

ADVANCED PROCESS MODELLING FORUM 22-23 APRIL 2015



gPROMS ProcessBuilder

Advanced Process Simulation

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gPROMS ProcessBuilder

Why did we create it? *

* Does the world need another process simulator?

Motivation 1



"We model the reactor in gPROMS then put a simplified version in Aspen Plus so we can design the separation system"

"We've created comprehensive libraries of all the basic unit operations – valves, compressors, pumps, etc." "I've got a guy starting on building a set of distillation models so we can build a whole plant model"

"We can provide the model to engineers via the CAPE-OPEN interface"

Situation until now



Traditional process simulators

- Easy to learn and use
- Rapid production of processwide heat & material balances

BUT

- Limited by Sequential Modular architecture
 - e.g. converging complex recycles
- Limited process model libraries
 - difficult to add own operations
- Limited or no optimisation capability

gPROMS ModelBuilder

- Very powerful modelling and solution
- Custom modelling for complete flexibility
- Powerful optimisation capability (including MIO)

BUT

- Limited by usability
- Need to write own models
- Difficult to learn preserve of 'expert modellers'



Need to ...

Provide all the power of the gPROMS platform and first-principles modelling ...

... without the need to write models

... but with a custom modelling capability where necessary

→ maximise competitive advantage

And make it easy to use!

gPROMS ProcessBuilder

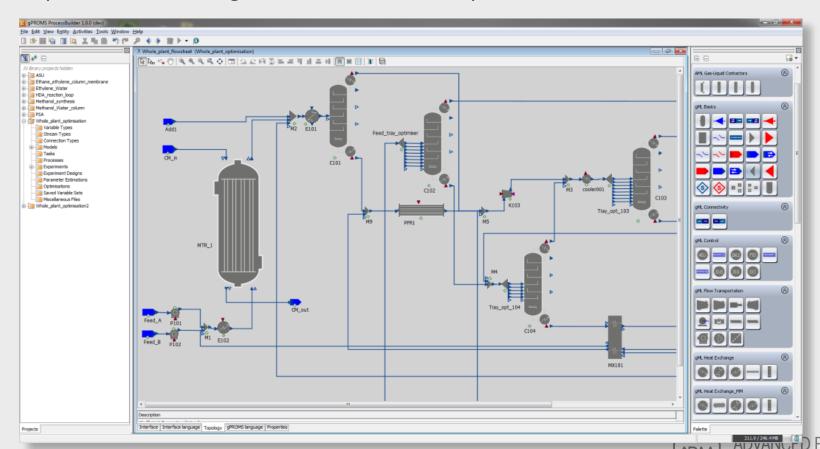




gPROMS ProcessBuilder

"Advanced Process Simulation"

A process modelling tool for chemicals & petrochemicals



Support for the basics ... and more



Support for the basics

- "Core" flowsheeting functionality
 - drag & drop flowsheeting based on model libraries
 - accurate and comprehensive physical properties
 - process analysis via steady-state& dynamic simulation
- Heat & material balance information
- Stream properties

... and more

- More comprehensive model libraries
 - higher fidelity
 - many more unit operations
- Steady state AND dynamic in same environment
- State-of-the-art custom modelling
- Powerful optimisation
- Equation-oriented solution power
 - complex integrated flowsheets
 - faster, more robust solution

Support for the basics ... and much more



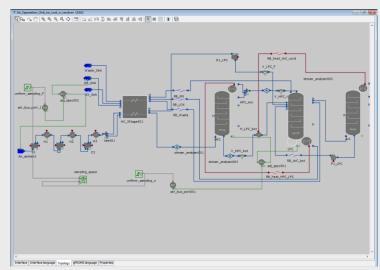
- BUT ProcessBuilder goes well beyond current practice
- Advanced applications that
 - add NEW value
 - create sustainable competitive advantage
- ... by enabling
 - rapid innovation
 - rigorous optimisation of process and equipment design
 - better management of technology risk
 - application across the process lifecycle



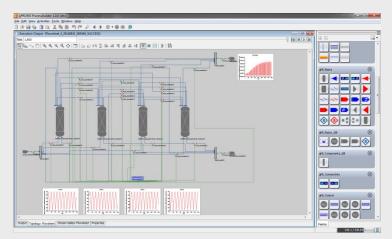


Solve new classes of problems

- Flowsheets with complex unit operations
- Flowsheets with complex recycles
- Large-scale optimisation complex reaction and separation section
- Mixed-integer optimisation
 problems process synthesis,
 equipment configuration
- Rigorous sensitivity analysis
- Online model-based applications with rigorous models
- Complex operating policies

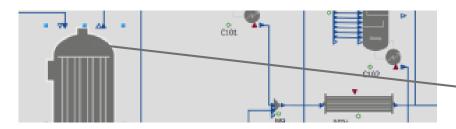


Complex recycles
Air Separation Unit (ASU)



