ADVANCED PROCESS MODELLING FORUM
LONDON
20–21 APRIL 2016

gPROMS ProcessBuilder v1.1

Full dynamic process modelling

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gPROMS

PSE's motivation for developing gPROMS ProcessBuilder

Aim to provide

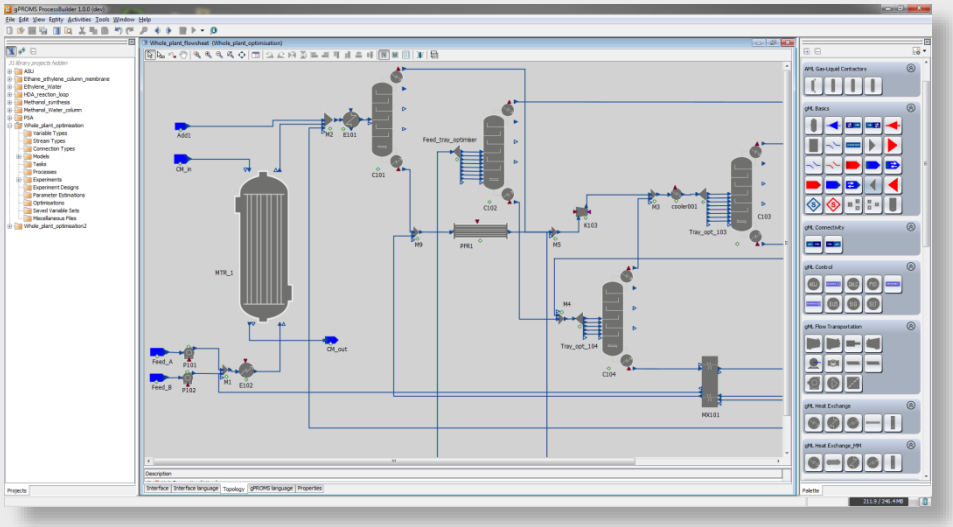
1. All the power of the gPROMS platform, first-principles modelling
   - *without the need to write every model*
2. Custom modelling capability *where necessary*
   - Plus sophisticated libraries of common unit operations
   - ➔ maximize competitive advantage
3. Optimisation power
   - find optima directly – no need for trial & error simulation
   - ➔ increase value, reduce time

➔ **Ease-of-use** combined with **equation-oriented power**

➔ g|PROCESS

gPROMS ProcessBuilder

Next-generation process simulation



v1.0 July 2015

v1.1 April 2016

What people were saying

"We need to …"

"… simulate the whole process flowsheet including a detailed model of the reactor"

"… do an economic optimisation of the whole plant so we can decide which is the most economic option"

"… perform hundreds of sensitivity studies over the next two weeks"

"… improve the reactor design to give better catalyst life"

"… look at operability"

"We need a simulator that can answer all our questions"

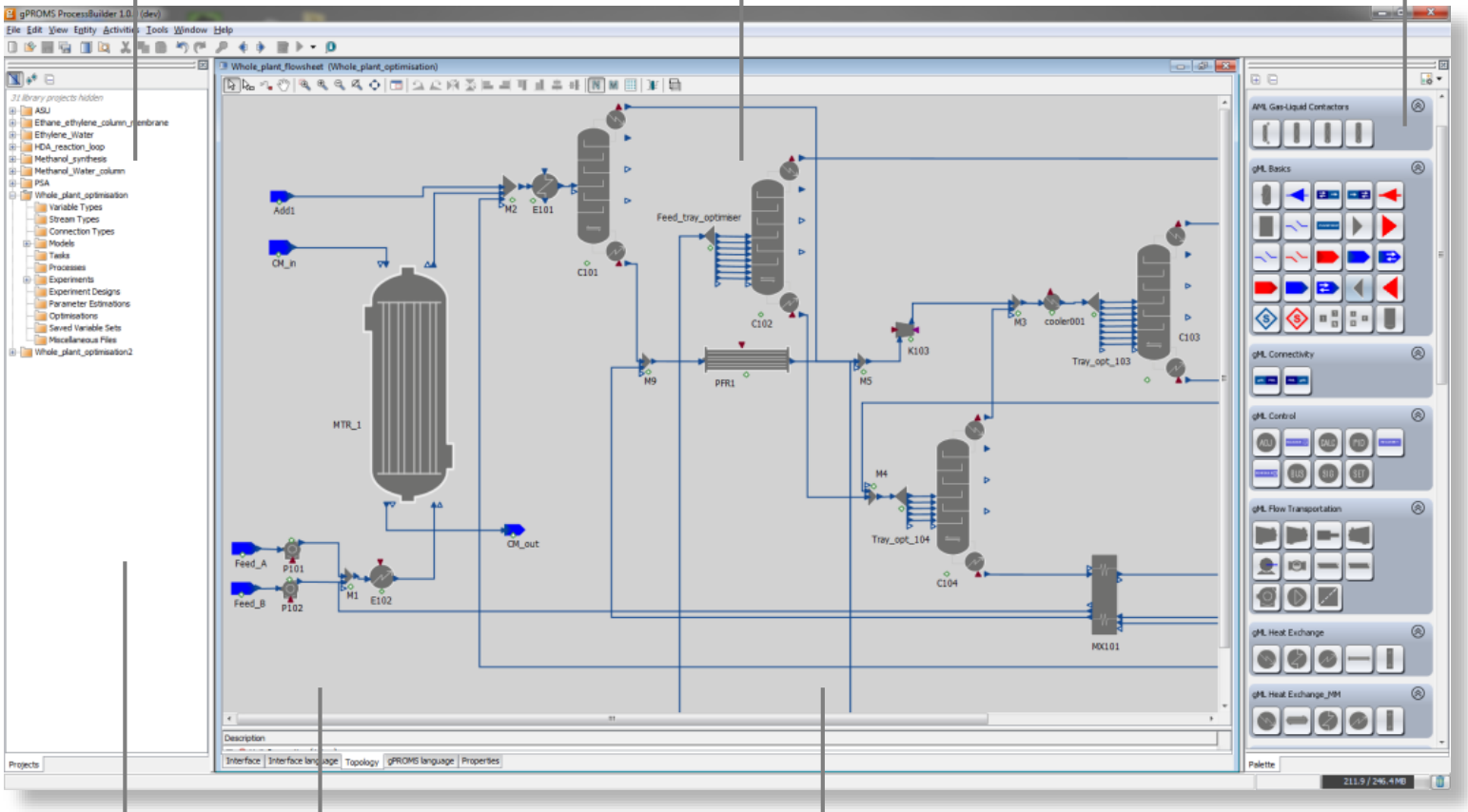
gPROMS ProcessBuilder at a glance

Project tree for easy control

Drag & drop flowsheeting

Library models
gPROMS Model Library
Advanced Model Libraries

Steady-state and dynamic



Easy custom modelling

Advanced platform capabilities
Parameter estimation
Model management

Built-in physical properties
Multiflash + DIPPR

Sophisticated numerical solution environment
Equation-oriented solution
Optimisation framework including MIO

Model Libraries – 1

1. gML:Separations – Fluid-Fluid

- Flash drum
- 3-phase separator
- Distillation column (tray, equilibrium)
- Distillation column (packed-bed, HETP)
- Column section (tray, equilibrium)
- Kettle evaporator
- 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

[1] (axial & radial flow)

3. gML:Reaction

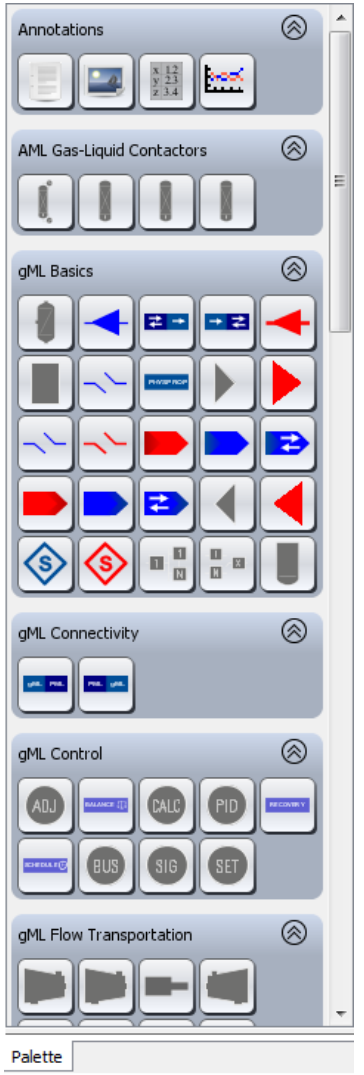
- Conversion reactor
- Gibbs reactor
- CSTR, single and two phase (kinetic & equilibrium reactions)
- PFR (kinetic & equilibrium reactions)

Reaction mechanisms

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

4. AMLs for Catalytic Reaction*

- Fixed-bed catalytic reactor (1D) [1]
- Fixed-bed catalytic reactor (1D + intra-particle)[1]
- Fixed-bed catalytic reactor (2D) [1]
- Fixed-bed catalytic reactor (2D + intra-particle)[1]
- Trickle-bed reactor
- Fischer-Tropsch reactor (fixed-bed)



Model Libraries – 2

5. gML:Heat Exchange

- Heater & Cooler
- Two-stream heat exchanger
- Multi-stream heat exchanger
- Shell-and-tube heat exchanger
- Double-pipe heat exchanger
- Condenser

6. gML:Flow Transportation

- Pipe
- Pipe (distributed)
- Pump
- Valve
- Pressure relief valve
- Compressor – Centrifugal & Reciprocating
- Expander
- Electric drive, drive shaft

7. gML:Signal

Controllers
- Gain, PID, delays

Logic
- Switches

Linear systems
- Transfer function, state-space model

Discrete
- Dead zone, hysteresis, saturation

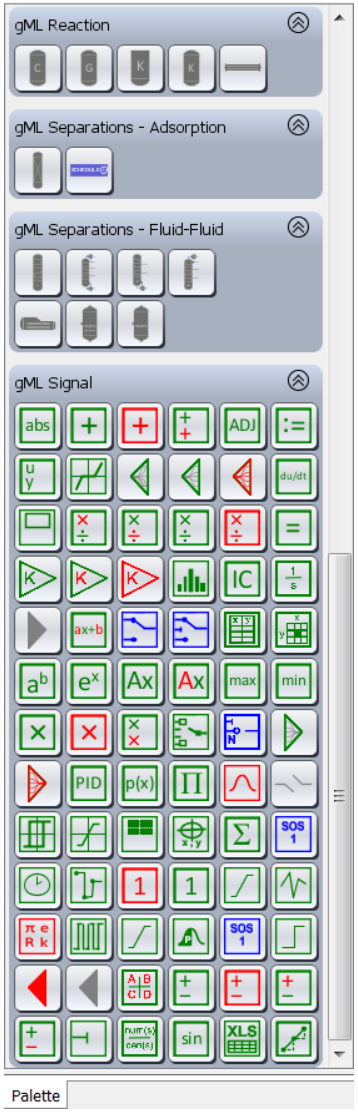
Mathematics
- Functions, basic operations

