ADVANCED PROCESS MODELLING FORUM
LONDON
20–21 APRIL 2016

Advanced Process Modelling

Transforming the way the process industries design & operate

Costas Pantelides – Managing Director

gPROMS

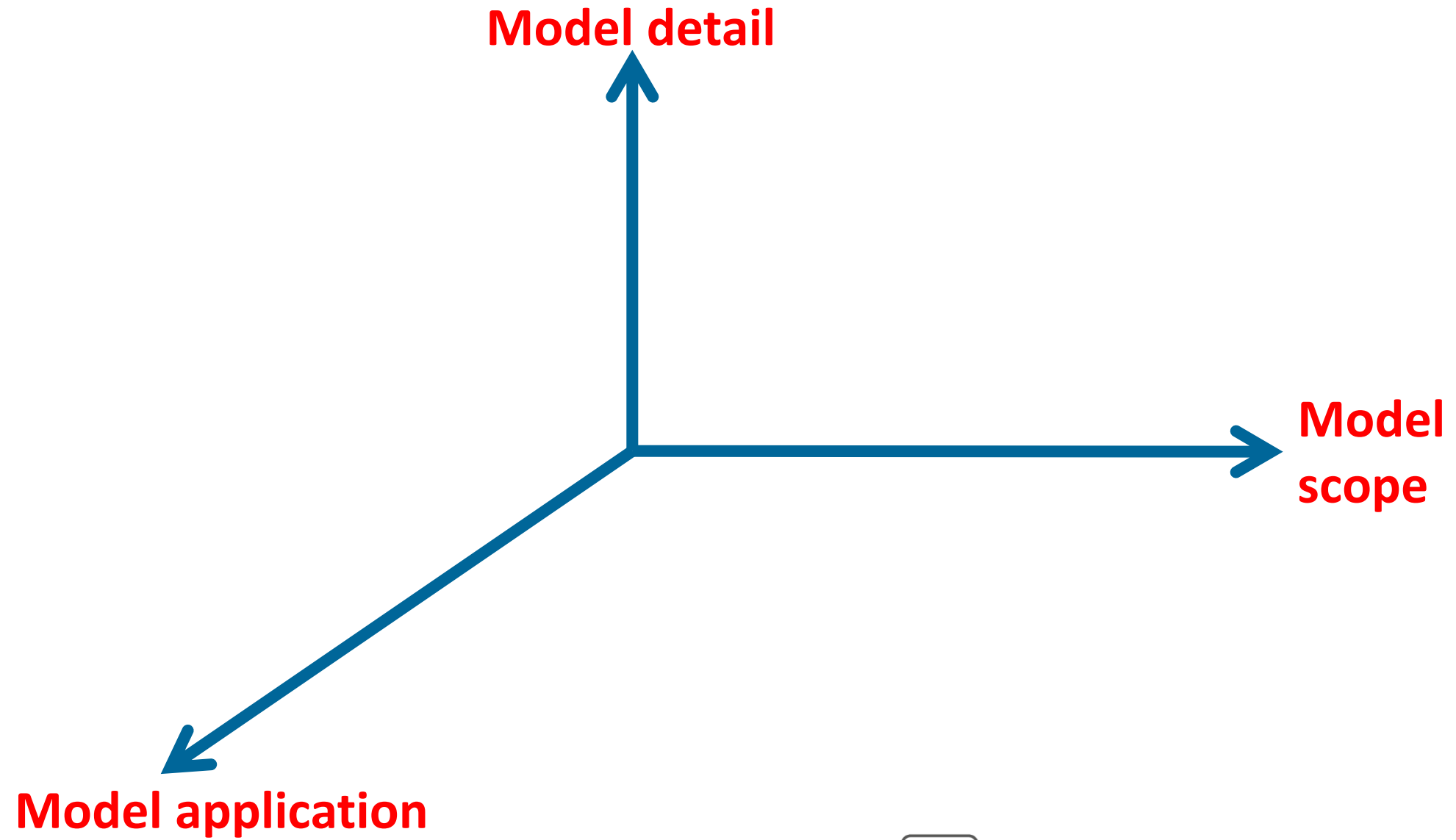
Advanced Process Modelling

1. What is it ?
2. What can it do ?
3. Why is it possible now ?

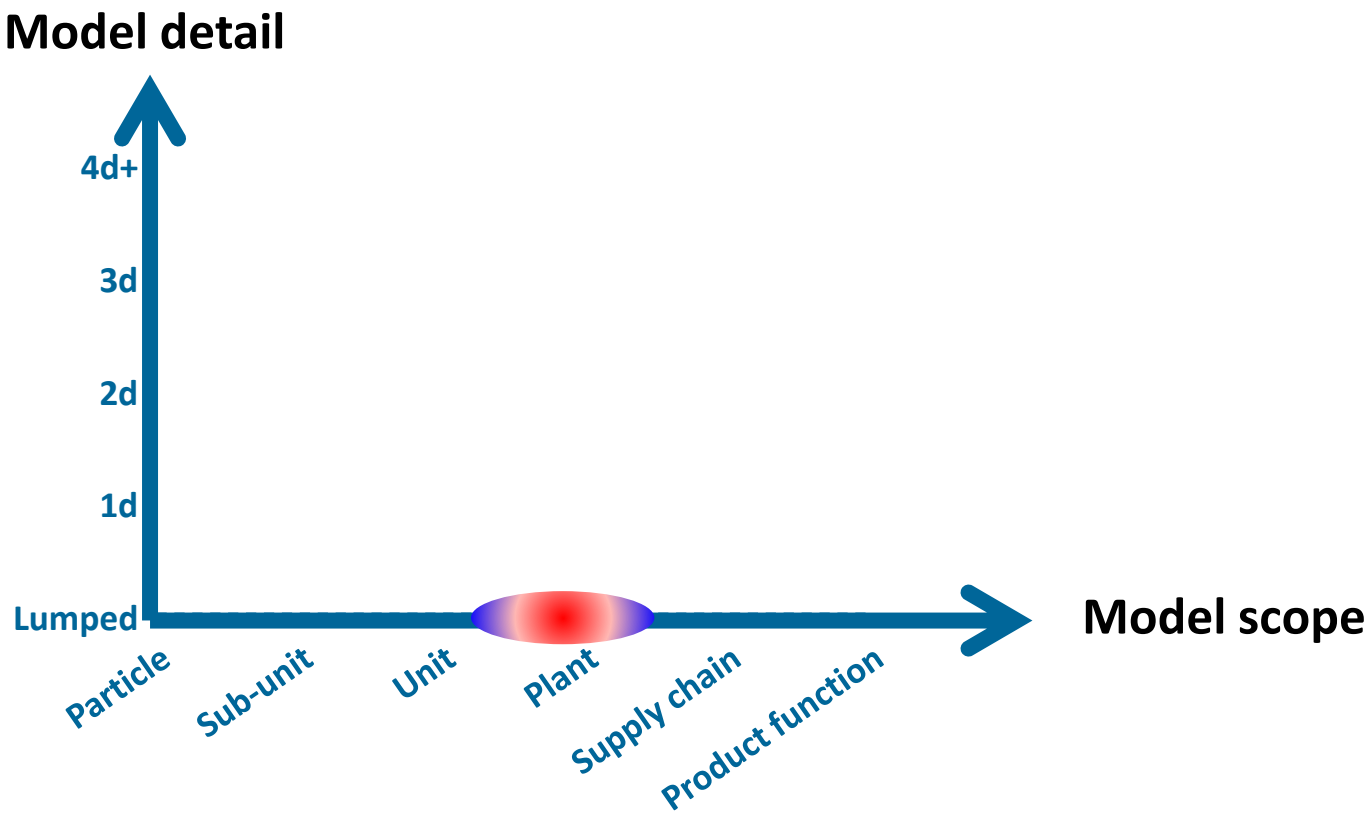
Advanced Process Modelling

What is it?

