ADVANCED PROCESS MODELLING FORUM

22–23 APRIL 2015

gPROMS ProcessBuilder

Advanced Applications

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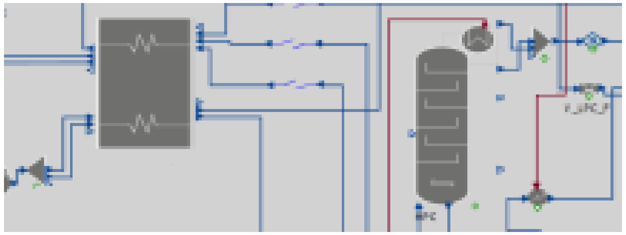
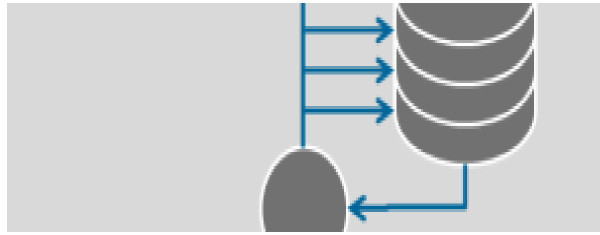
gPROMS ProcessBuilder - Advanced Applications



Detailed reactor design

- Full reactor modelling
  - standalone or within flowsheet
- Any level of complexity
- Start-up, shutdown, transition analysis
- Reduce cost of ownership of reactor, catalyst design

➔ **Potential $M benefit**



Optimal equipment configuration

- Rigorously optimise configurational aspects
  - distillation stages, feed and draw locations
  - batch equipment sizes
- Reduce CAPEX & OPEX

➔ **Potential $M benefit**

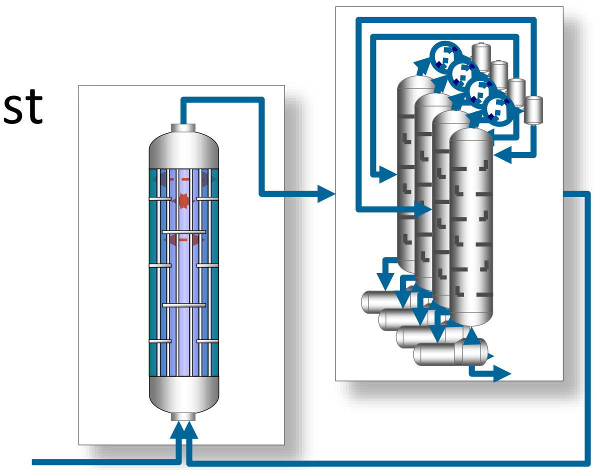
Whole-plant optimisation

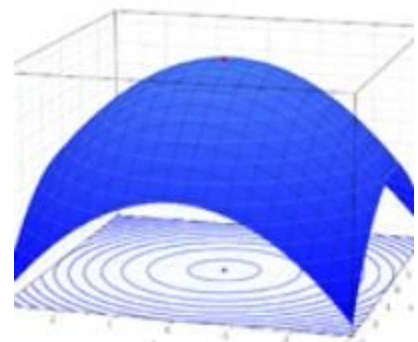
- Consider entire plant simultaneously
- Detailed reactor and separation modelling
- Multiple decision variables
- Economic objective function

➔ **Potential $M benefit**

Advanced Application: Whole-plant optimisation

1. Include major trade-offs
   – minimise reactor cost vs minimise separation cost
2. Get results you can trust
   – use high-fidelity models
   – validate with lab and/or plant data
   – accurately represent constraints
3. Find truly optimal design
   – include all relevant decisions
   – explore multi-dimensional problem efficiently
   – come up with solutions you hadn't considered
   – don't waste time with trial-and-error simulations
4. Benefits
   – realise $millions of additional revenue/cost savings





Example

Styrene monomer production

Styrene monomer (SM) production

- SM is precursor to polystyrene, ABS, SBR, and many others
- Usually produced by dehydrogenating ethylbenzene (EB):