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

Signal Sinks
- Display, plot, X-Y plot

Data
- Lookup table

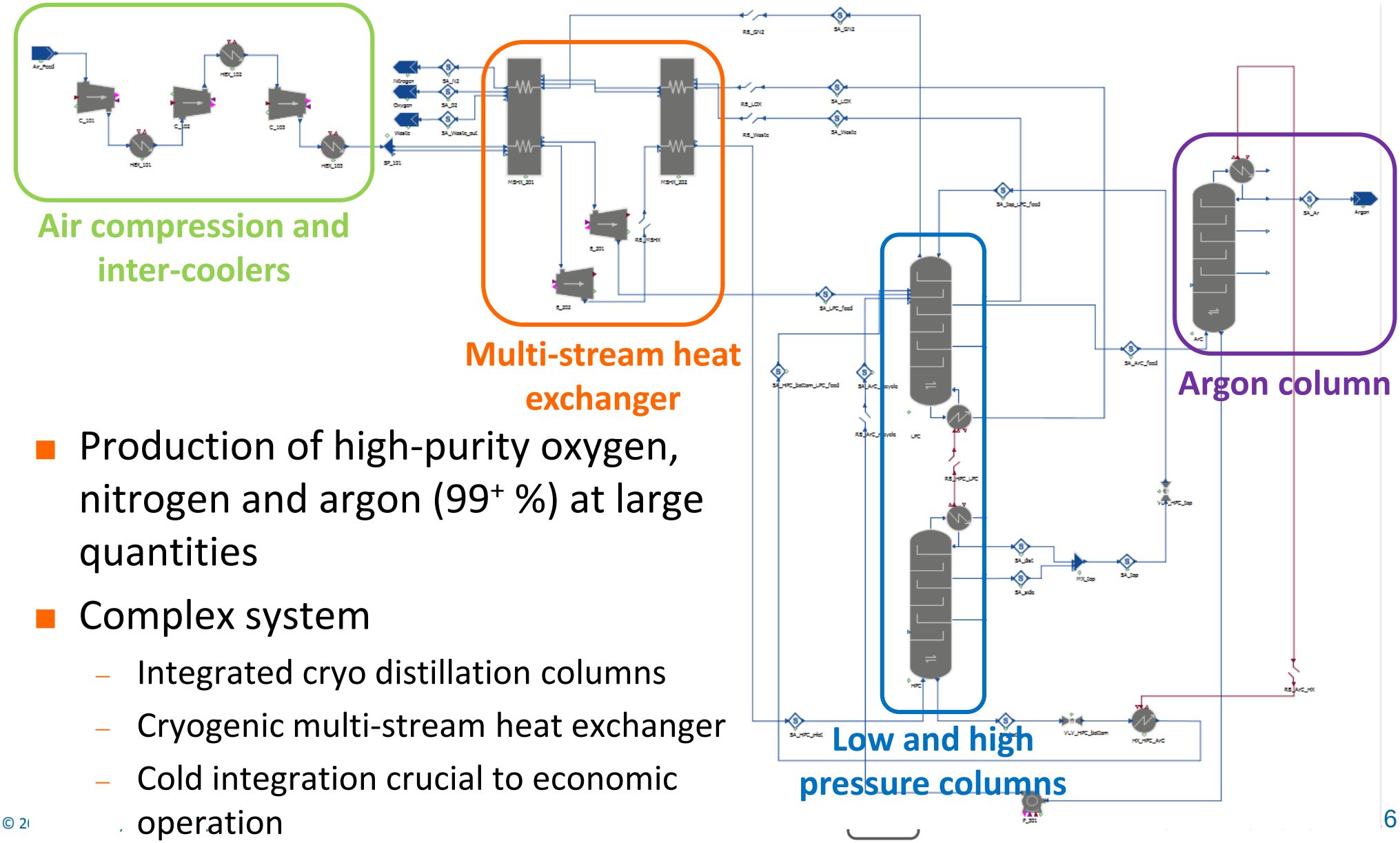
Logic programming
- Special Ordered Set (SOS1)



What is now possible?

Application examples

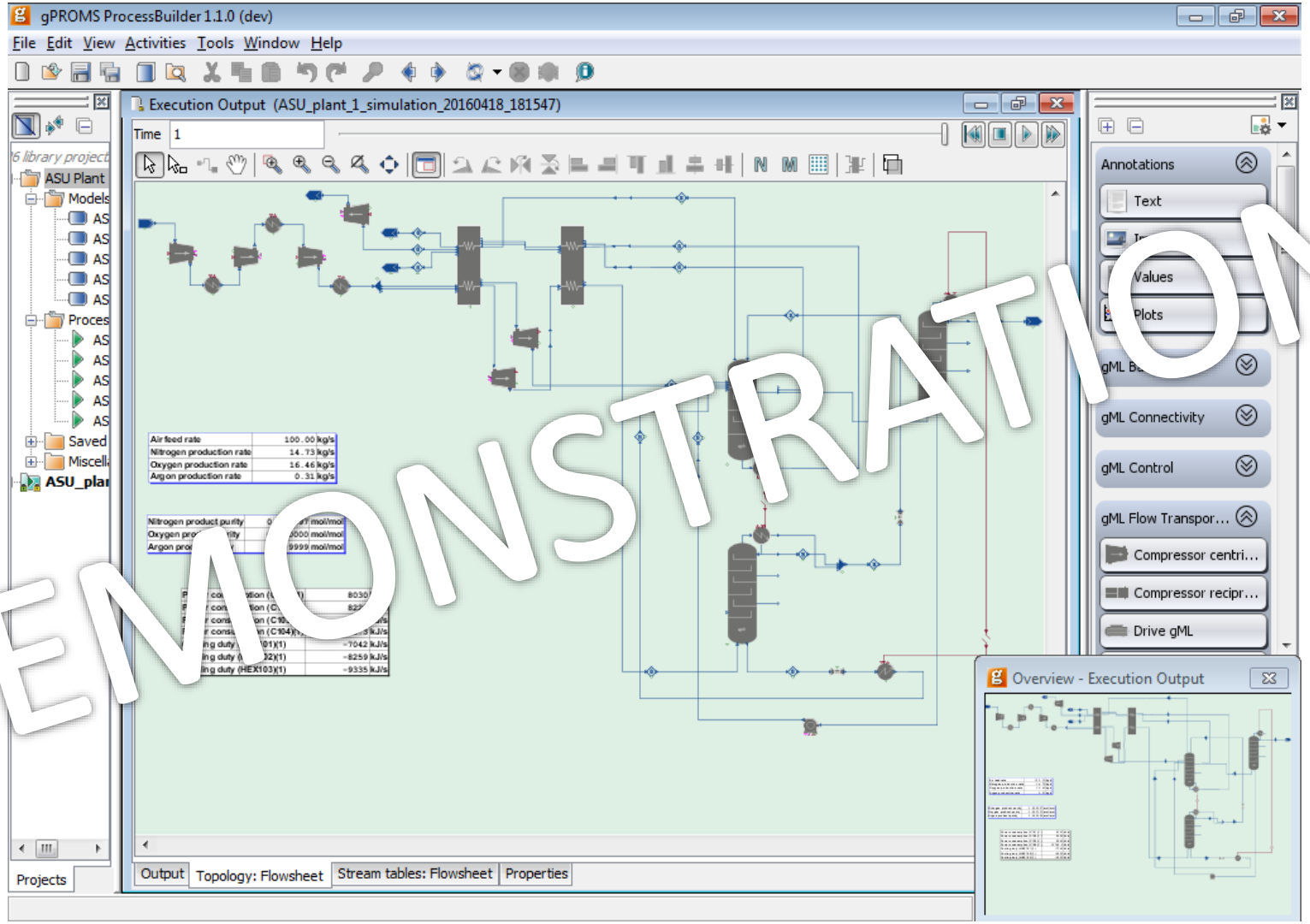
What is now possible?
Cryogenic Air Separation Unit (ASU)



- Production of high-purity oxygen, nitrogen and argon (99⁺ %) at large quantities
- Complex system
  - Integrated cryo distillation columns
  - Cryogenic multi-stream heat exchanger
  - Cold integration crucial to economic operation

Equation-oriented Solution Robustness

Initialise ASU model without any user-provided initial guesses



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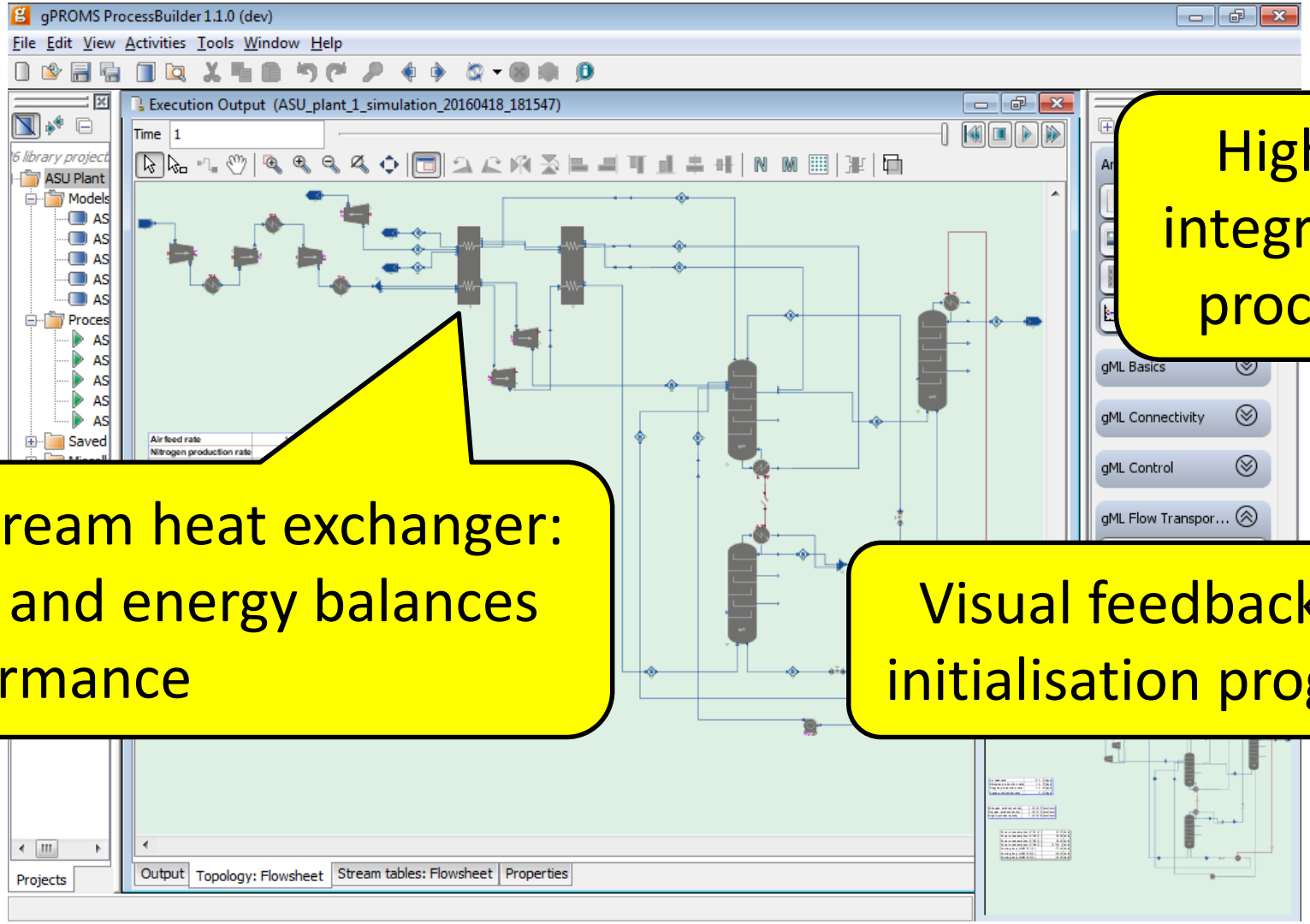