Dimensions of process modelling

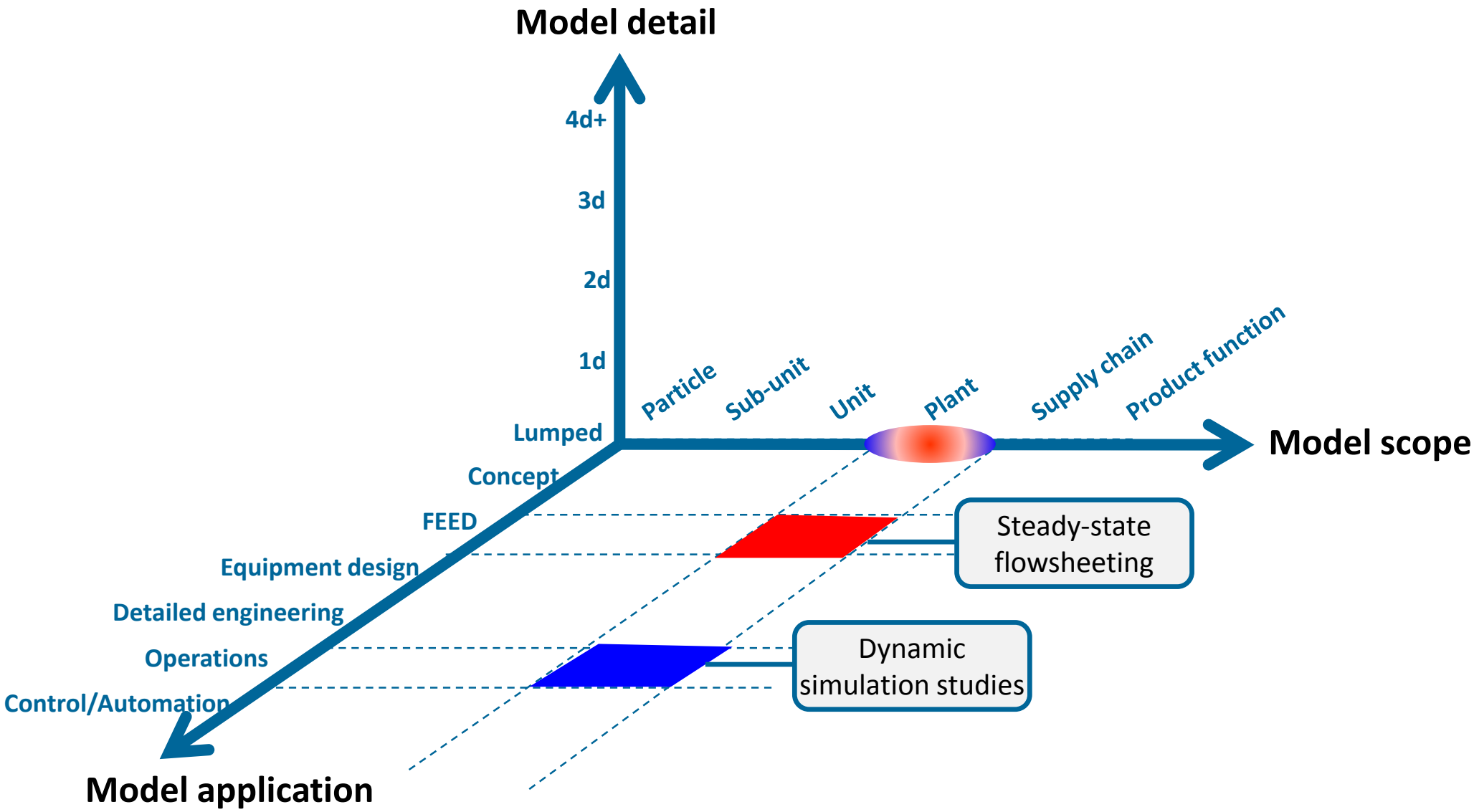


Process Modelling
Flowsheeting tools



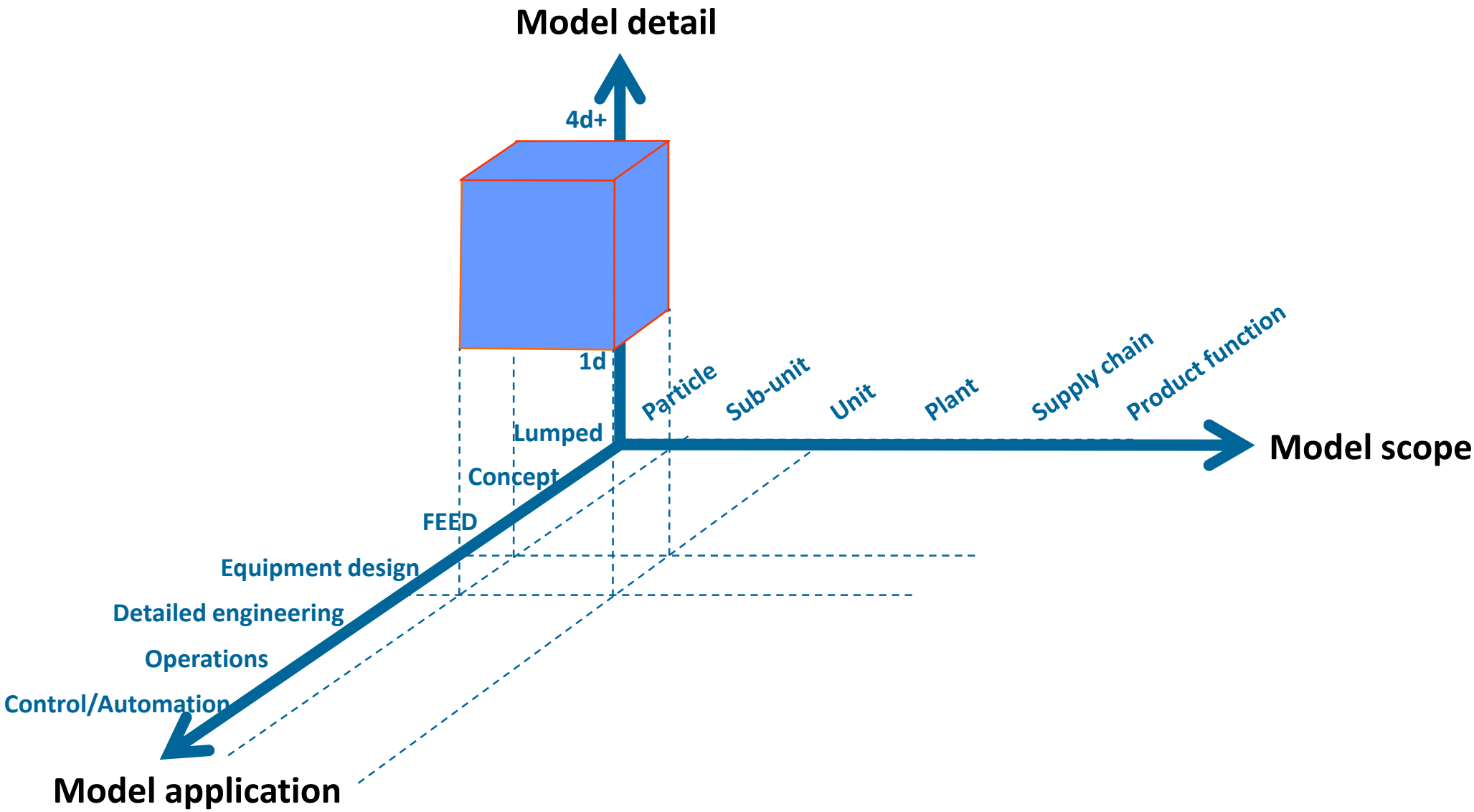
Process Modelling

Flowsheeting tools

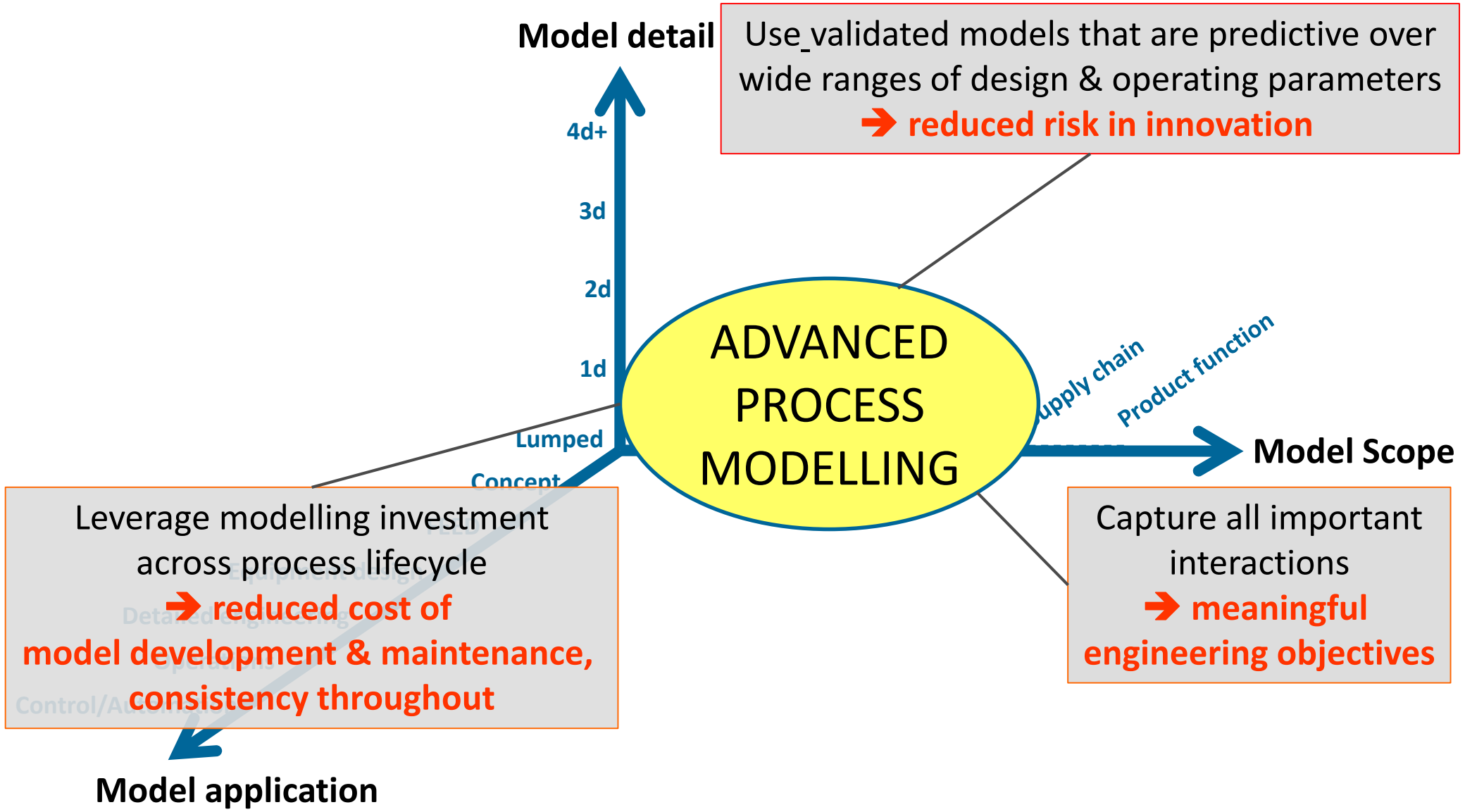


Process Modelling

Computational Fluid Dynamics & “multiphysics” tools



Current drivers for process modelling technology



Use validated models that are predictive over wide ranges of design & operating parameters