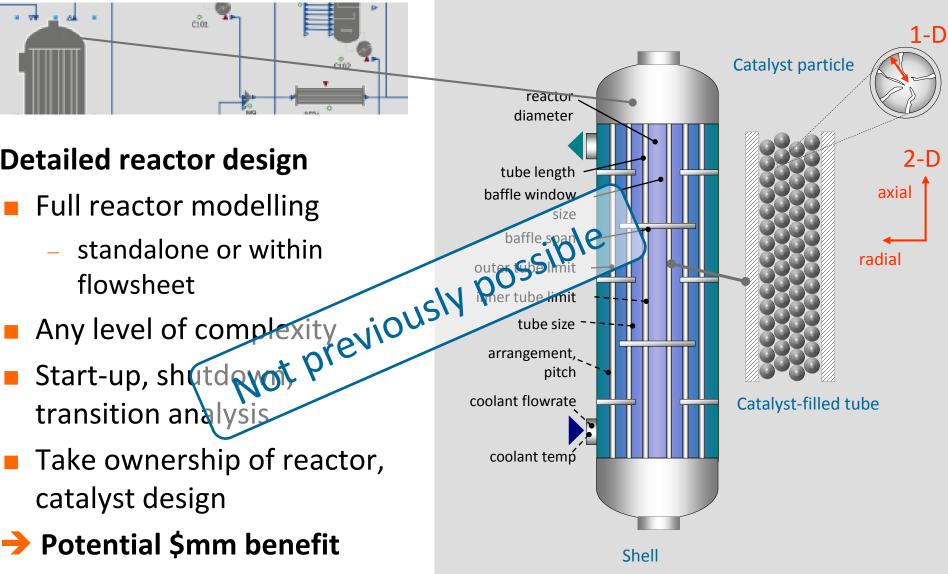
Complex dynamics
Pressure-Swing Adsorption (PSA)





Detailed reactor design

- Full reactor modelling
 - standalone or within
- transition analys
- Take ownership of reactor, catalyst design
- Potential \$mm benefit





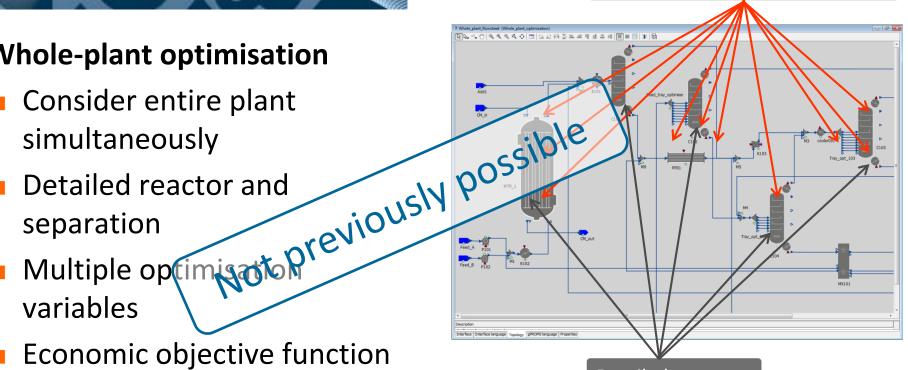


Whole-plant optimisation

Consider entire plant

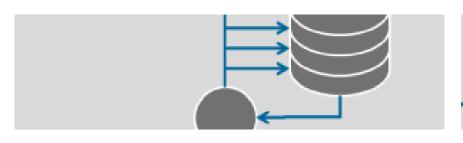
- **Economic objective function**
- Potential \$mm benefit

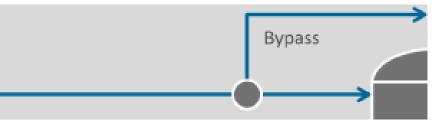
Optimisation (including mixedinteger) with multiple integer & continuous decisions



Detailed reactor & separation







Optimal equipment configuration

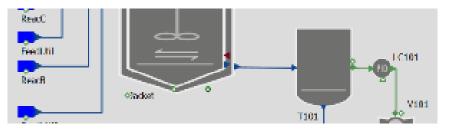
- Rigorously optimise configuration aspects
 - distillation stages draw locat
 - batch equ
 - Number of trains ...
- **Reduce CAPEX & OPEX**
- Potential \$m-\$mm benefit

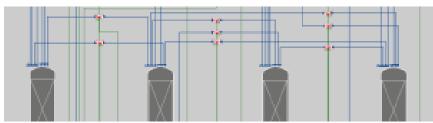
Process synthesis

- n of reaction and Not previously Possible Com quipment nser chooses between proposed process options
 - Find optimal process configuration
 - Potential \$m-\$mm benefit over lifetime