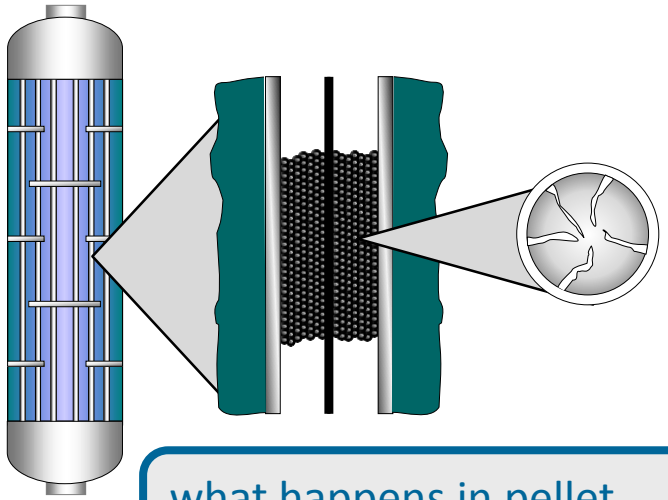
Highly integrated process

Multi-stream heat exchanger:
1. Mass and energy balances
2. Performance

Visual feedback on initialisation progress

What is now possible?

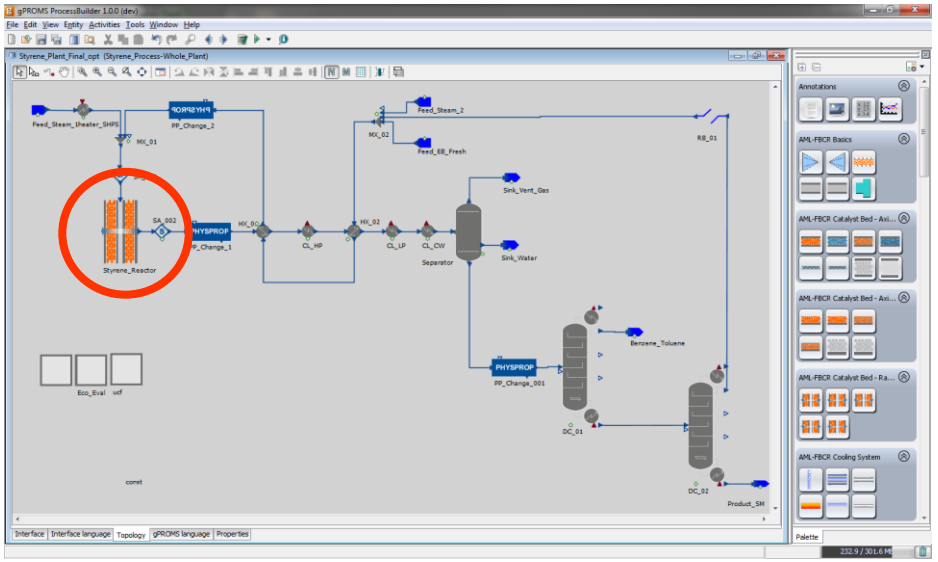
Detailed reactor design in a flowsheeting environment



what happens in pellet
can affect reactor performance

- Better conversion and selectivity
- Easier control
- Run at higher overall temperature
- Reduced hot-spot formation
- Longer catalyst life

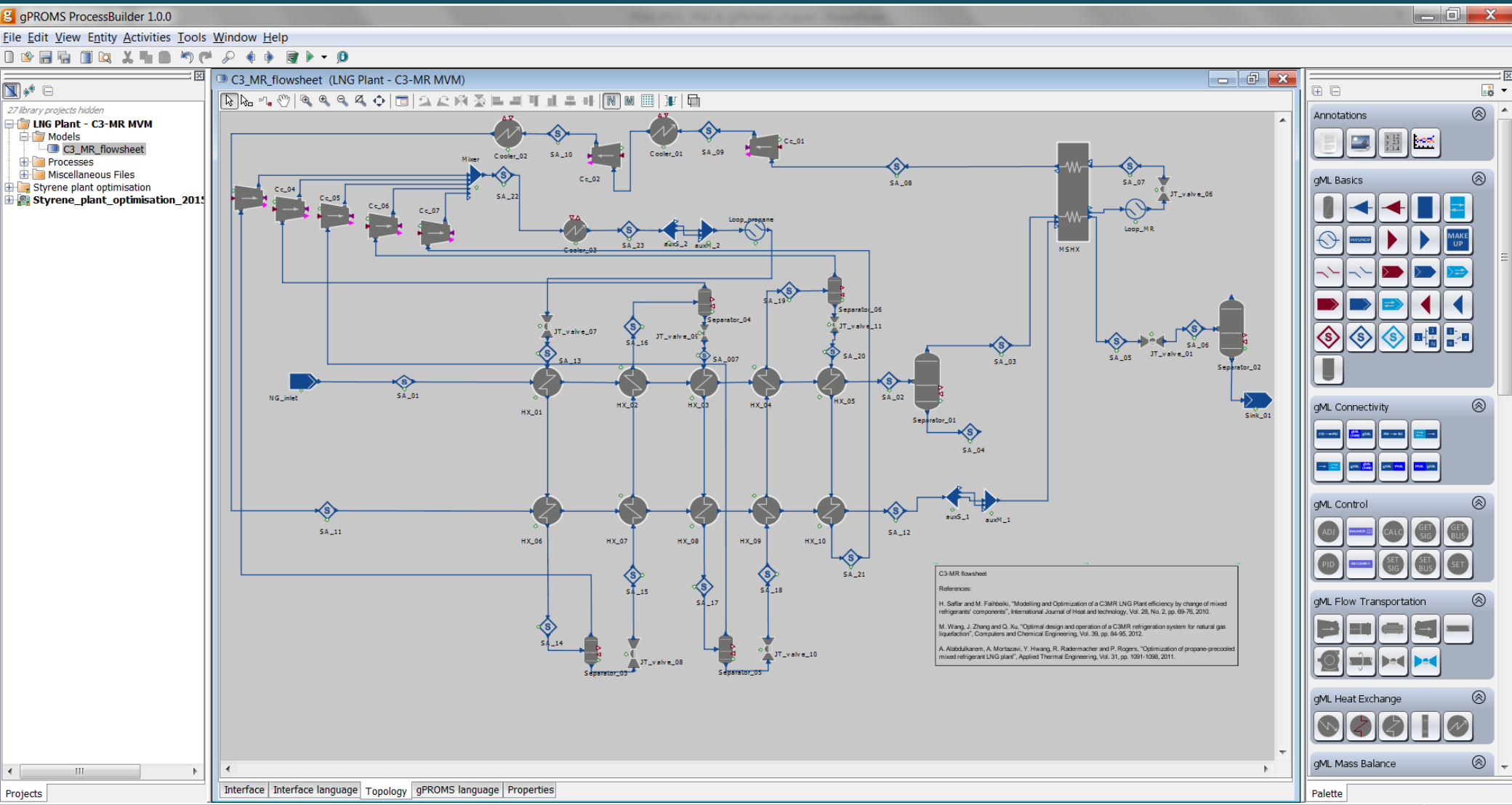
… now include in whole-plant optimisation



Styrene plant

What is now possible?

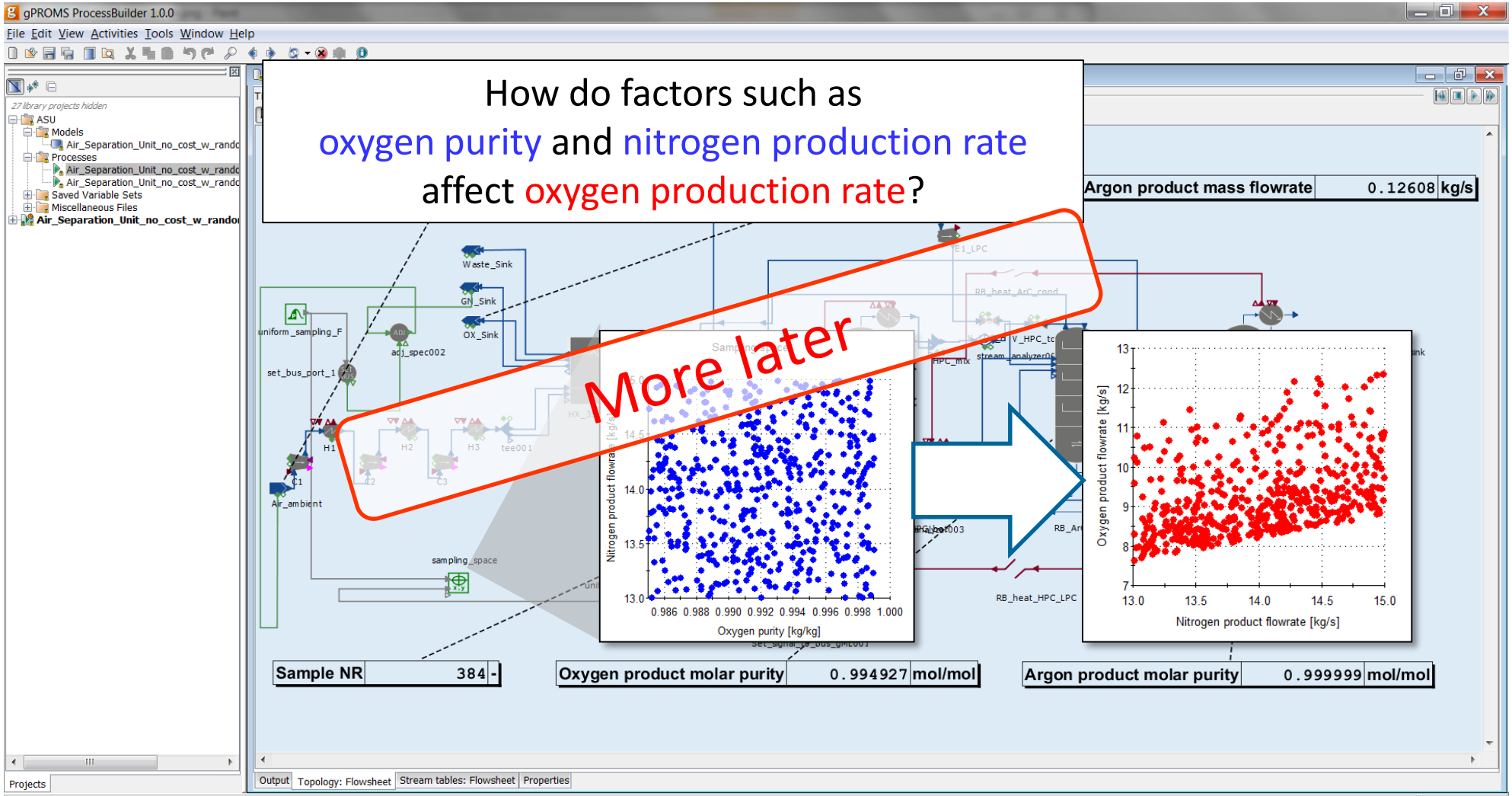
Easy solution of systems with complex recycles: LNG (C3/MR)