$$C_6H_5\text{-}CH_2\text{-}CH_3 \leftrightarrow C_6H_5\text{-}CH{=}CH_2 + H_2$$

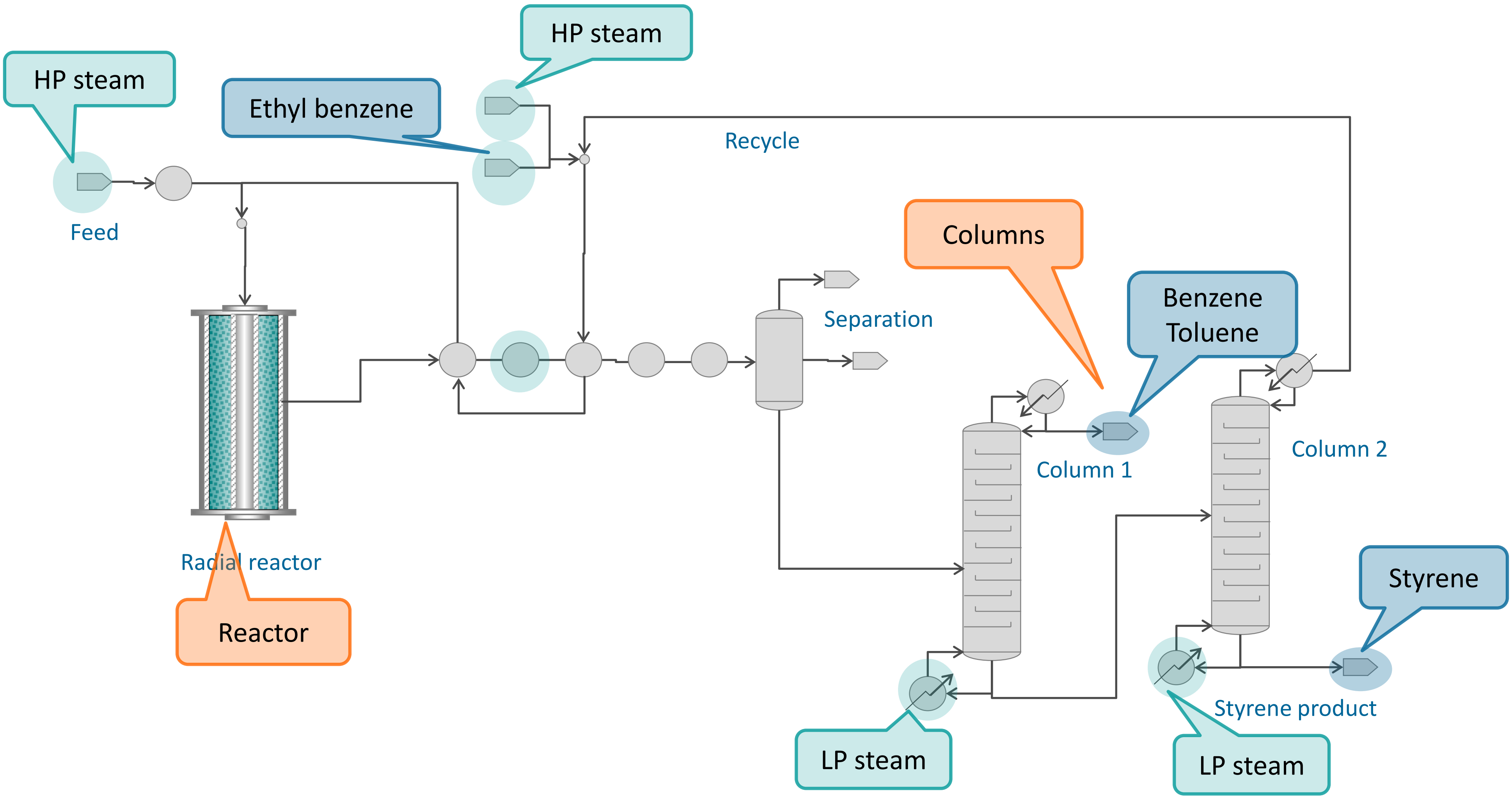
- Side reactions yield toluene and benzene

$$C_6H_5\text{-}CH_2\text{-}CH_3 + H_2 \rightarrow C_6H_5\text{-}CH_3 + CH_4$$

$$C_6H_5\text{-}CH_2\text{-}CH_3 \rightarrow C_6H_6 + C_2H_4$$

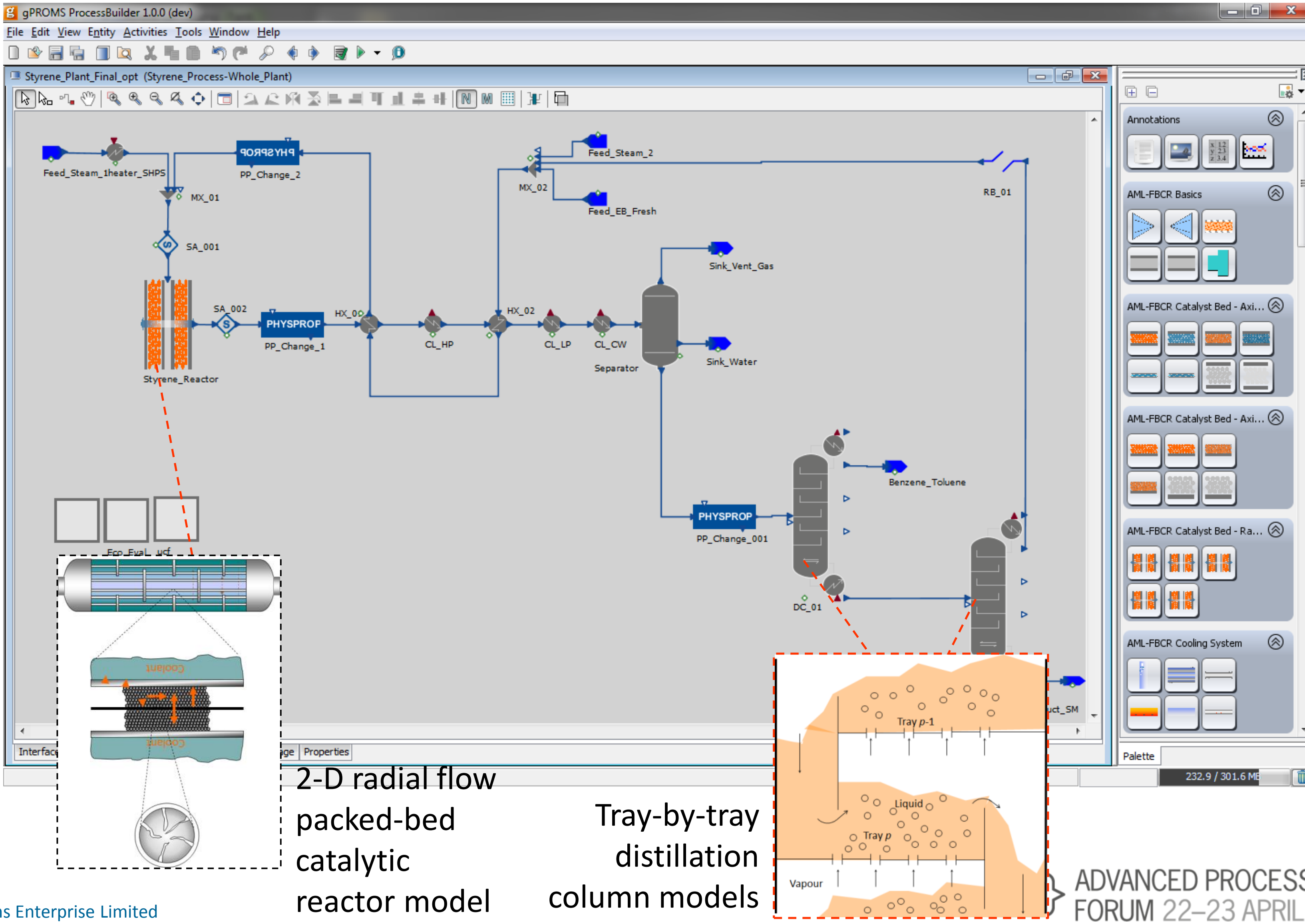
- Vapour-phase endothermic reaction
  - catalyst: Fe_2O_3 with K_2O or K_2CO_3
  - heat supplied by steam
- Challenges
  - difficult separation of SM (bp 145°C) and unreacted EB (bp 136°C)
  - large recycle (30% unreacted EB)