Batch process optimisation

- Rigorously optimise batch schedule
- Based on rigorous modules, schedule

 Schedule

 Maintain
- Maintain or except duality constraints
- Increase throughput
- → Potential \$m-\$mm benefit

Complex process design

- Dynamic processes eg. cyclic separation
- Wery difficult to design!
- Runtimes reduced from days/weeks to hours
- Optimise, not just simulate
- Potential \$m-\$mm savings in operating costs



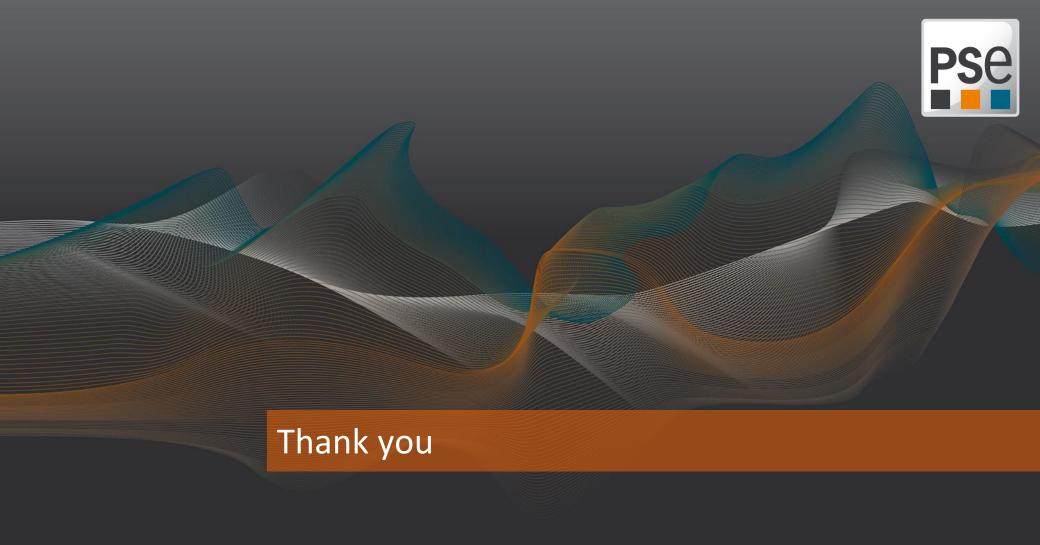
We believe that these are very important new capabilities that will become a standard part of engineers' tools and engineering workflows in the future

All made possible by the gPROMS platform

gPROMS ProcessBuilder – Launch



- ProcessBuilder launch in EMEA/Americas
- 'New product', but we have some history
 - APAC launch mid-2014
 - Already have 10+ customers
 - Feedback, improvement
- Next up
- 1. gPROMS ProcessBuilder: what's in it? Maarten Nauta
- gPROMS ProcessBuilder: advanced applications Bart de Groot





















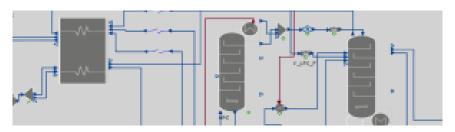


gPROMS ProcessBuilder



A new product







Detailed reactor design

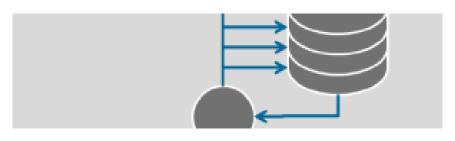
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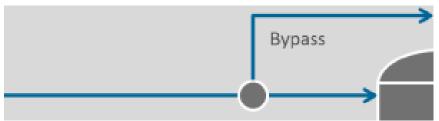
Whole-plant optimisation

- Consider entire plant
- ailed reactor and separation
- Multiple optimisation variables
- Economic objective function
- Potential \$mmm benefit









Optimal equipment configuration

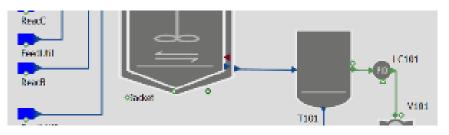
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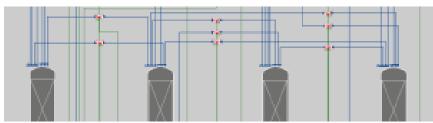
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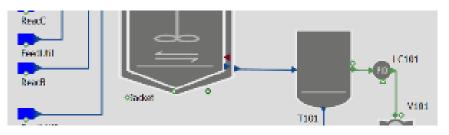
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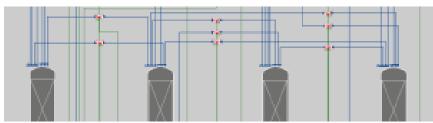
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Motivation 3 – exploring further



"We need to ..."

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

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

"... do an economic optimisation of the whole plant so we can decide which option to go for"

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

"... look at operability"

"We need a simulator that can answer <u>all</u> our questions"