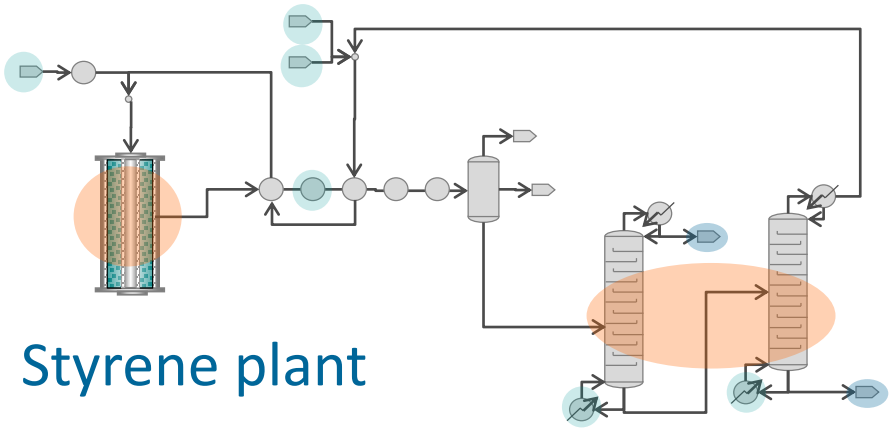
What is now possible?

Sensitivity analysis to explore multidimensional design space

- E.g. Air Separation Unit



What is now possible?
Whole-plant optimisation



Styrene plant

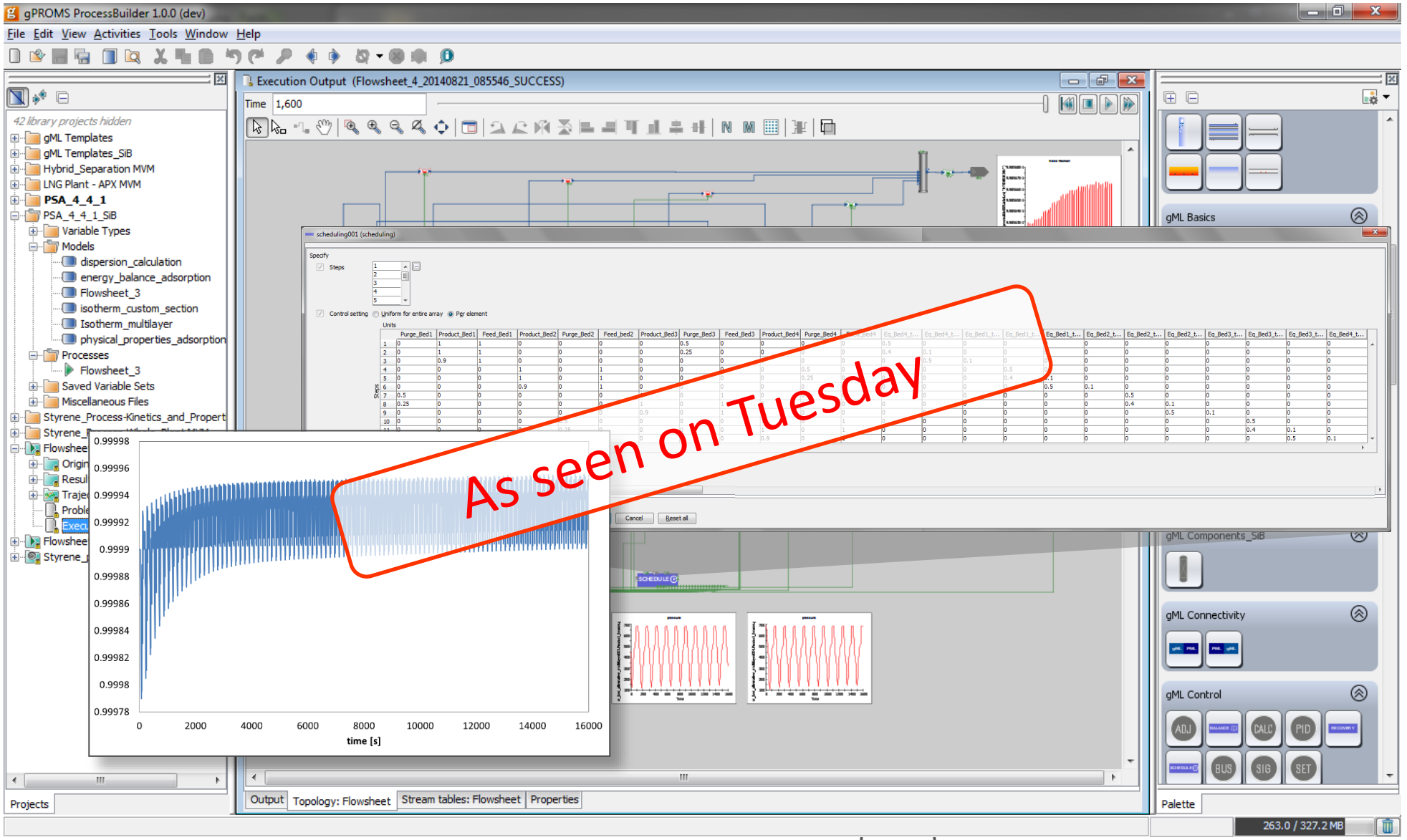
- High predictive capability
- Includes all interactions and trade-offs
- Comprehensive and efficient exploration of design space

	Initial	Optimal
Total annualised profit (MM$)	**19.72**	**25.15**
Feed stage of 1st column	40	34
# stages of 1st column	100	90
Boil up ratio of 1st column	1.00	0.60
Fresh EB flowrate(kg/sec)	4.70	5.89
Reactor radius(m)	1.37	1.34

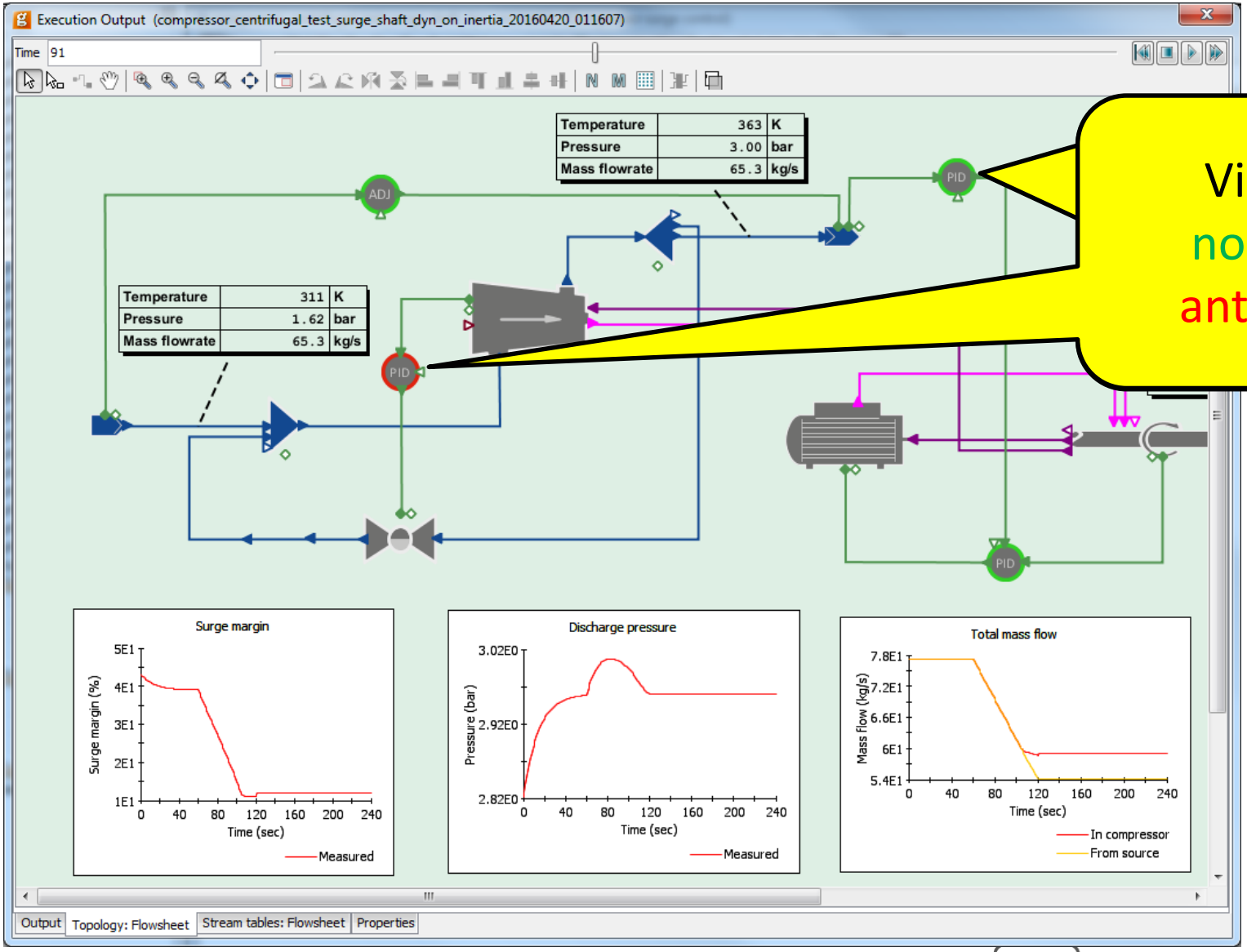
- **Higher-quality, lower-cost** designs
- More **profitable, safer** operations
- Lower **risk**

What is now possible?

Complex dynamic systems: PSA



What is now possible?
Compressor surge control



Visual warnings:
normal operation
anti-windup active

What is now possible?