➔ **reduced risk in innovation**

Leverage modelling investment across process lifecycle
➔ **reduced cost of model development & maintenance, consistency throughout**

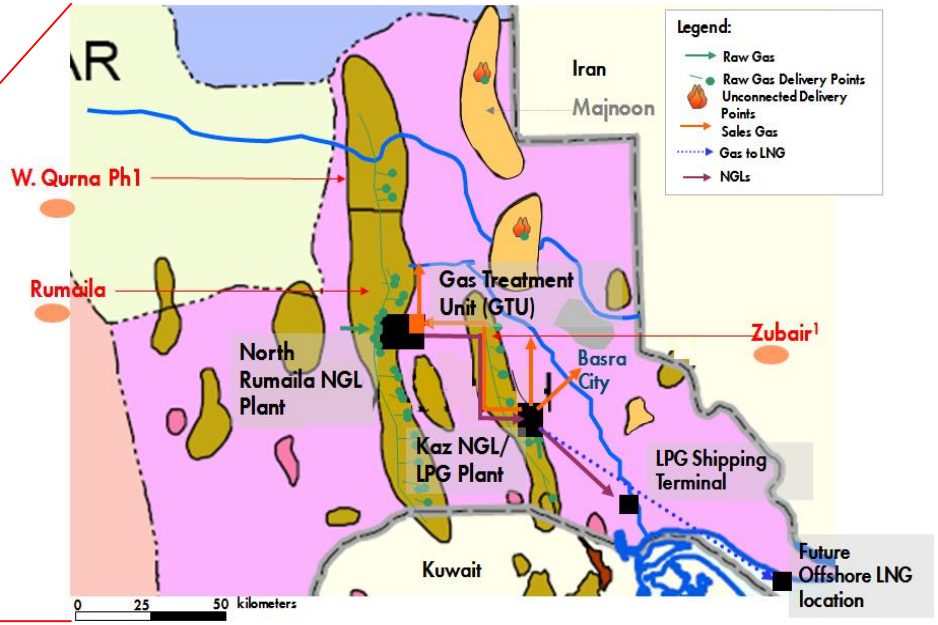
Capture all important interactions
➔ **meaningful engineering objectives**

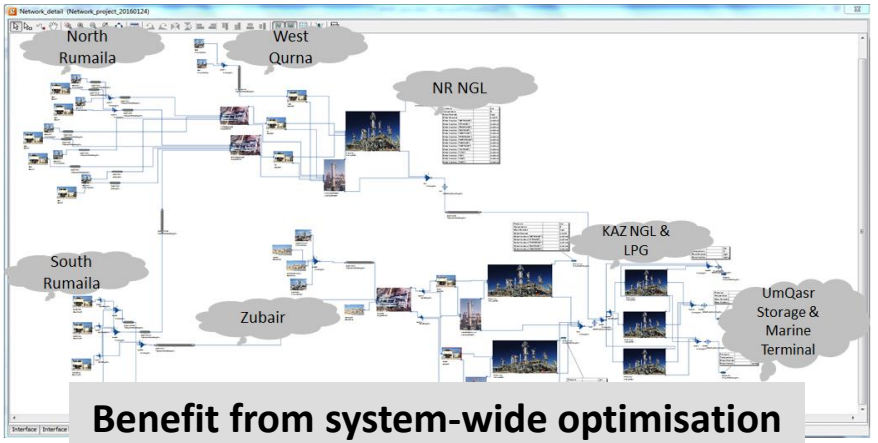
Advanced Process Modelling

What can it do?