Styrene monomer production process



Styrene monomer production process

Modelled in gPROMS ProcessBuilder



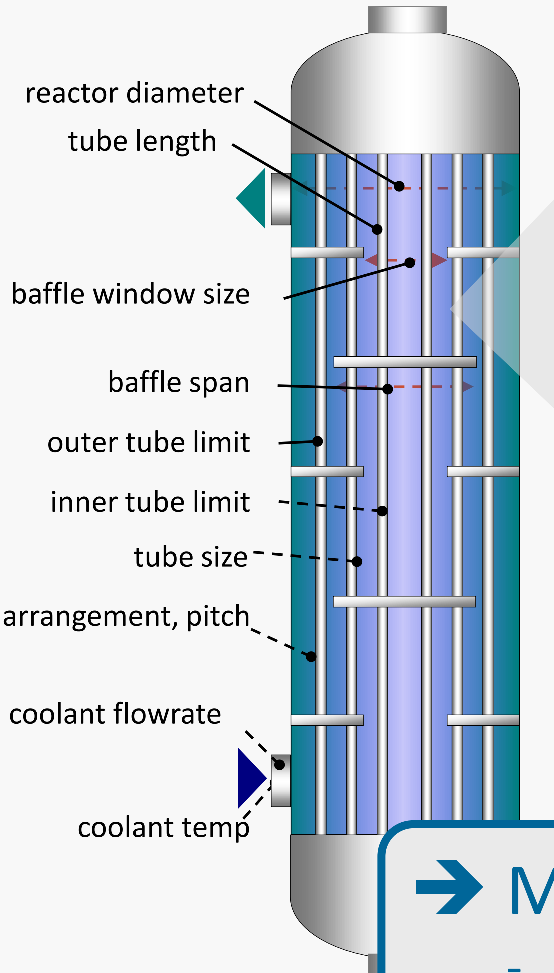
2-D radial flow packed-bed catalytic reactor model