Real-time monitoring & optimisation – e.g. olefins plant

Objective function

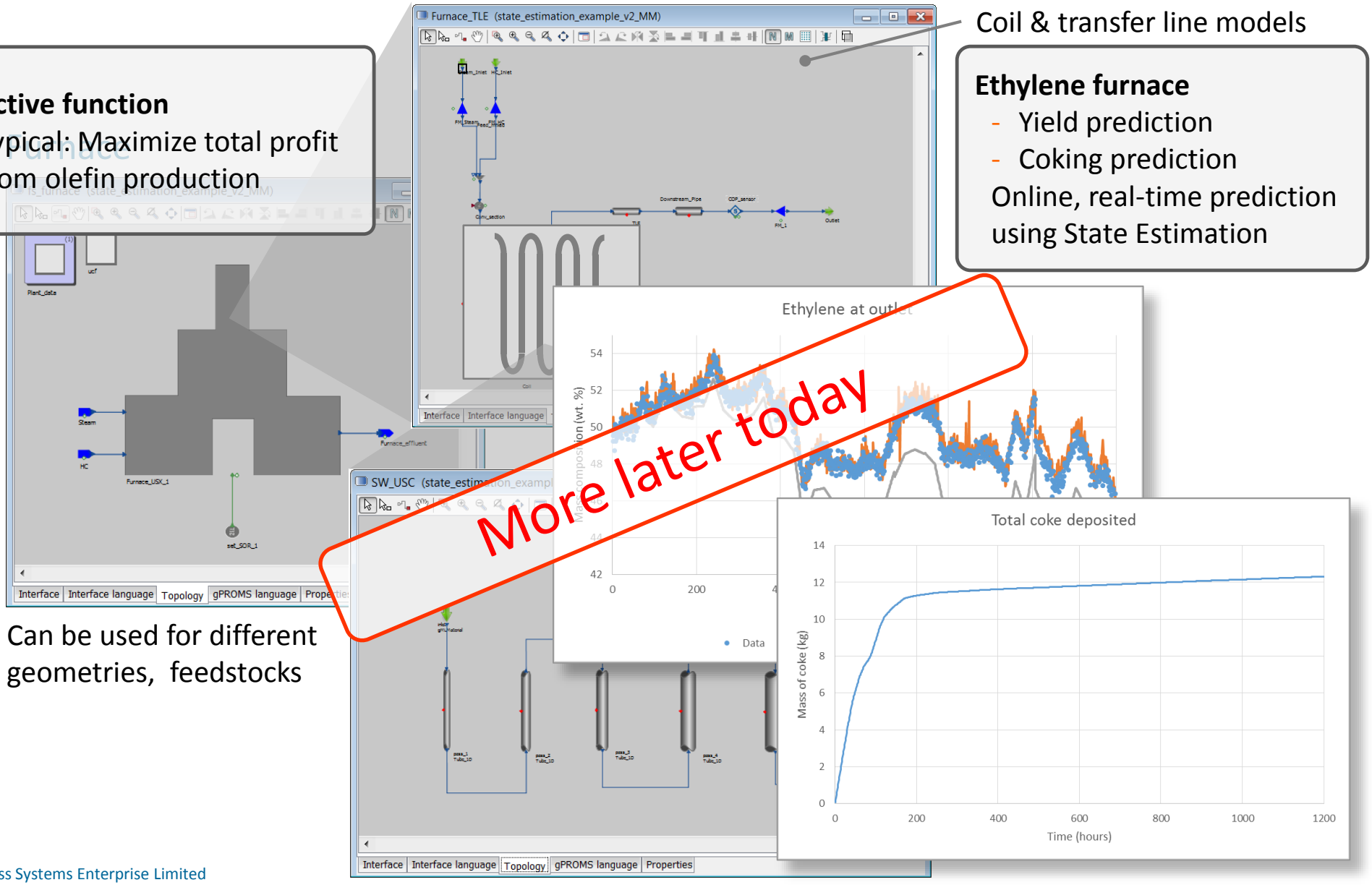
- Typical: Maximize total profit from olefin production

Coil & transfer line models

Ethylene furnace

- Yield prediction
- Coking prediction

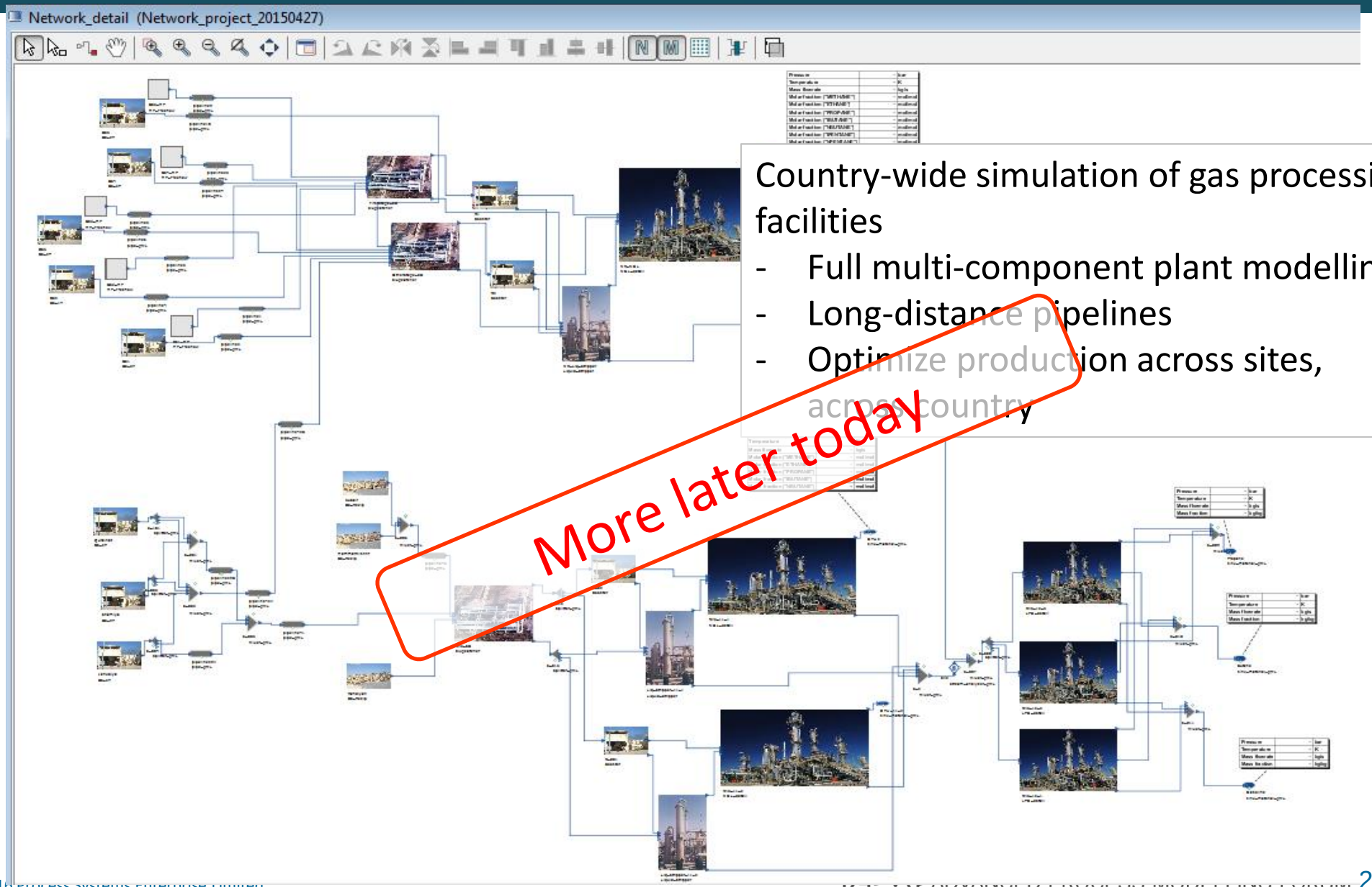
Online, real-time prediction using State Estimation



Can be used for different geometries, feedstocks

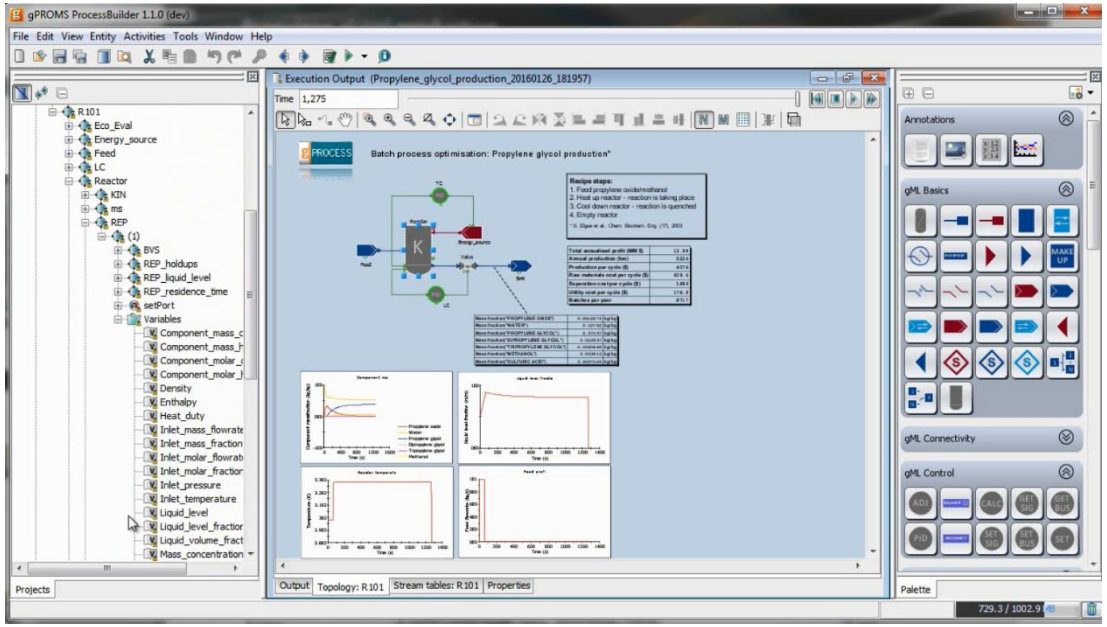
What is now possible?

Large-scale optimisation, e.g. country-wide gas production



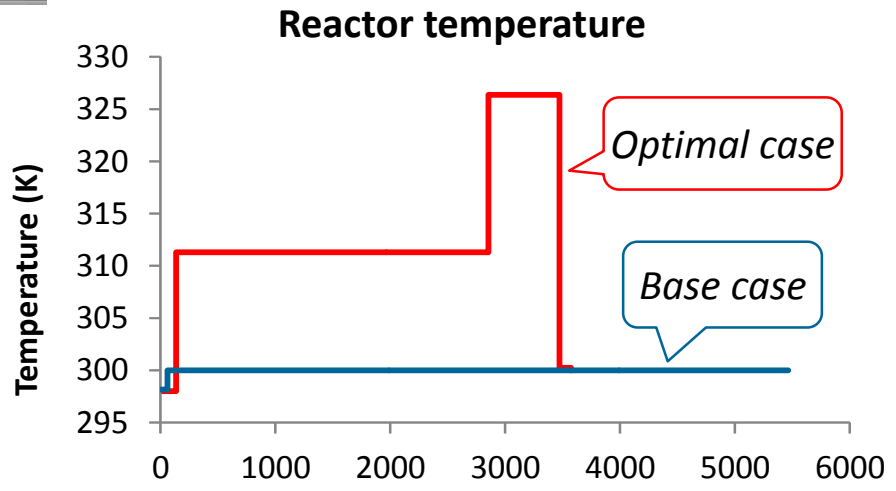
What is now possible?