Advanced Process Modelling – Example #1

Region-wide optimisation of natural gas production & processing





Presentation by Daniel Aluma tomorrow afternoon

Benefit from system-wide optimisation O($100m/year)

Advanced Process Modelling – Example #2

Systems-based Pharmaceutics

Decisions & Disturbances

Critical Process Parameters (CPPs)

solvent/additive, unit ops, recipes, *impurities…*	dosage form wet/dry granulation…	dose & dosage regimen *patient-to-patient variability*	
Drug substance manufacturing	**Drug product manufacturing**	**Drug delivery: Oral absorption & PK**	**Drug delivery: pharmacodynamics**
Polymorph, Morphology, PSD, Purity Process KPIs	Content Uniformity Tablet hardness/ porosity Flowability (FFC)	C_{max} AUC	Efficacy Safety

Objectives & Constraints

Product KPIs: Critical Quality Attributes (CQAs)

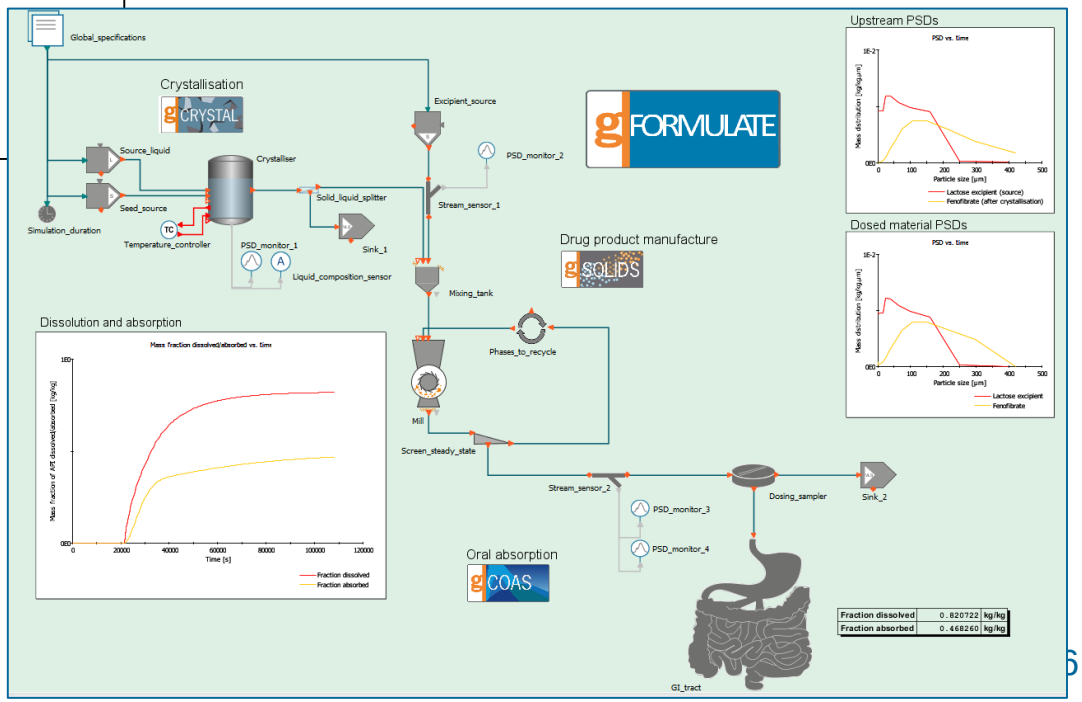
Process KPIs: Economics, Safety, Operability, Environmental Impact

Systems-based Pharmaceutics

A holistic, integrated view of drug manufacturing & biological effect

↓

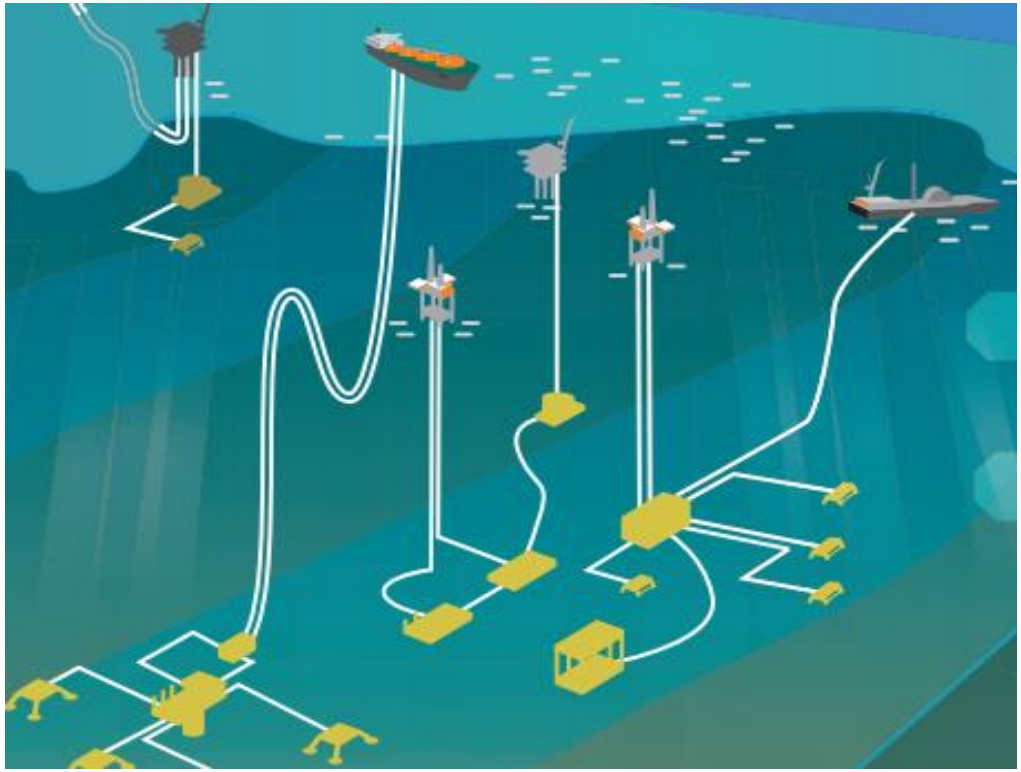
Accelerated development of **higher-quality** pharmaceuticals

