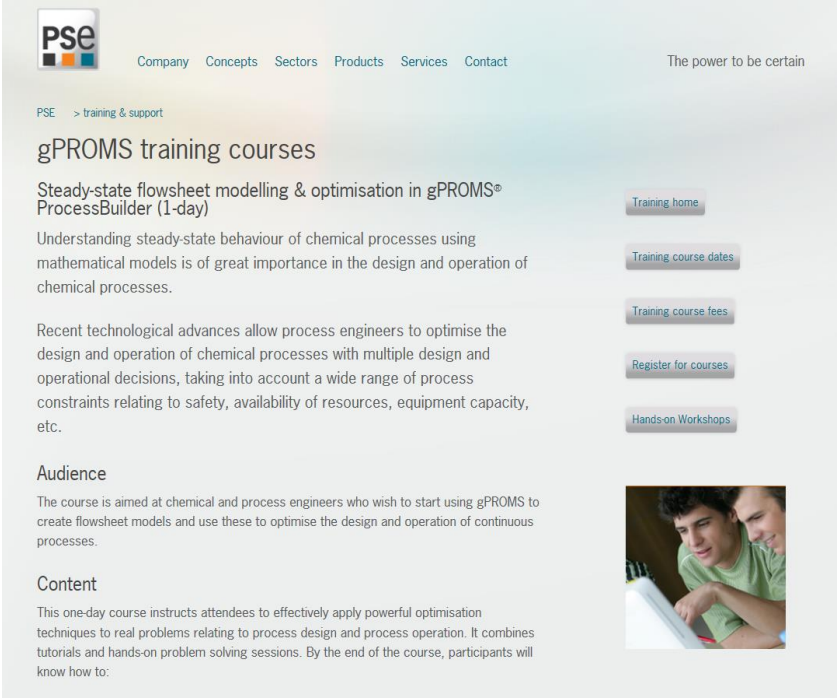
Training courses

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)



See PSE website for course schedule

Conclusions

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Product formulation

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2. **Physical properties**
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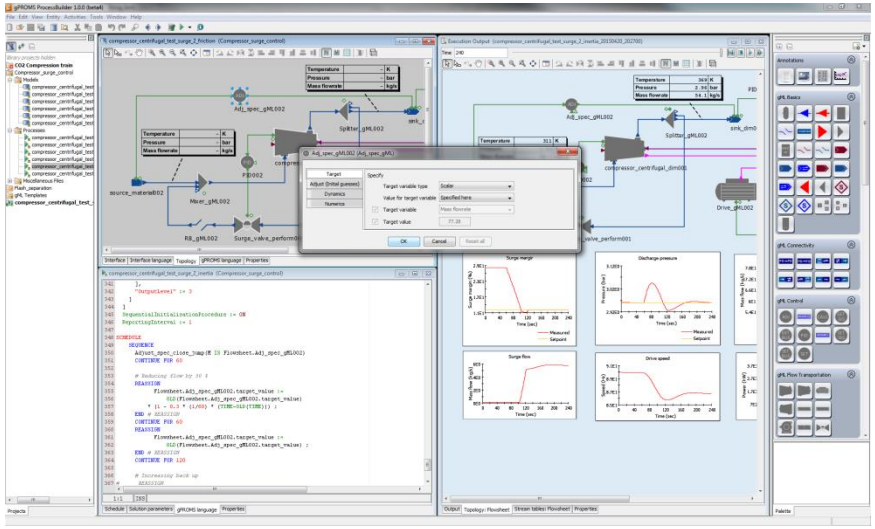
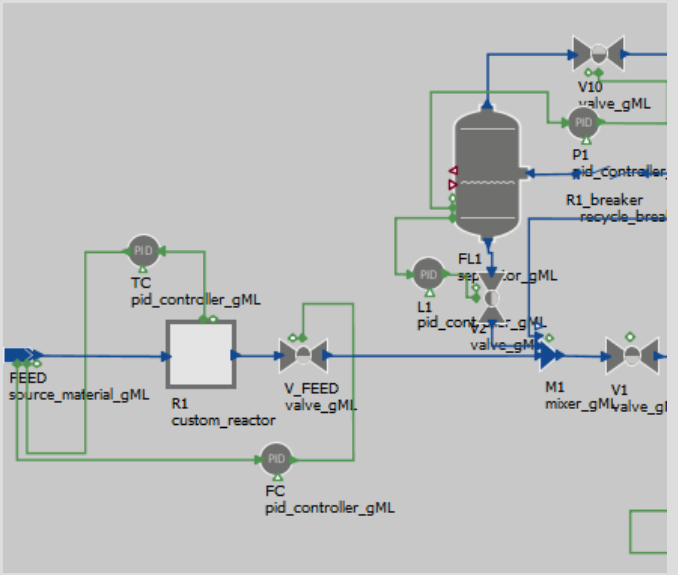


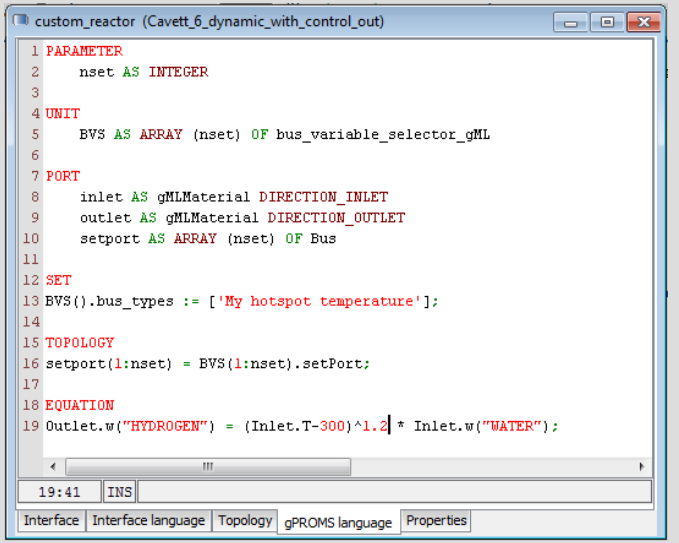
Planned official release date
15 May 2015

gPROMS ProcessBuilder v1.0

Extensibility: using your own models

- 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





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Extensibility: Customising standard models

- 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