Batch process optimisation, e.g. propylene glycol

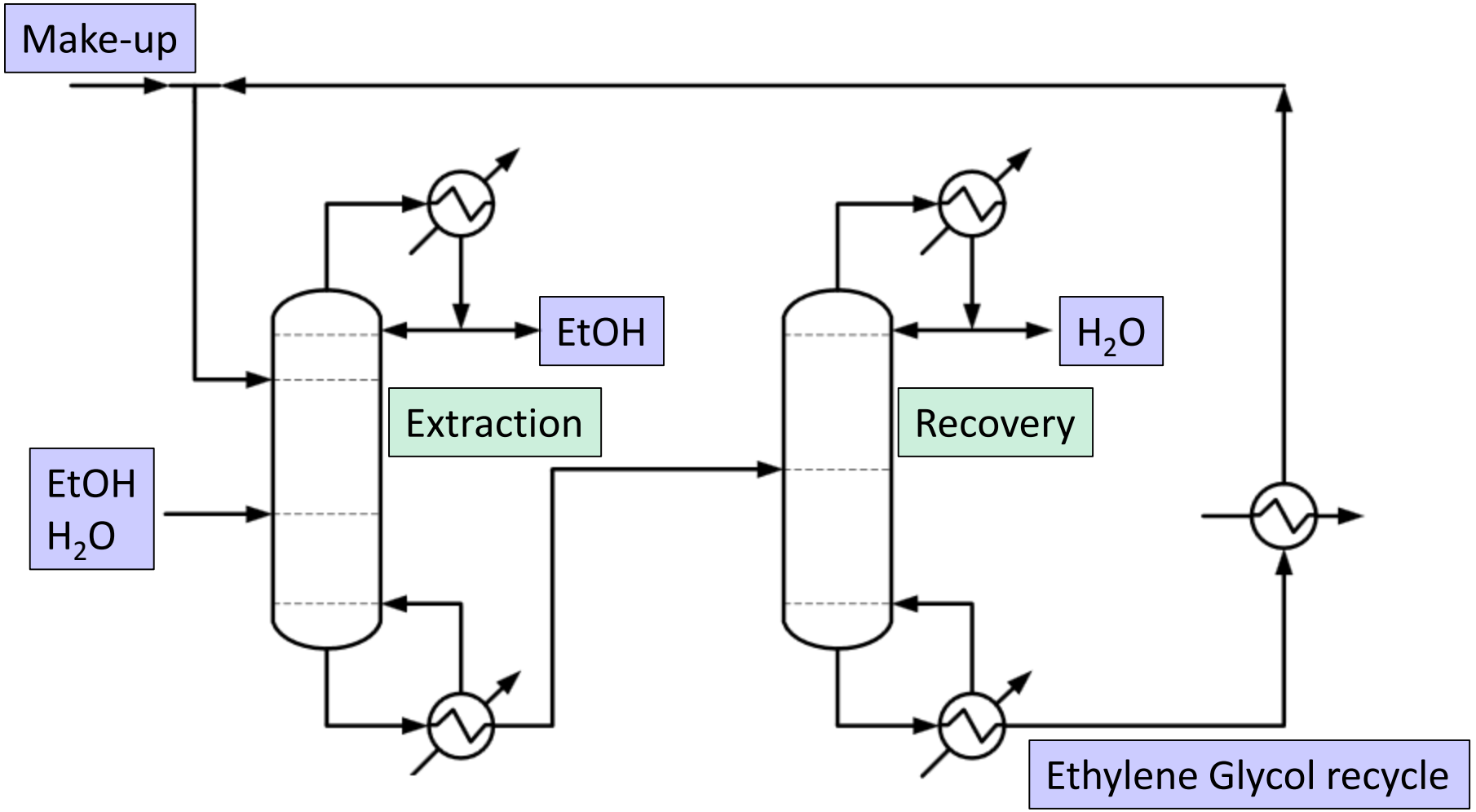


- Detailed reaction kinetics for accuracy
- Optimize batch recipe

	Base case	Optimized
Profit (MM $ / y)	3.6	9.9
Production (ton / y)	2018	3839
Batches per year	3690	4984
2PG in product [%w]	2.79	7.9
3PG in product [%w]	<0.1	0.6

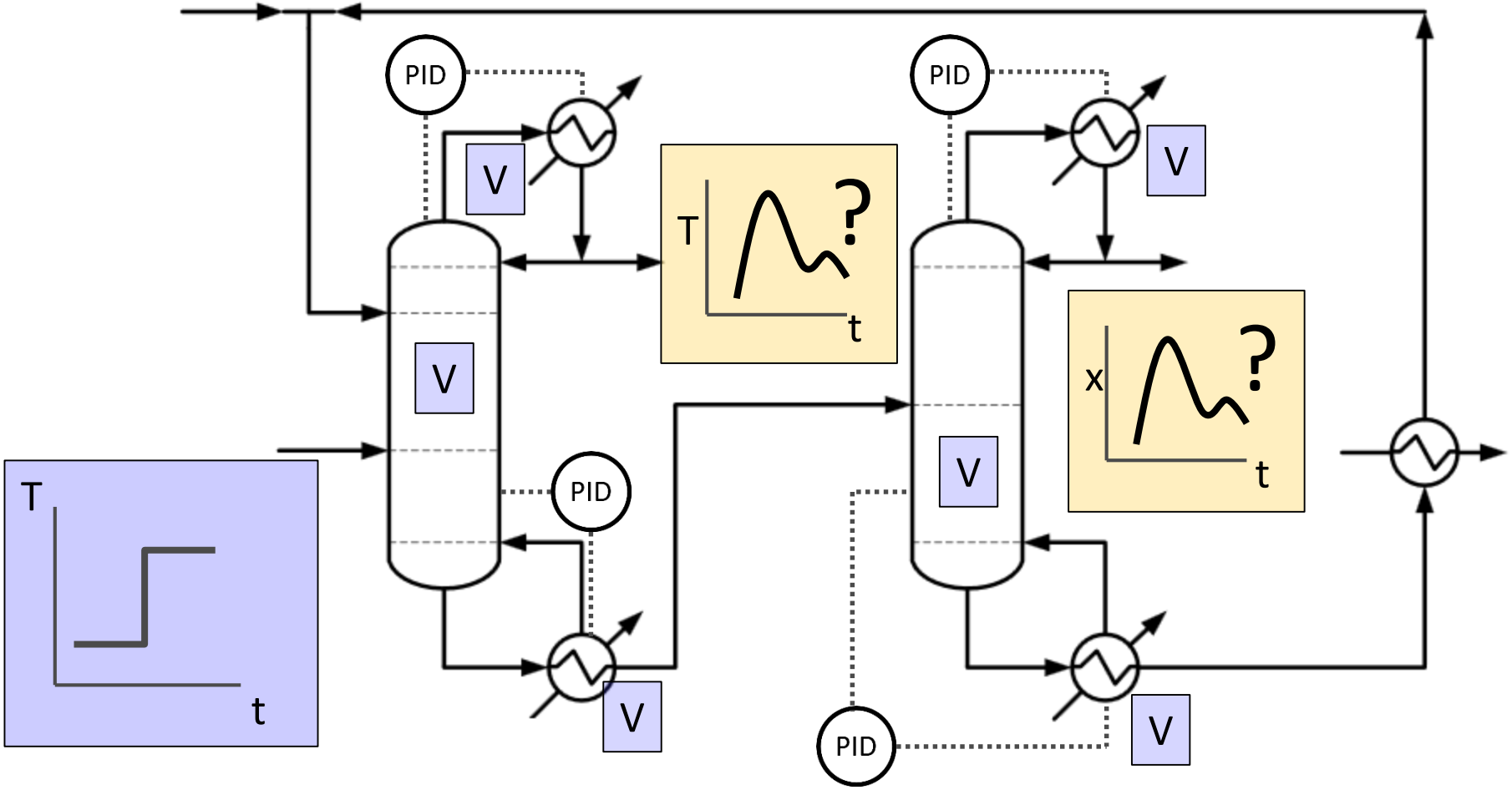


What is now possible?
Dynamic distillation



Bastidas P.A., Gil I.D., Rodriguez G., "Comparison of the main ethanol dehydration technologies through process simulation", ESCAPE 20 proceedings

What is now possible?
Dynamic distillation



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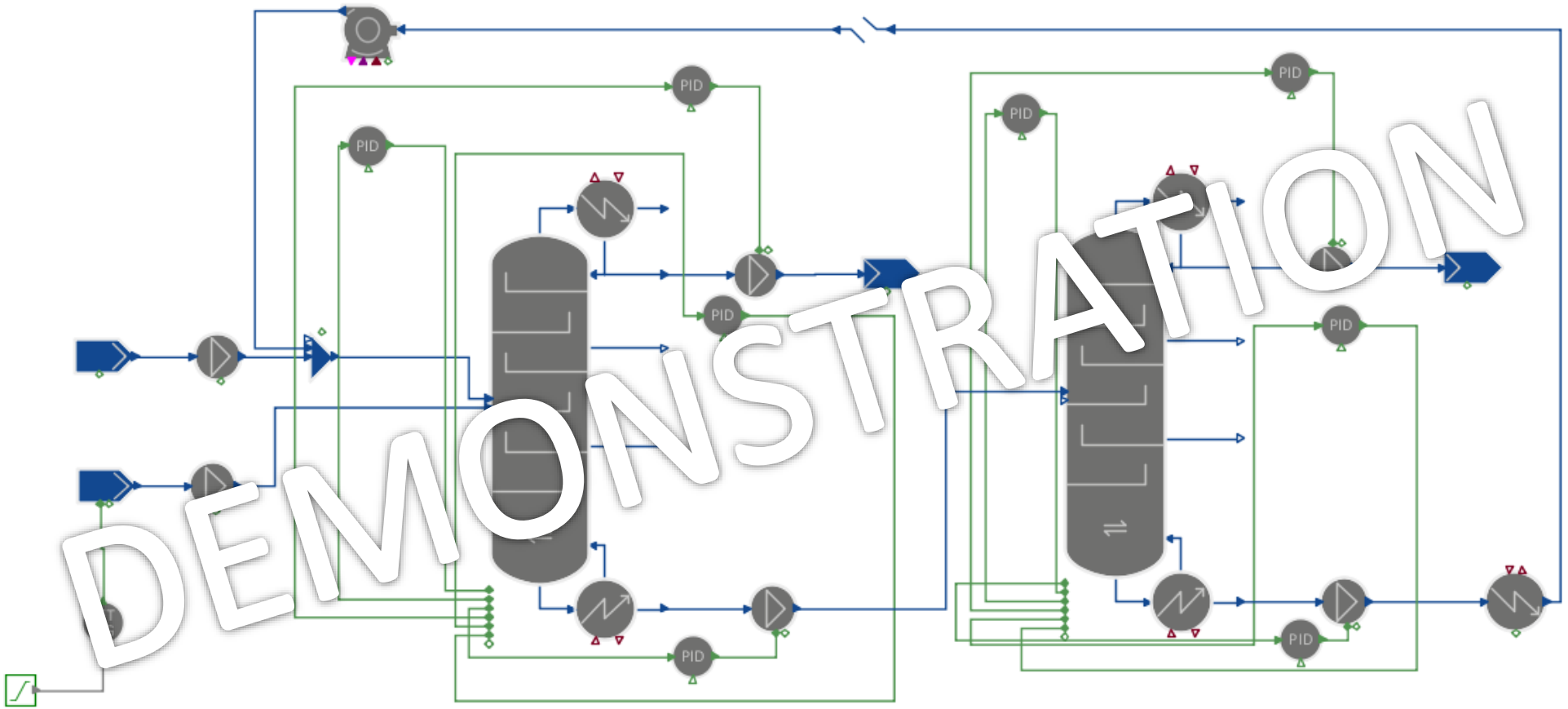