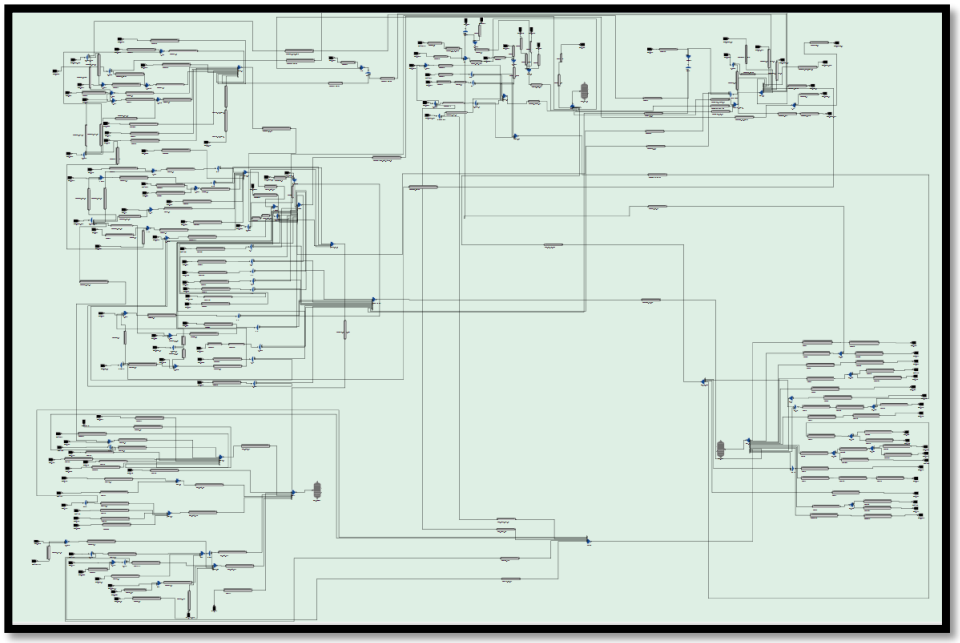


Presentation
by Sean Bermingham
& sessions on Formulated Products today

Advanced Process Modelling – Example #3

Oilfield optimisation





Presentation by James Marriott tomorrow afternoon

Oilfield Production Optimisation

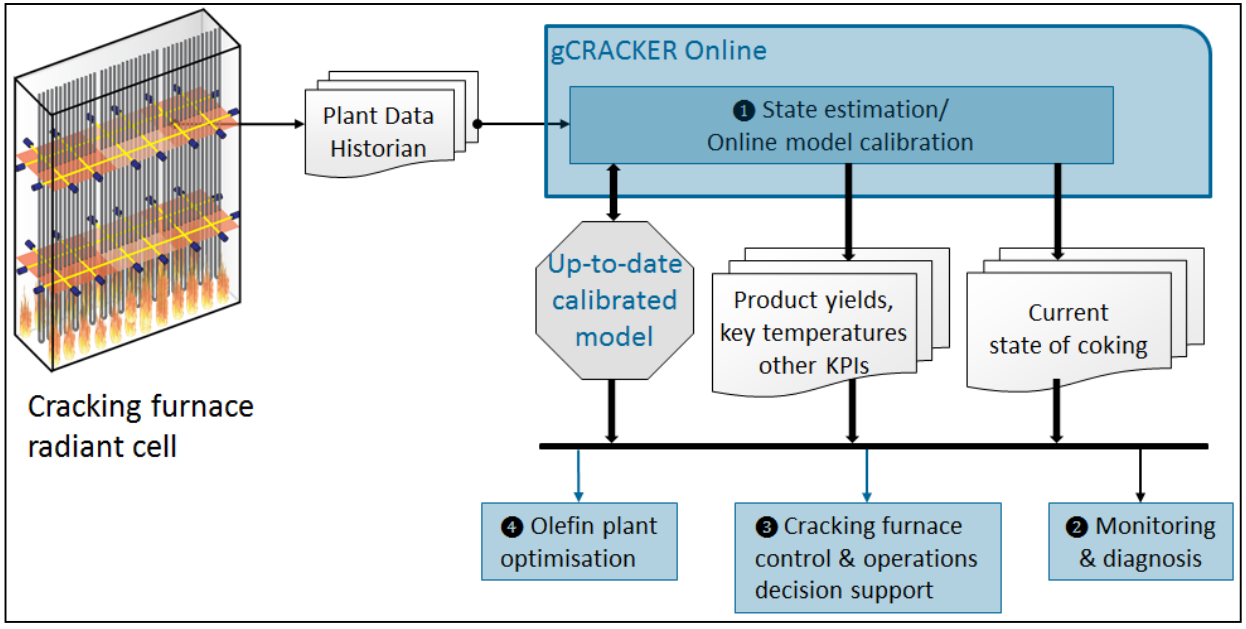
New advanced optimisation technology leading to higher-quality solutions

↓

O($m/day) benefit

Advanced Process Modelling – Example #4

Online monitoring of olefins steam cracking furnaces



Presentation by Mark Matzopoulos tomorrow morning

Model-based monitoring

Accurate real-time estimates of product yields

Real-time monitoring of accumulated coke & coking rates

↓

Improved severity control in cracking furnaces

More realistic basis for day-to-day olefin plant optimisation

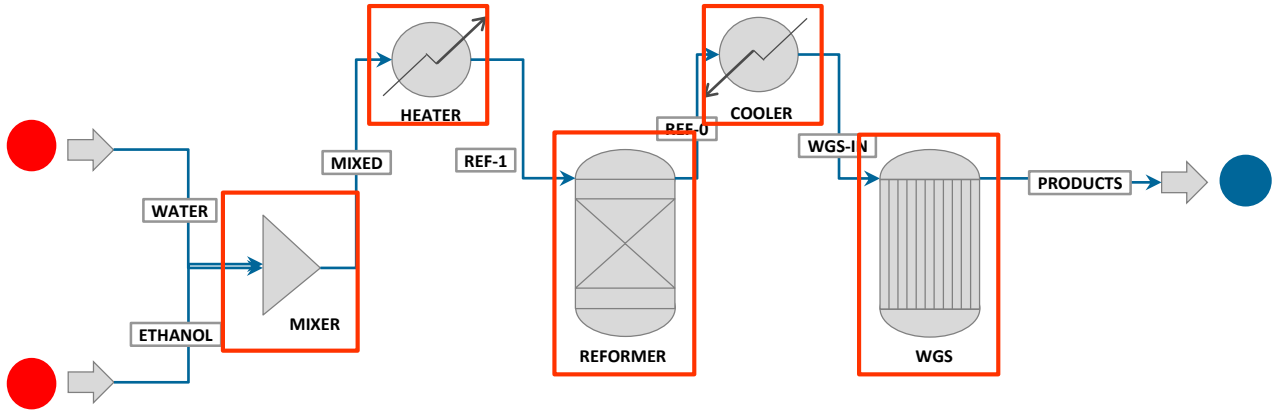
Safer operation

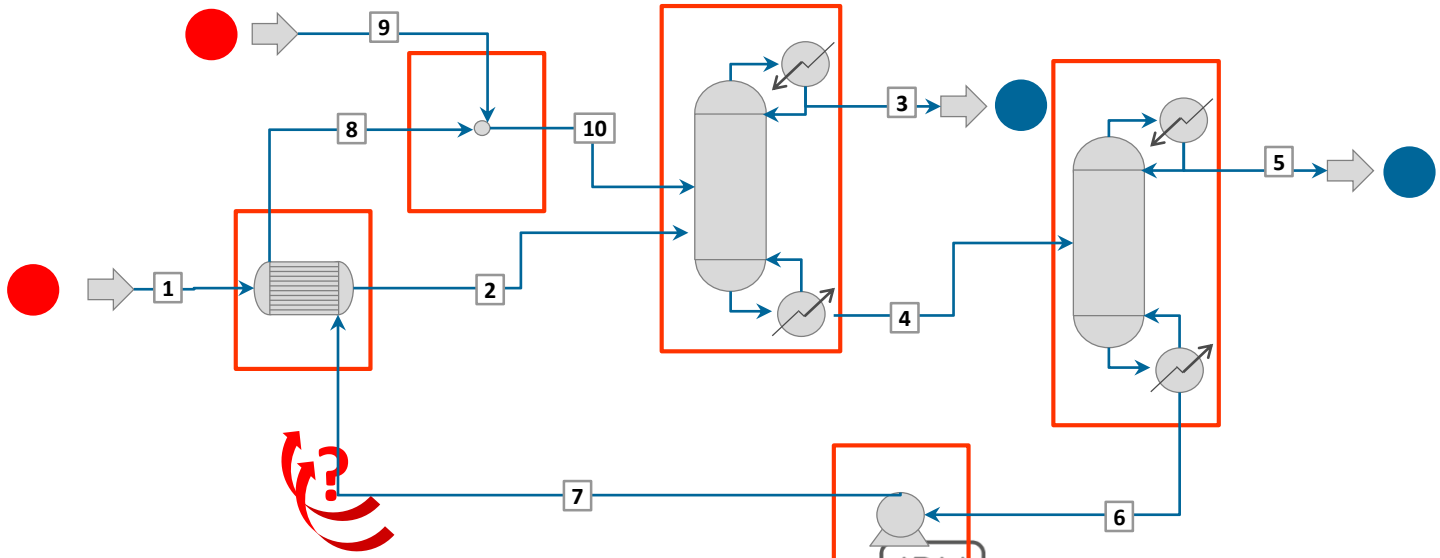
Advanced Process Modelling

Why is it possible now?