Tray-by-tray distillation column models

Detailed reactor models:
Advanced Model Library for Fixed-Bed Catalytic Reactors

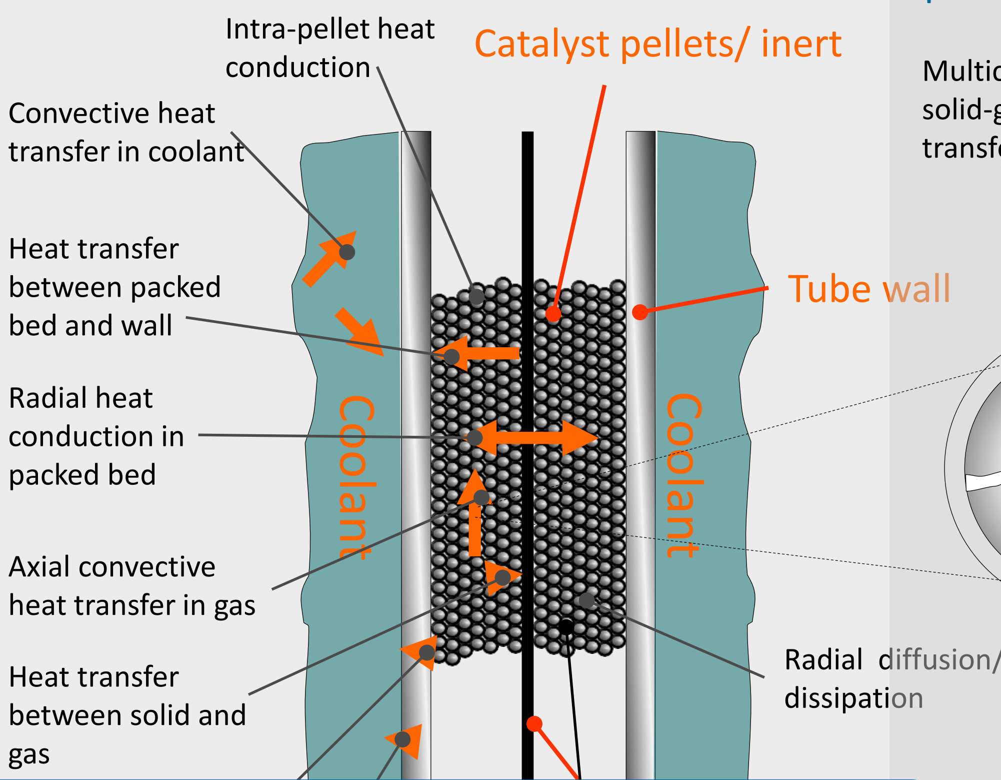
Reactor unit

Design variables



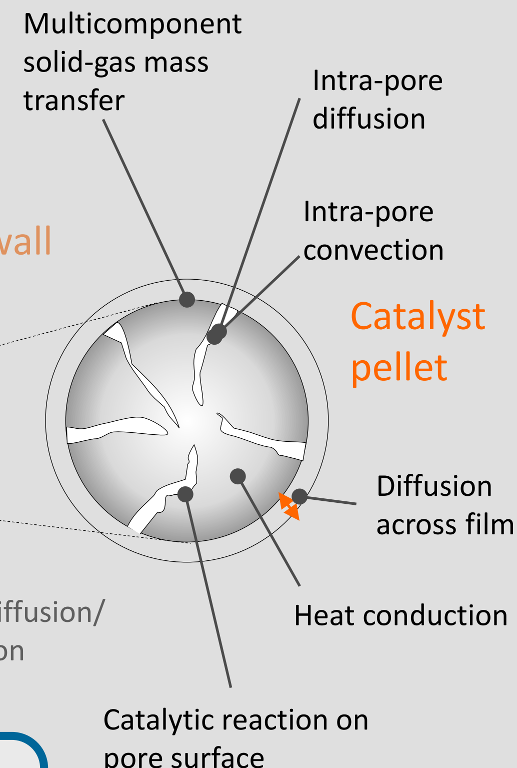
Tube

Bed heat and mass transfer phenomena



Catalyst pellet

Heat and mass transfer phenomena

