ADVANCED PROCESS MODELLING FORUM 2017
London 25–26 April

Advanced Process Modelling

From vision to realisation

Mark Matzopoulos – Deputy Managing Director

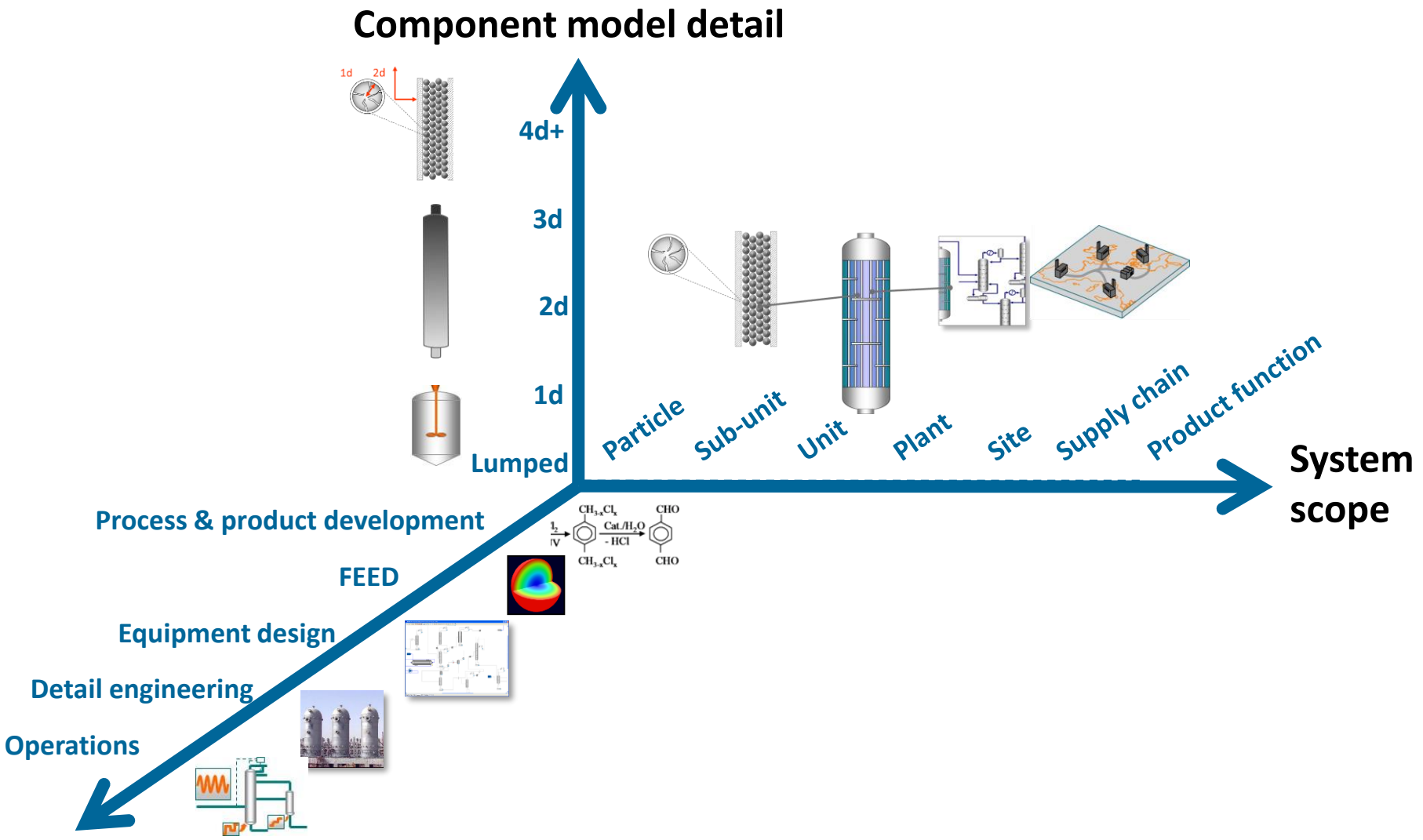
gPROMS

Advanced Process Modelling (APM)
Outline

- Advanced Process Modelling: the vision
  - Current drivers & trends
  - Proof of Concept studies
- Advanced Process Modelling: from vision to realisation
- Advanced Process Modelling: where to next ?