Sequential Modular vs. Equation Oriented modelling

The Sequential Modular (SM) approach



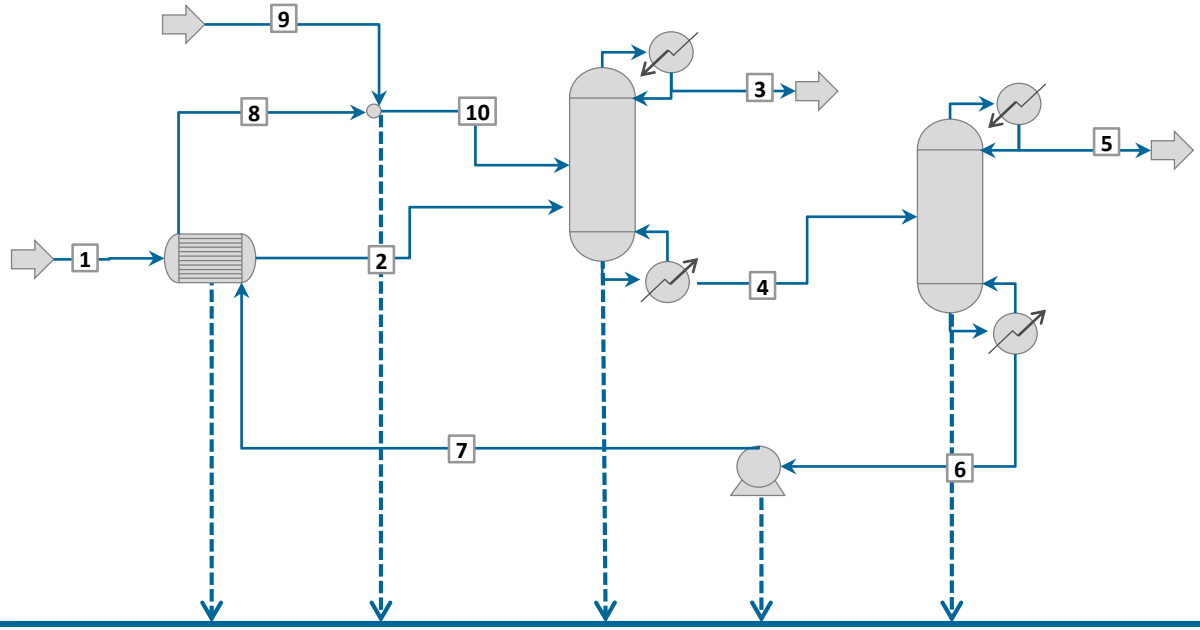


SM vs EO – 1

Sequential Modular

- Advantages
  - **easy to use**; quick for simple calculations
  - **failure is rare**; clear diagnostics issued
- Disadvantages
  - 'downstream' specifications difficult to handle
  - **recycles slow to converge**; multiple recycles **difficult**
  - adding **new custom models** – need to code solution method
  - poor **optimisation** capability
  - **many** other limitations

The Equation Oriented (EO) approach



f(x) = 0

One large set of equations (10^3-10^6 variables)
Solved simultaneously

Conceptually much simpler …

SM vs EO – 2

Sequential Modular

- Advantages
  - **easy to use**; quick for simple calculations
  - **failure is rare**; clear diagnostics issued
- Disadvantages
  - '**downstream**' specifications
  - **recycles slow to converge**; multiple recycles **difficult**
  - adding **new custom models** – need to code solution method
  - poor **optimisation** capability
  - **many** other limitations

Equation-oriented

- Advantages
  - can **specify any variable** subject to degrees of freedom – 'downstream' specifications **easy**
  - **fast, robust convergence of multiple recycles**
  - powerful **custom modelling** – easy to create new unit operations
  - very **powerful optimisation**
- Disadvantages
  - may **fail to find an initial solution** easily
  - often **difficult to diagnose reason** for failure

Sequential Modular vs. Equation Oriented

A 30+ year consensus

Sequential Modular

- Robustness (real/perceived)

Key consideration

Equation Oriented

Well-understood advantages

- Recycle handling
- Non-standard (e.g. design) specifications
- Optimisation
- Custom modelling

Aspen HYSYS®
Aspen Plus®
CHEMCAD®
Petro-SIM®
PRO/II®
Prosim®
UniSim®

A well-understood & widely accepted trade-off since the early 1980s

SPEEDUP® → ACM®
gPROMS ModelBuilder®

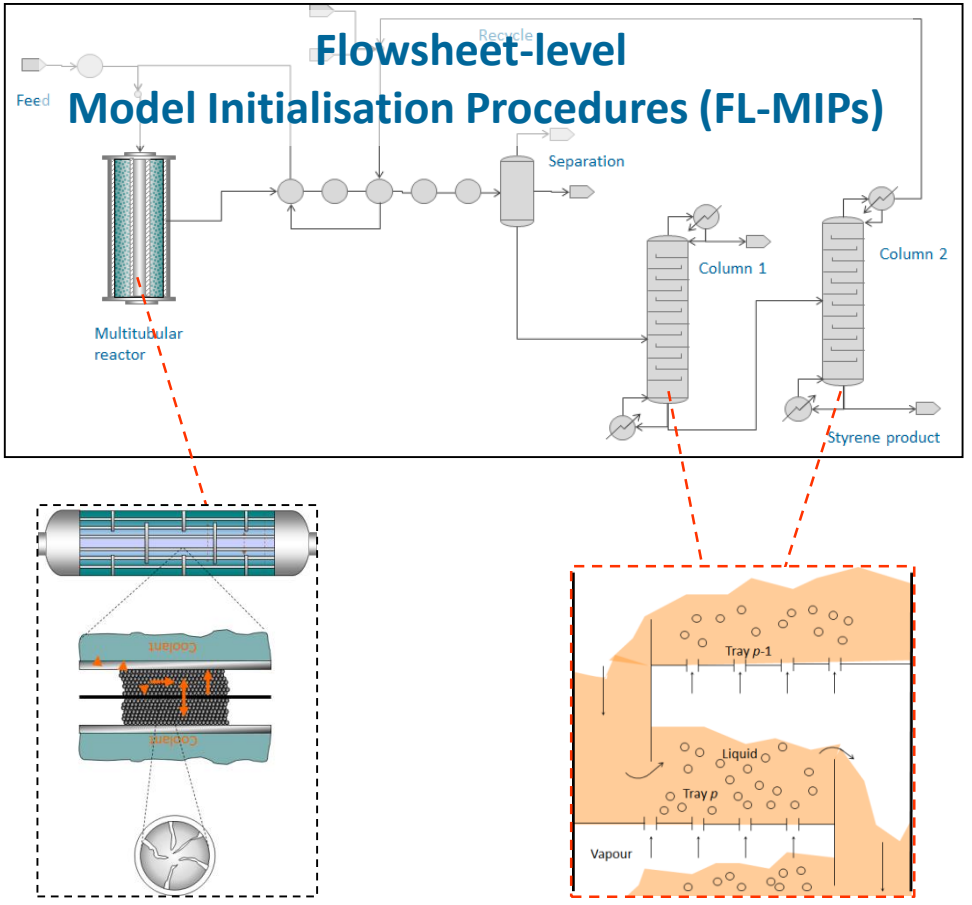
Aspen Plus® (EO mode)
RomEO®

So what's changed?

Model Initialisation Procedures (MIPs)

- **Objective: comprehensively address robustness issues in EO flowsheeting technology**
  - a long-term fundamental R&D project

- Complexity arises at two levels
  - **Flowsheet-level complexity**
    - increasingly wider envelopes
    - tighter integration of material & energy
  - **Unit-level complexity**
    - increasingly detailed models of process equipment



Sequential Modular vs. Equation Oriented

A 30+ year consensus

Sequential Modular

- Robustness

Equation Oriented

- Recycle handling
- Non-standard (e.g. design) specifications
- Optimisation
- Custom modelling

➔Robustness

Potentially disruptive technology

➔Enables many of the things you will see in this APMF

Advanced Process Modelling

In summary…

Advanced Process Modelling

- **What is it?**

  APM is about describing process systems…

  - to a breadth that ensures that all relevant interactions are within the model envelope
  - to a depth that provides confidence in the model predictions
  - in a way that allows the modelling investment to be leveraged across the process lifecycle and the organisation in a consistent, cost-effective manner

- **What can it do?**

  APM allows significant value to be extracted at all stages of the process lifecycle via the combination of

  - process models that are sufficiently broad & deep (see above)
  - advanced computational techniques that allow comprehensive exploration of large decision spaces

- Why is it possible now ?