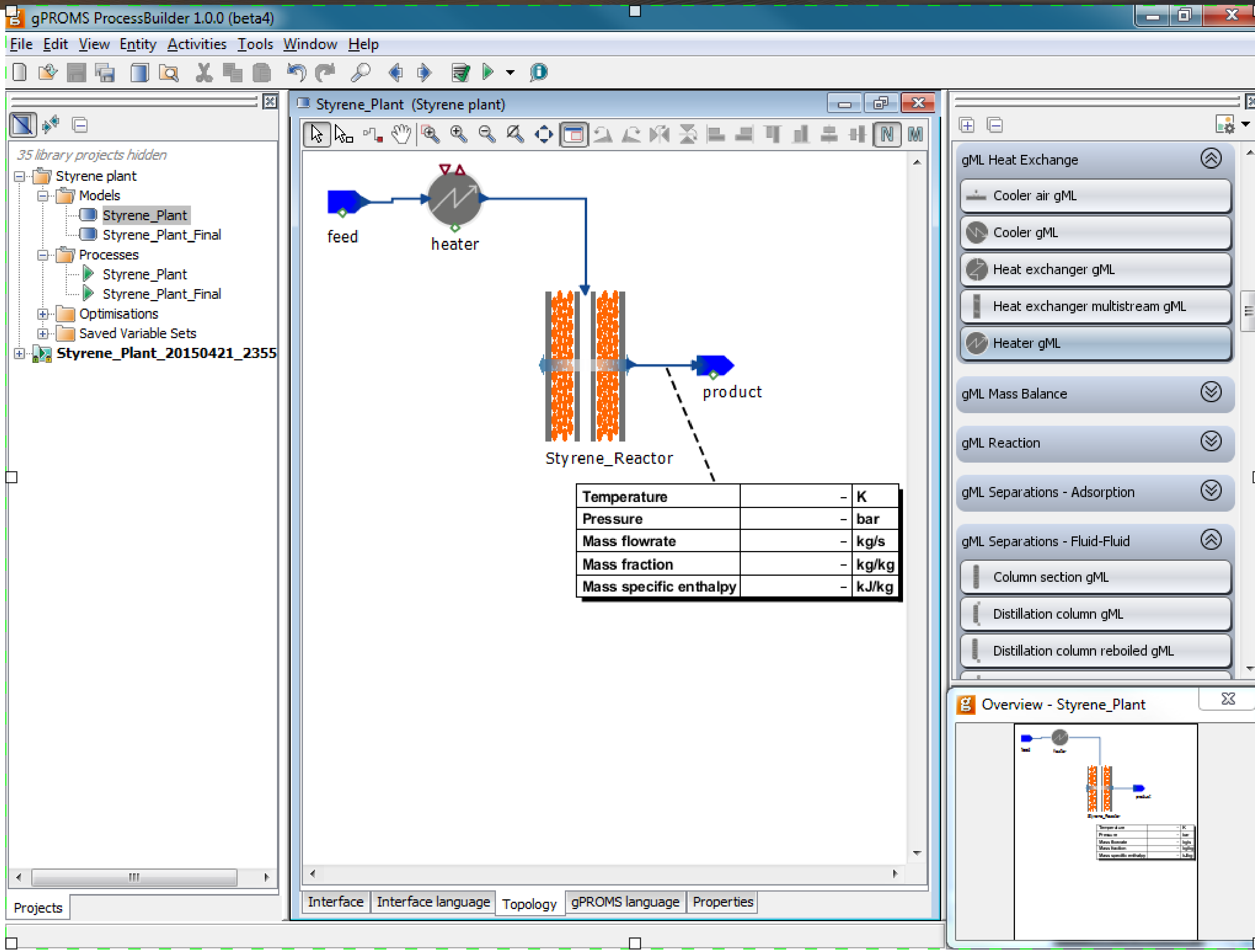


➔ Multiscale modelling approach

- microns to meters

Demonstration #1
Building the SM process model

Click on the image to watch the demo

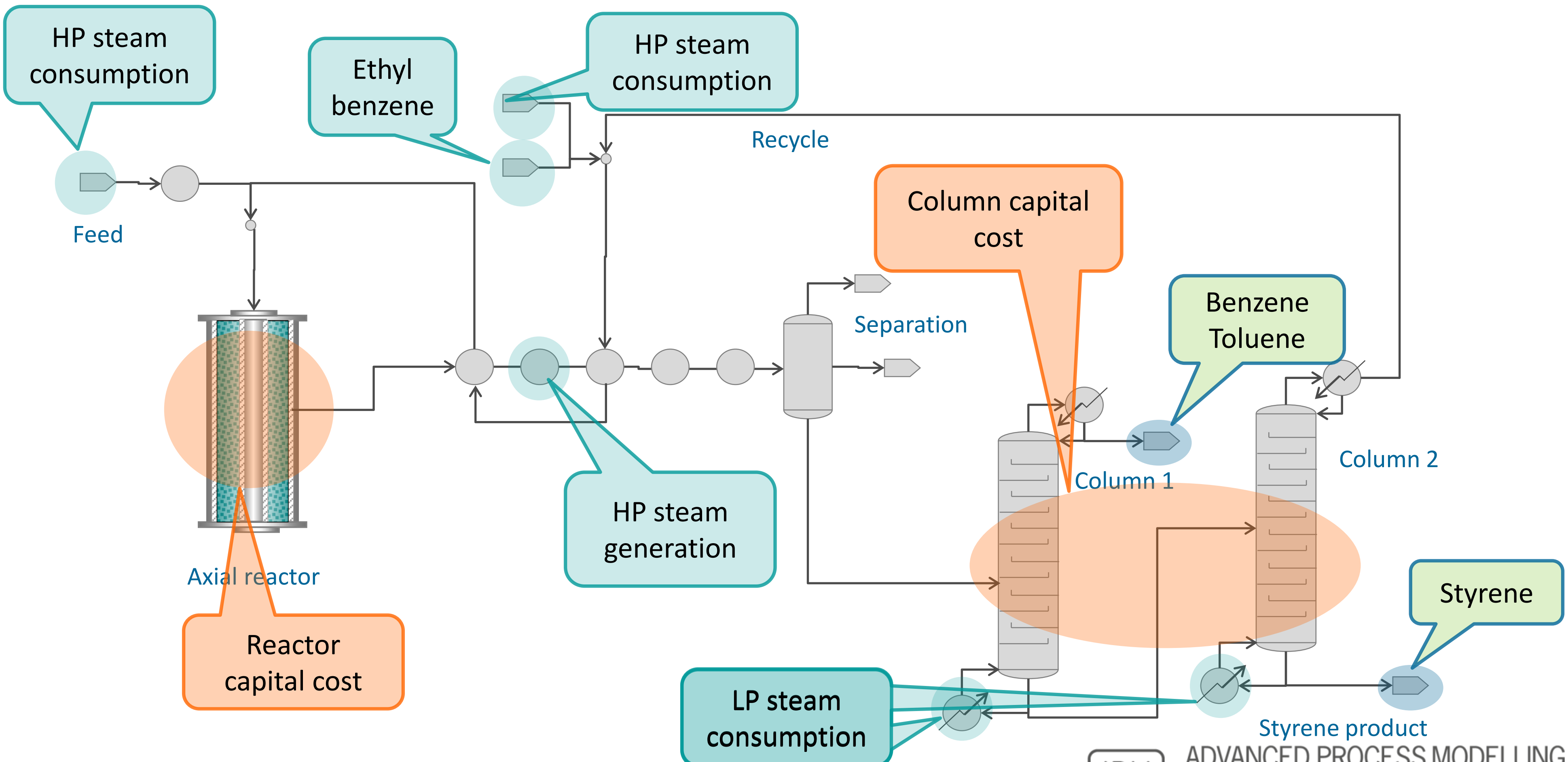


Whole-plant optimisation

Objective function

- Total annualised profit (MMUSD)