Advanced Process Modelling: the vision

Dimensions of process modelling

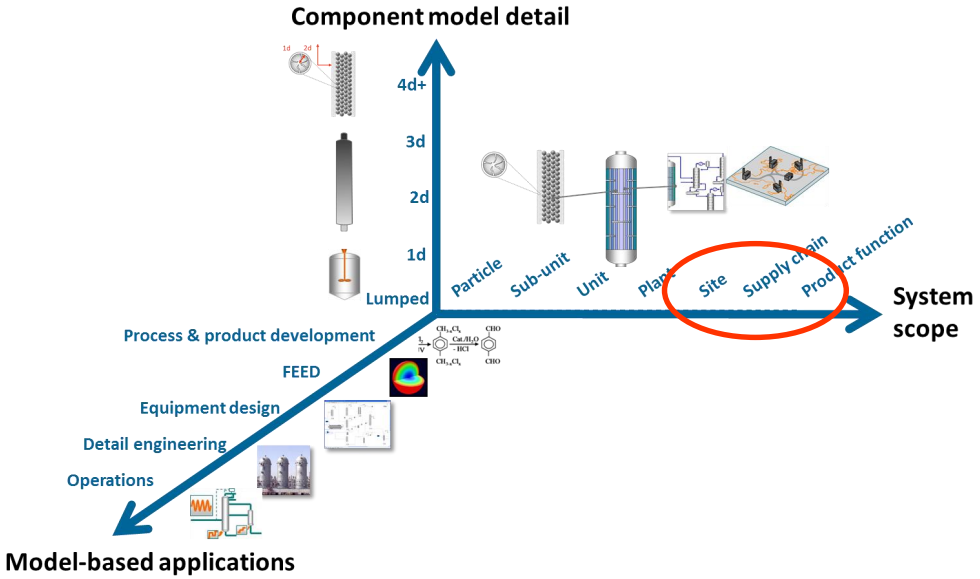


Advanced Process Modelling

Current drivers & trends

Use validated models that are predictive over wide ranges of design & operating parameters

➔ **increase reliability/reduce risk in model-based decisions**



Capture all important interactions

➔ **formulate meaningful engineering objectives**

Leverage modelling investment across process lifecycle

➔ **reduce cost of model development & maintenance**

“Capture all important interactions”

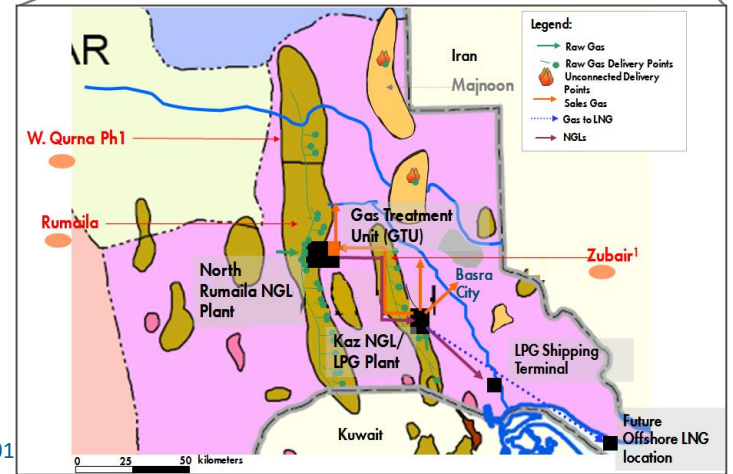
Optimisation of integrated
natural gas production & processing systems