  APM has been made possible

  - by significant recent breakthroughs in modelling methodologies & solution methods
  - coupled with advances in computing hardware and software engineering

Thank you

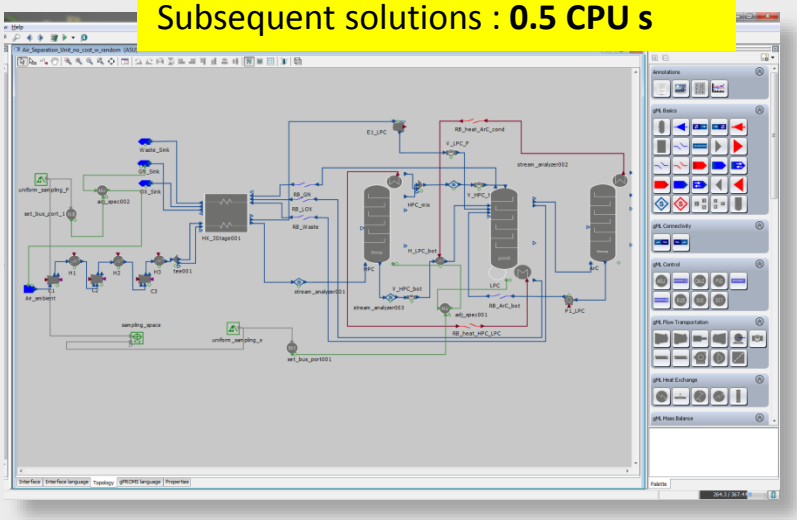
The gPROMS ProcessBuilder

gPROMS ProcessBuilder

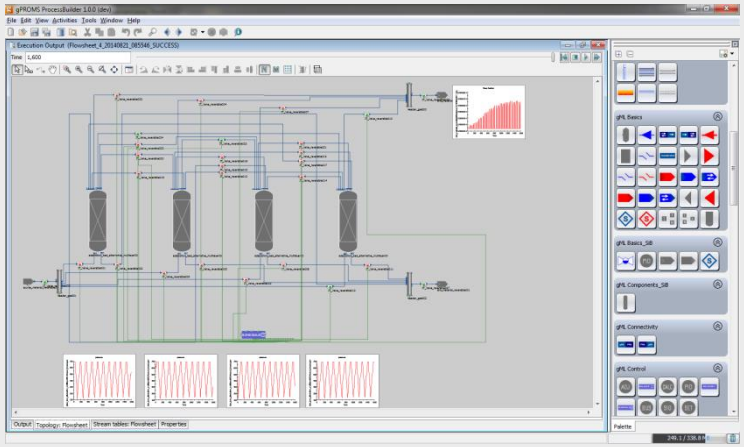
Equation-oriented process flowsheeting

1. Equation-oriented technology
   - Convergence of tightly integrated flowsheets
     - multiple recycles, thermal couplings etc.
     - fast solution ➔ rigorous sensitivity analysis
   - Handling of non-standard specifications
2. Drag-and-drop flowsheeting
   - Standard model libraries
   - User-defined custom models
2. Analysis of process behaviour via steady-state & dynamic simulation
3. Optimisation of design & operation via steady-state & dynamic optimisation
   - Rigorous mathematical optimisation
     - no need for trial & error simulation
   - Continuous and discrete decisions

Detailed model, ~18,000 equations
First solution : **35 CPU s**
Subsequent solutions : **0.5 CPU s**



Complex recycles
Air Separation Unit (ASU)

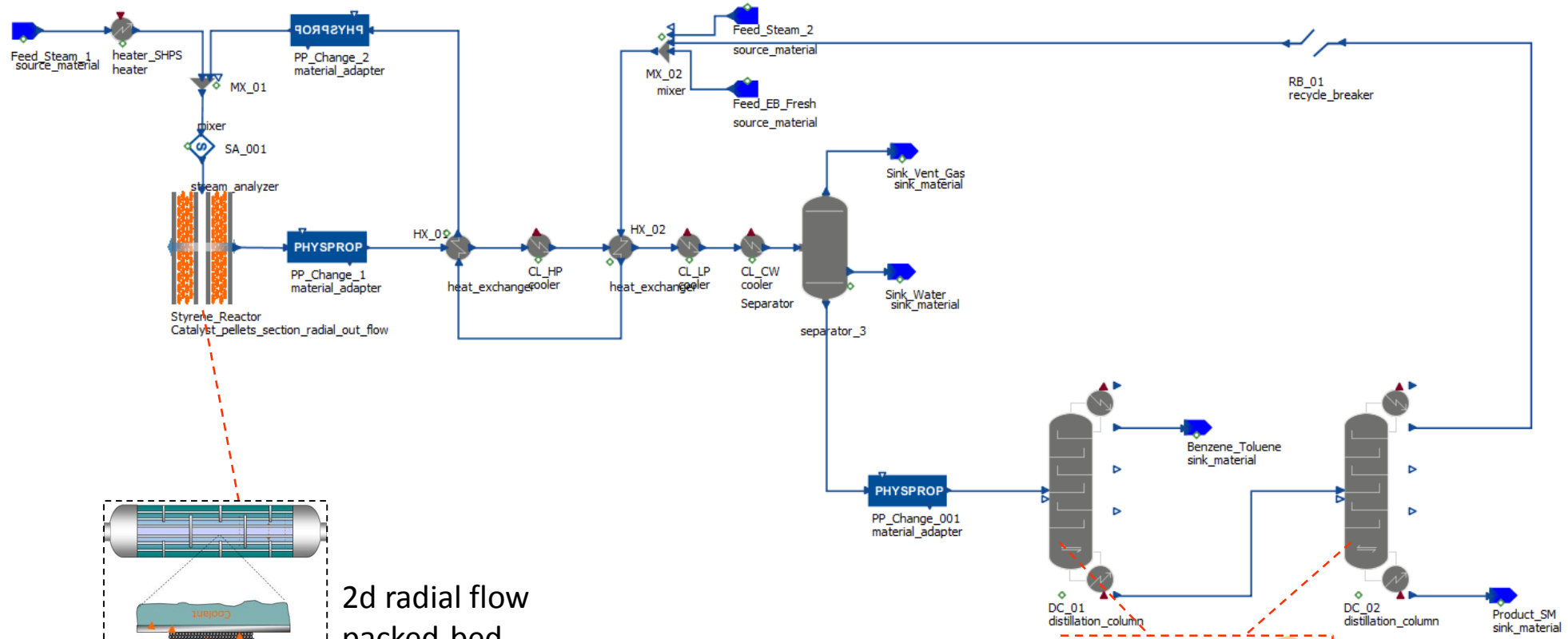


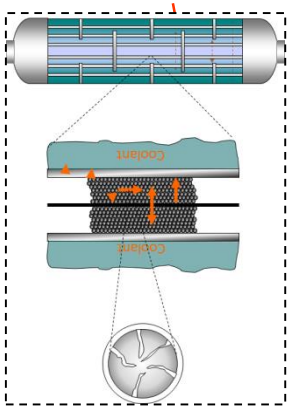
Complex dynamics
Pressure-Swing Adsorption (PSA)