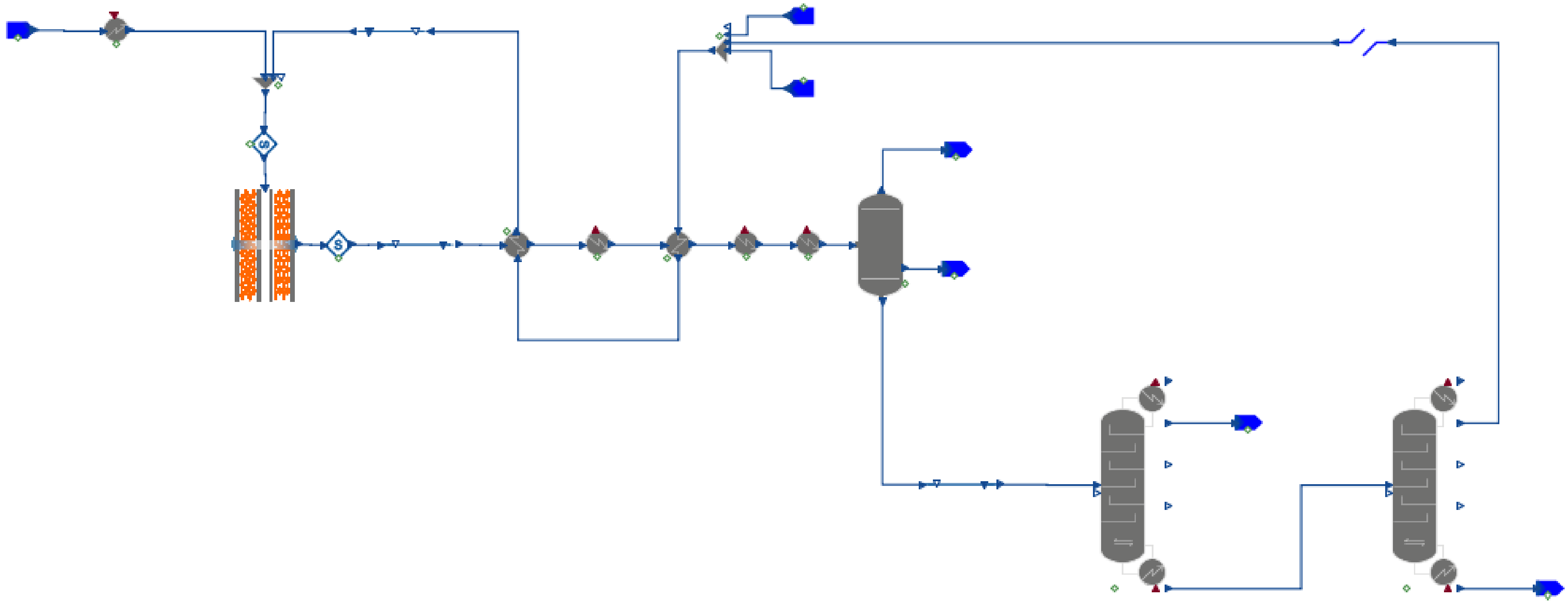
  = Annual revenue – annualised capital cost – operating cost



Demonstration #3

Defining an economic performance measure

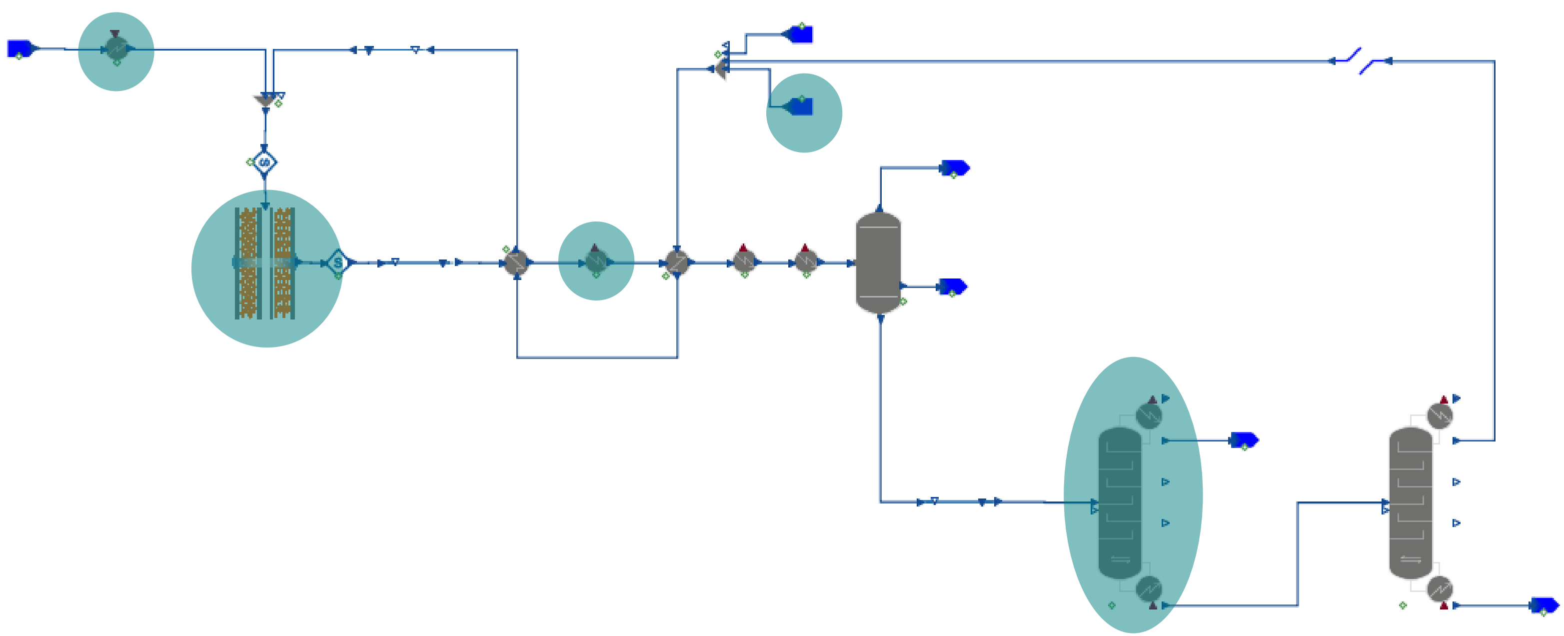
Click on the image below to watch the demo