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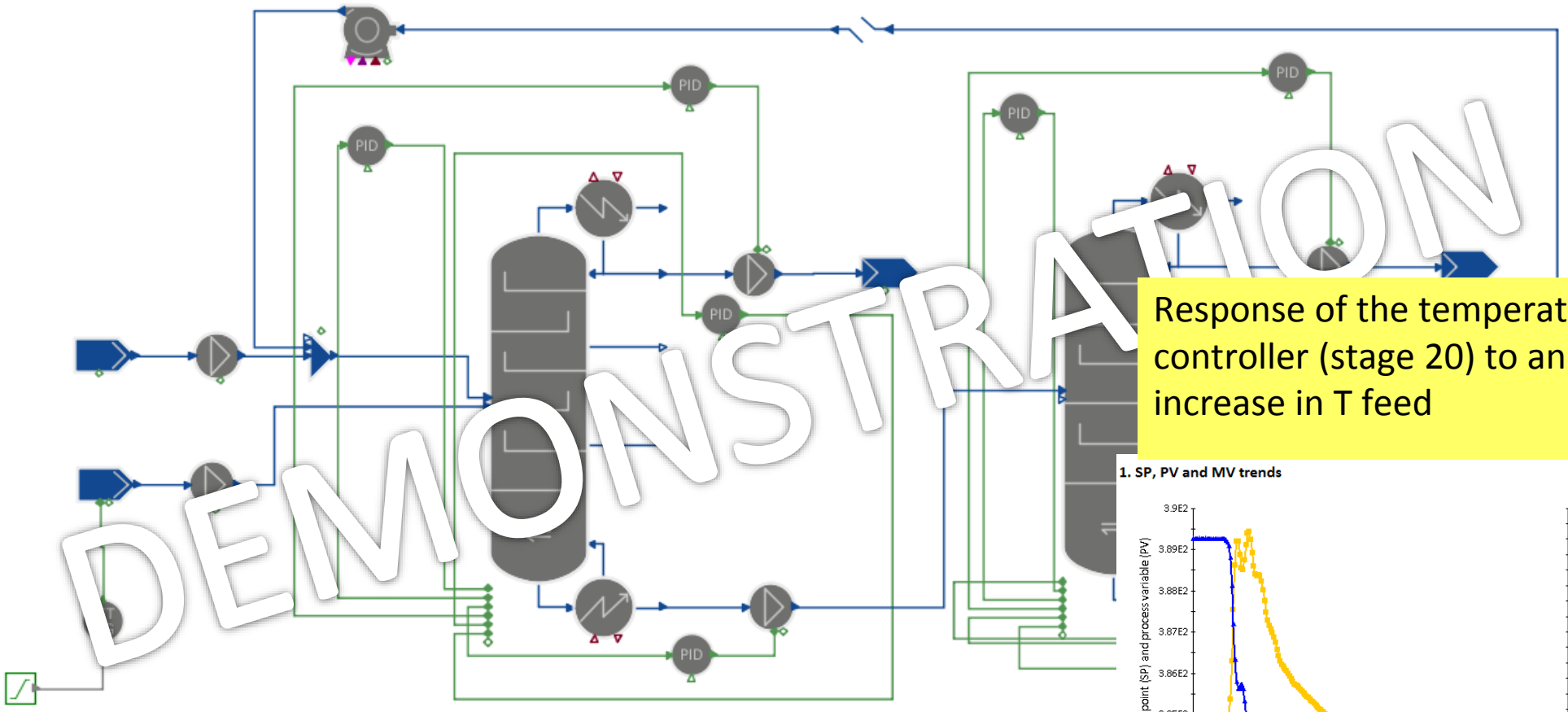
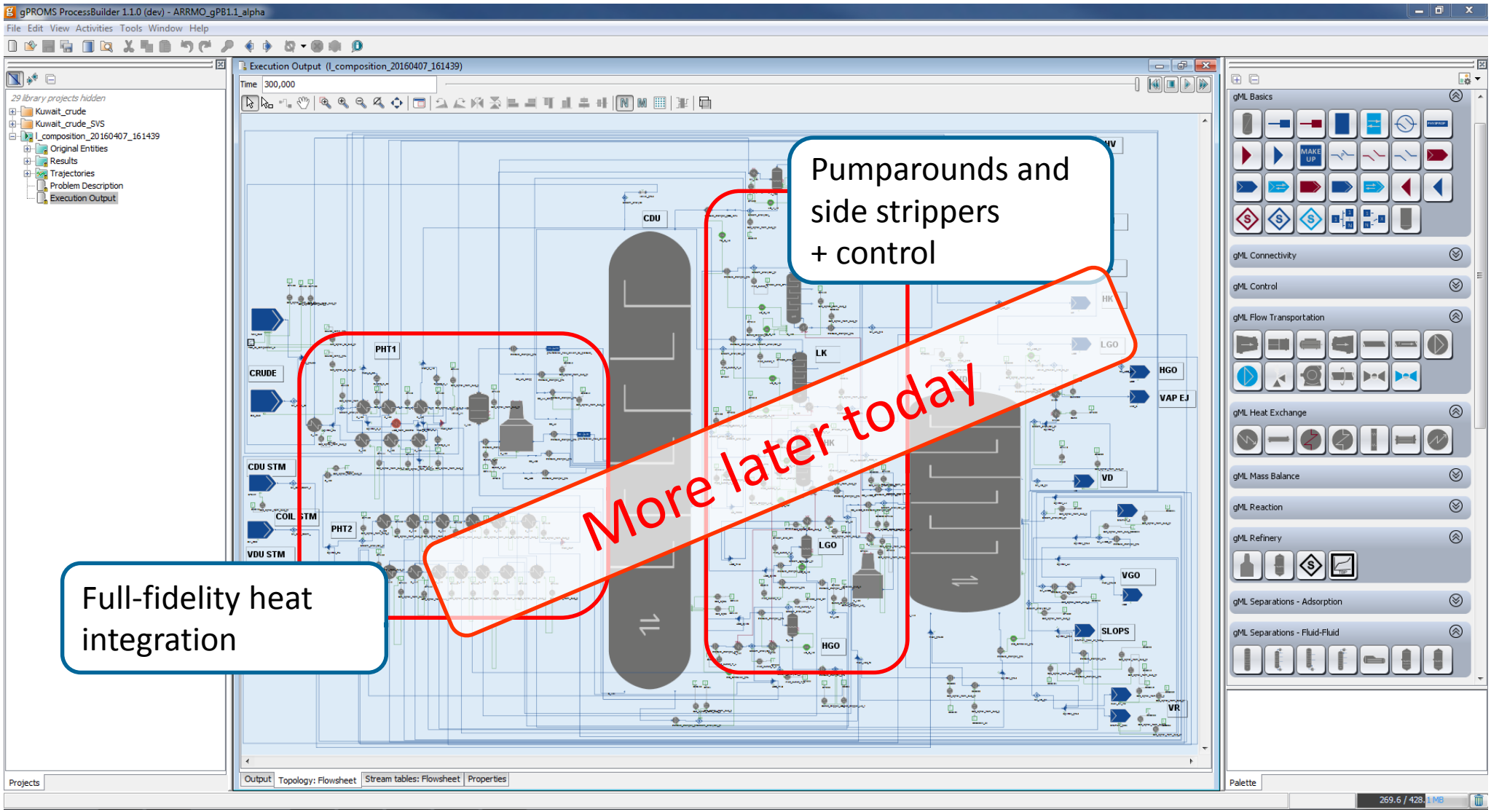
Dynamic distillation



Response of the temperature controller (stage 20) to an increase in T feed

What is now possible?

Dynamic model of crude distillation unit (CDU)

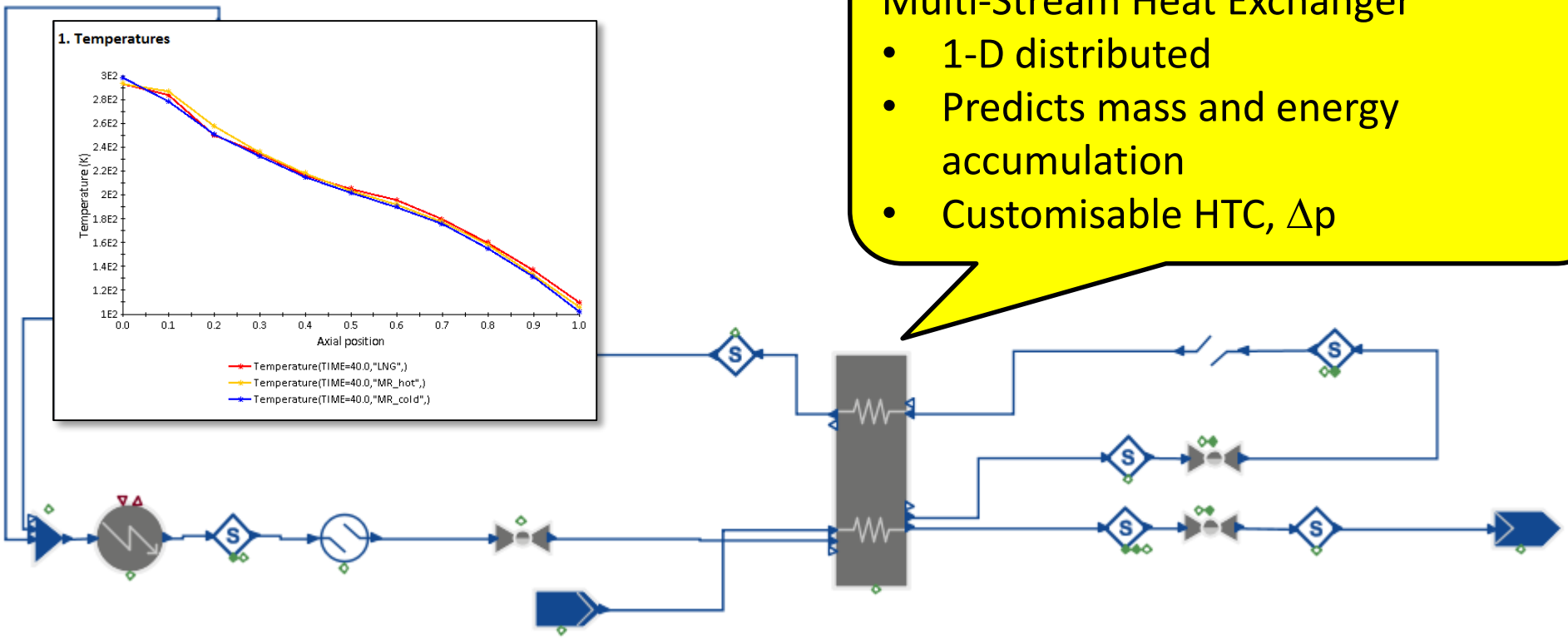


Why look at process dynamics?