gPROMS ProcessBuilder

1. Use of detailed, validated equipment models within integrated flowsheets

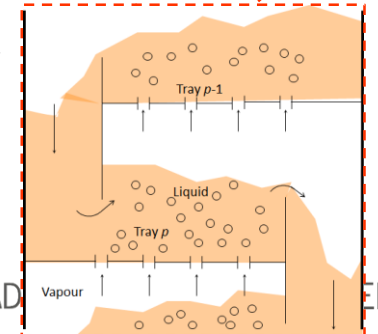
Styrene monomer plant





2d radial flow packed-bed catalytic reactor model

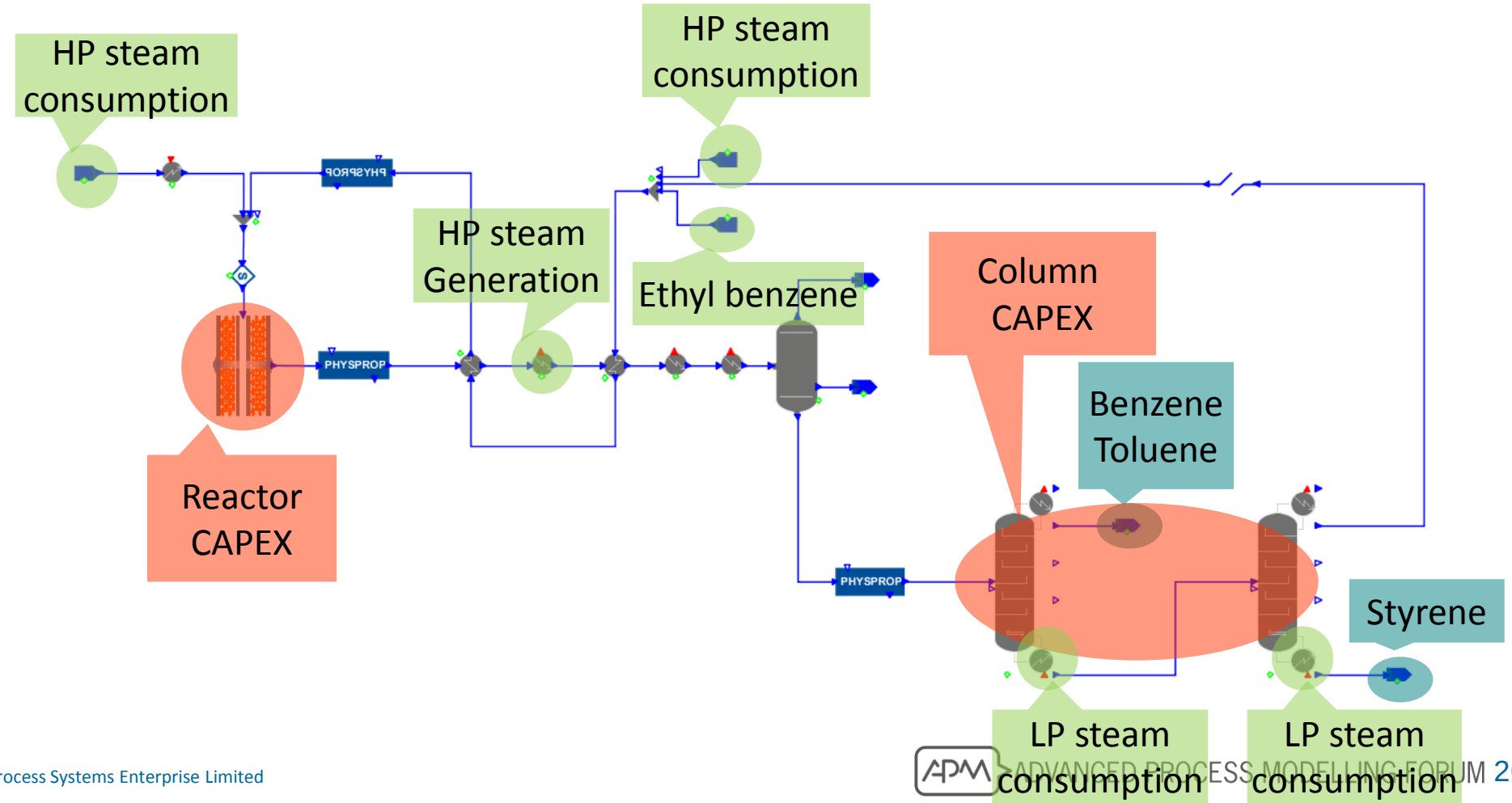
Tray-by-tray distillation column models



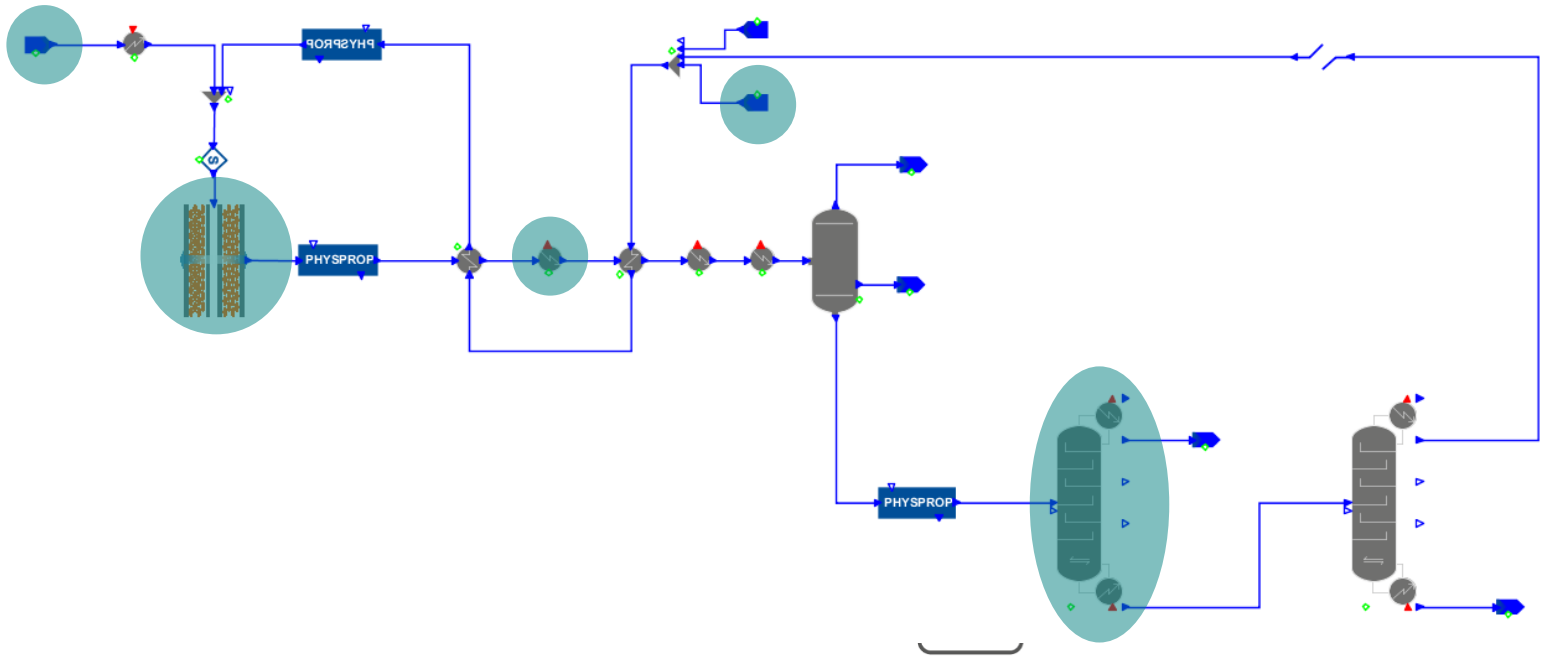
Standard library models

- Objective function : Total annualised profit (MMUSD)

  = Annual revenue – annualised capital cost – operating cost



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



gPROMS ProcessBuilder

Applications presented at this Advanced Process Modelling Forum