Whole-plant optimisation

Optimisation decision variables

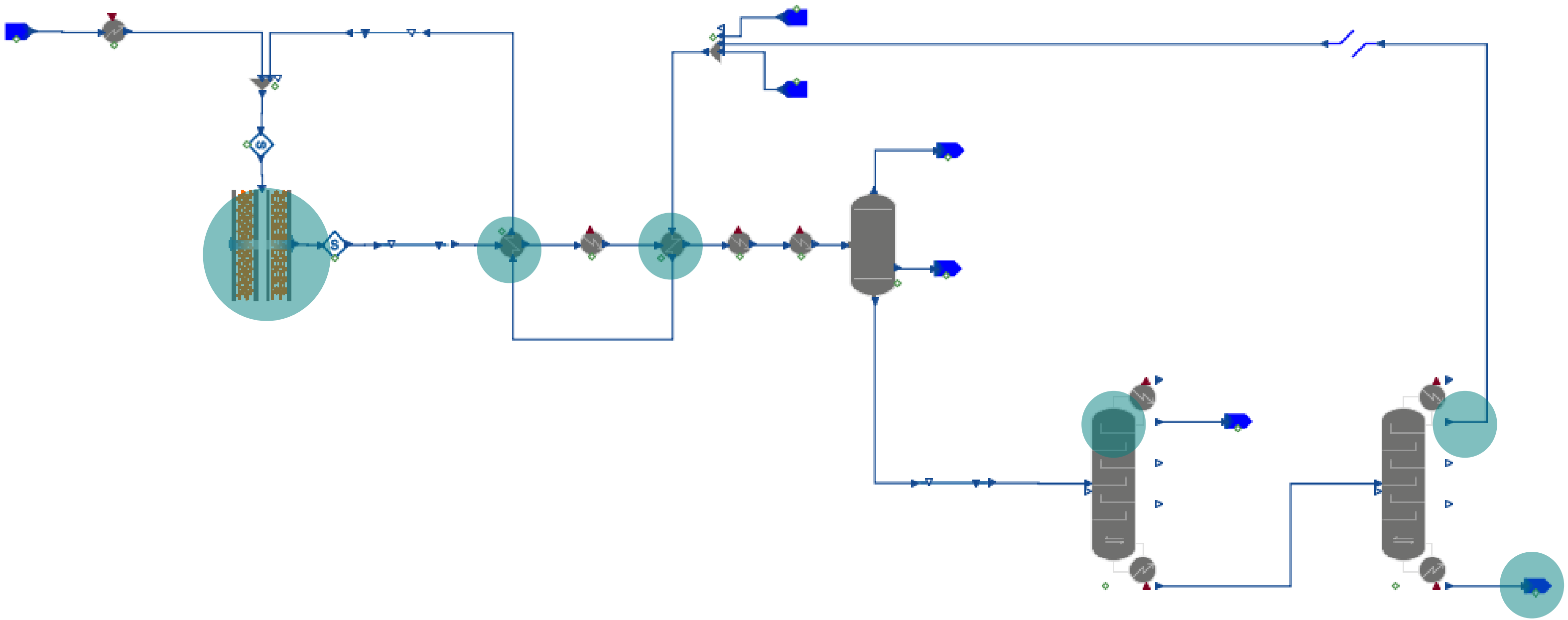
- High-pressure steam generation
- Feed stage and total number of stages of 1st column
- Boil-up ratio of 1st column
- Fresh EB flowrate
- Superheated high-pressure steam flowrate
- Reactor radius



Whole-plant optimisation

Constraints

- Conversion of ethyl benzene
- Selectivity of styrene
- Maximum temperature of reactor
- Minimum temperature difference of two stream heat exchangers
- 0.1mol% ethylene benzene at top liquid stream of 1st column
- 1000 mol ppm ethylene benzene at styrene product
- 1 mol% styrene at top liquid stream of 2nd column