- Perform start-up / shutdown scenarios
- Study safety scenarios / abnormal operation
- Test different control configurations
- Design control system
- Assess effects of disturbances on KPIs
- Assess effect of heat integration on system stability
- Optimise grade changes

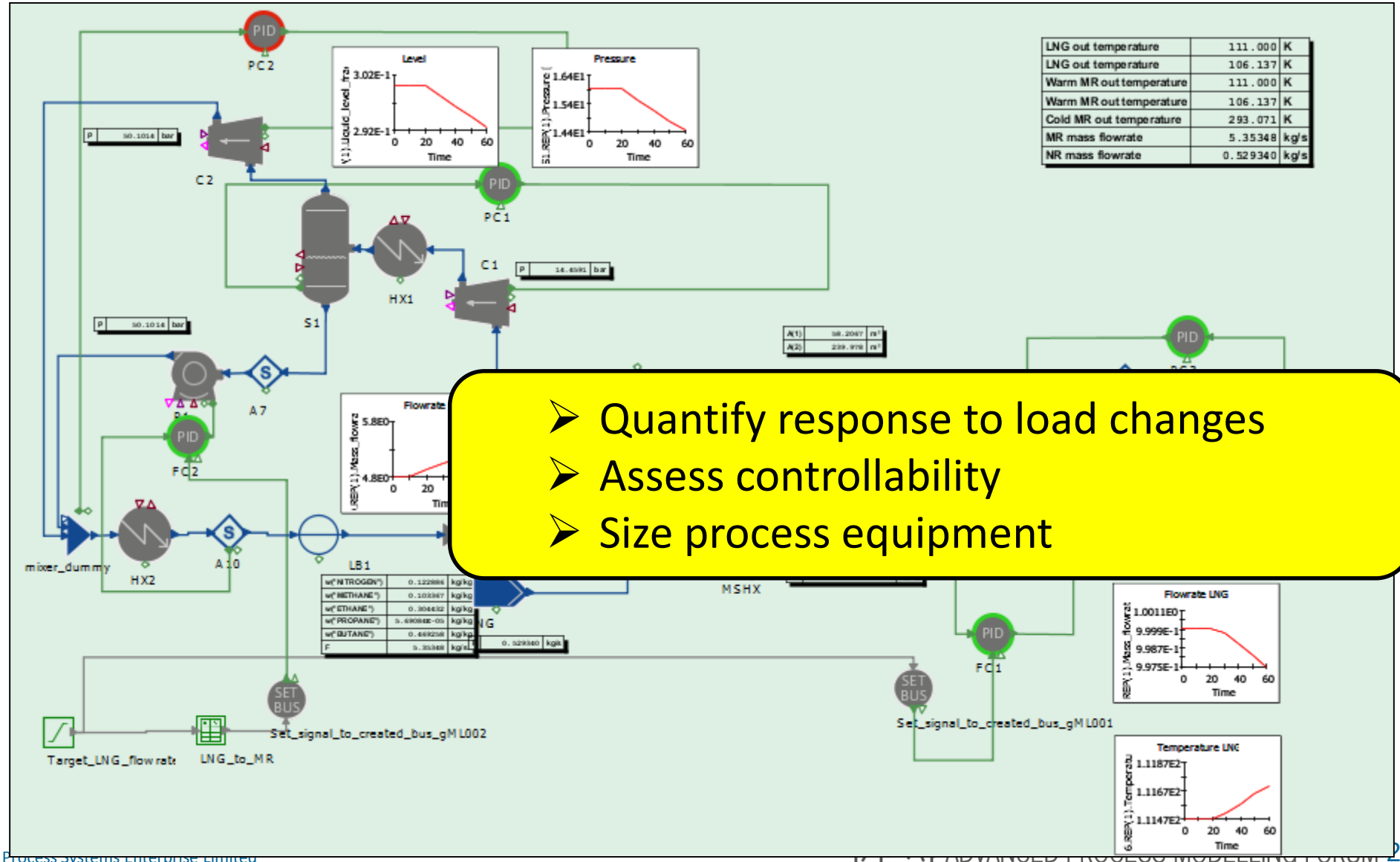
SMR process

Multi-Stream Heat Exchanger
- 1-D distributed
- Predicts mass and energy accumulation
- Customisable HTC, Δp



What is now possible?

Assess natural gas liquefaction process **dynamics**

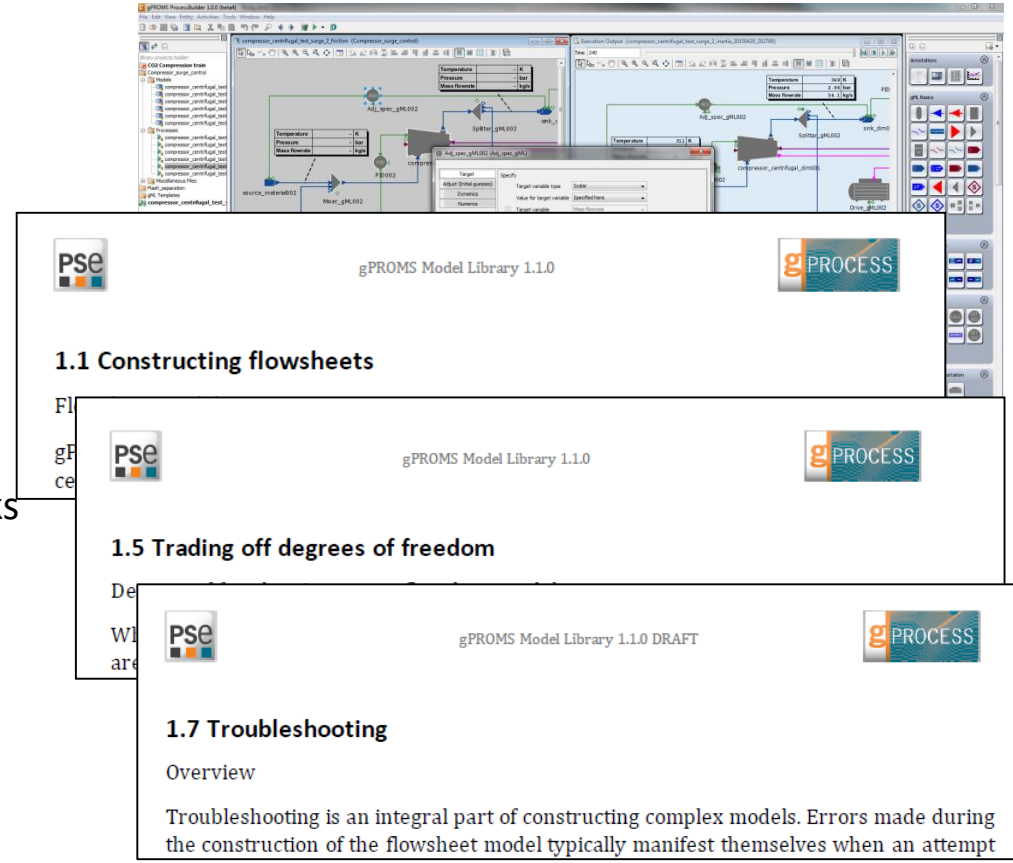


- Quantify response to load changes
- Assess controllability
- Size process equipment

gPROMS ProcessBuilder v1.1

What's available now?

1. Model libraries
   - unit operation MODELs
   - documentation
2. Physical properties
   - Multiflash + DIPPR databank
   - gSAFT
     - SAFT-VR SW + SAFT-γ Mie databanks
     - Custom Databank Management
3. Workflow guides
4. Examples
5. Custom modelling templates
   a. Kinetics, heat transfer, pressure drop, …
   b. Unit operation models
6. Regular training courses

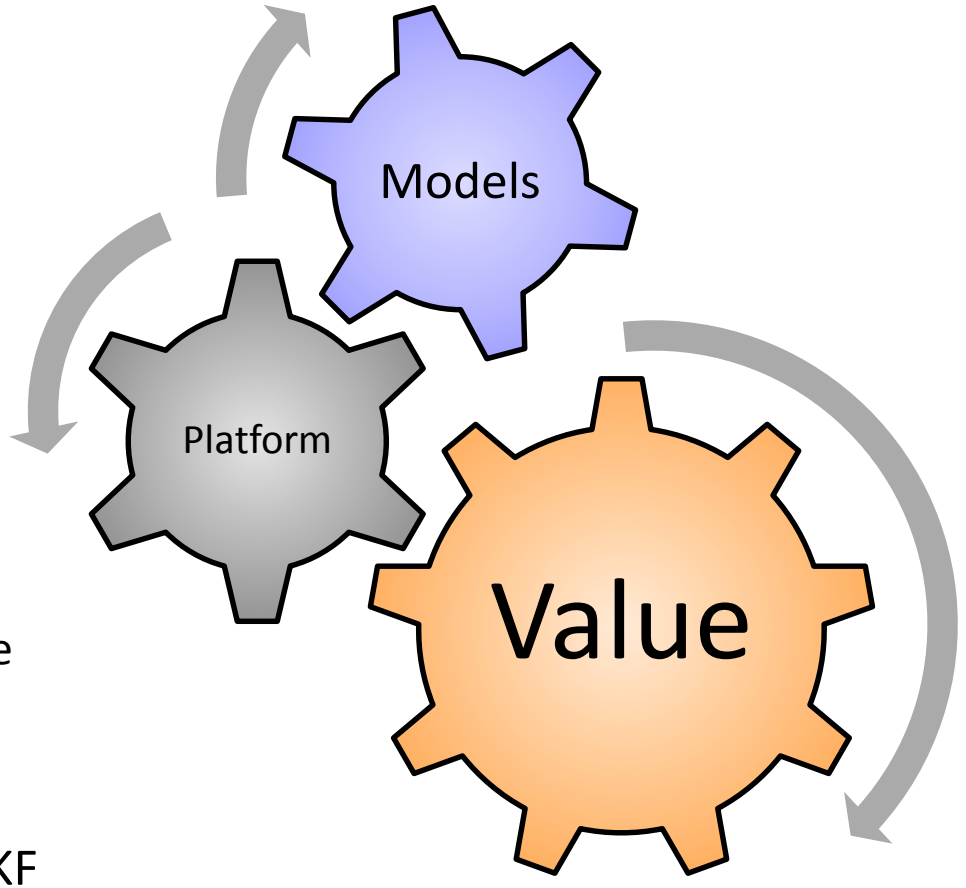


Conclusion

Conclusion

gPROMS ProcessBuilder 1.1 brings

- comprehensive model libraries + property package
  - some detailed high-fidelity models not seen elsewhere
- option to extend with own custom models
  - capture and use your organisation's unique knowledge
- clear workflow guides for key activities
- steady state and dynamic calculations
  - same models, same environment → save time
- powerful equation-based solvers
  - save time converging tightly coupled systems
- all other platform developments, e.g. GSA, EKF
- optimisation, optimisation, optimisation
  - identify real bottom-line value



Thank you