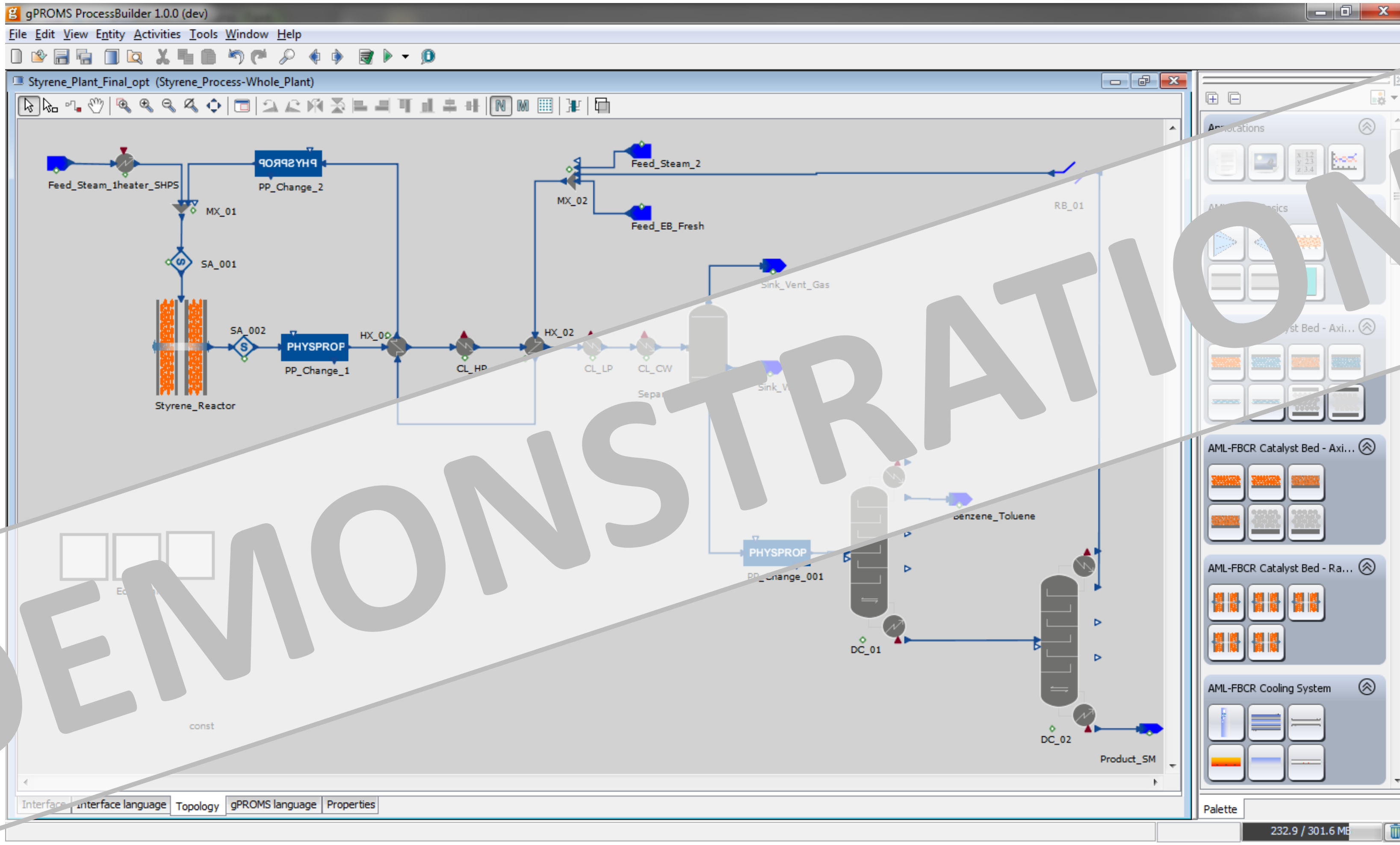
Demonstration #3

Performing an economic optimisation

PSE

Styrene monomer plant

Click on the image to watch the demo



Whole-plant optimisation

Key results

	Initial	Optimal
Objective function - Maximise		
Total annualized profit ($m)	**13.34**	**25.13**
Annual revenue (+)	50.49	58.33
Annualised capital cost (-)	8.33	7.07
Operation cost (-)	28.82	26.11
Control variables		
High pressure steam generation (kJ/sec)	-	6895
Feed stage of 1st column	40	34
Total number of stage of 1st column	100	90
Boil up ratio of 1st column	1.00	0.59
Fresh Ethyl Benzene flowrate (kg/sec)	4.70	5.89
Flowrate of superheated HP (kg/sec)	9.20	13.40
Styrene reactor radius (m)	1.372	1.339

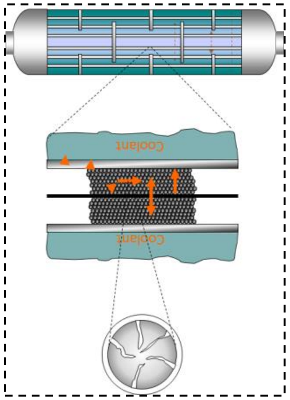
Conclusions

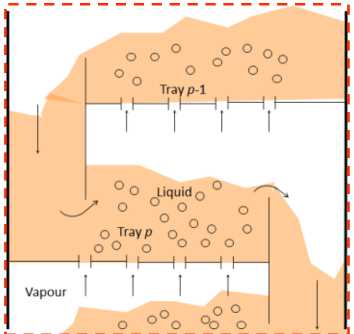
gPROMS ProcessBuilder

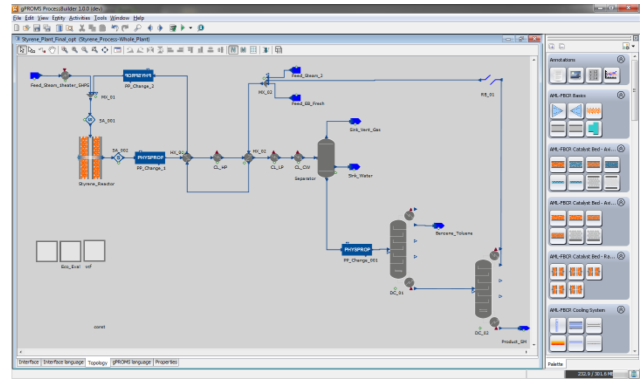
A step change in process flowsheeting

Detailed unit operation models…

…integrated within whole-plant models…







higher confidence in predictions

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

all important interactions & trade-offs taken into account

comprehensive & efficient exploration of decision space

…used for rigorous whole-plant optimisation

Thank you