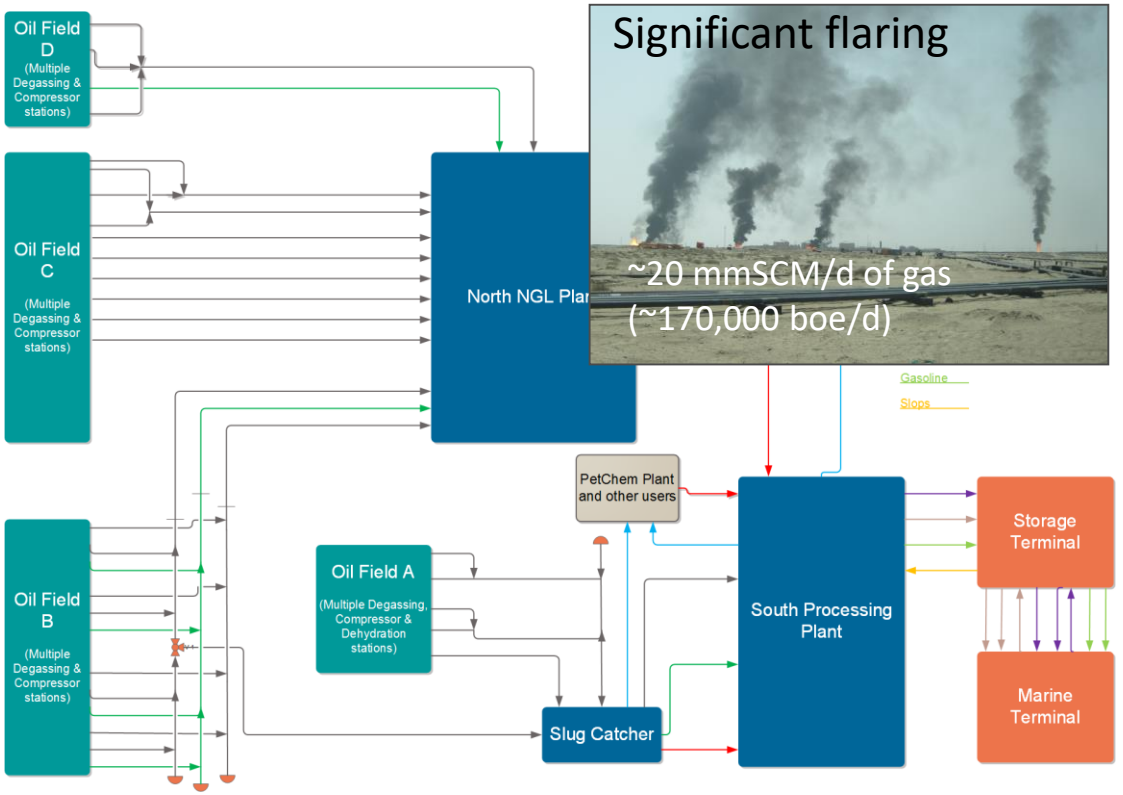
APM Proof of Concept

D. Aluma, N. Thijssen, K.M. Nauta, C.C Pantelides, N. Shah
Optimize an integrated natural gas production and distribution network
Gas Processing News, October 2016

APM Proof of Concept study: Shell/Basrah Gas Company

Integrated gas production & processing networks

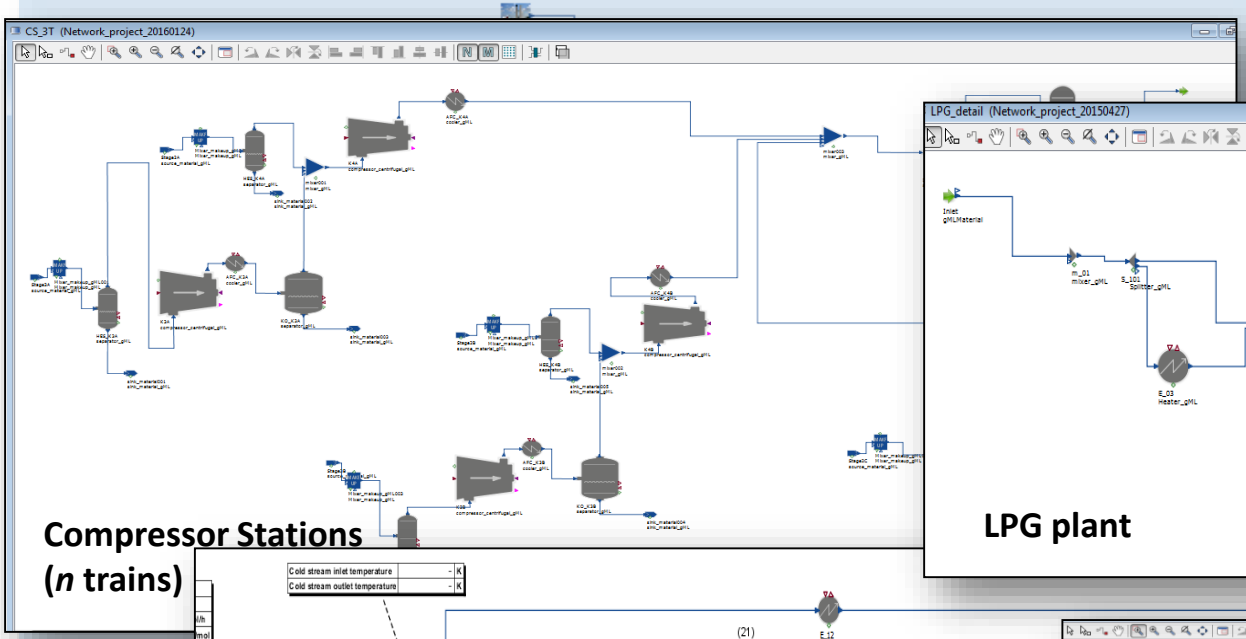




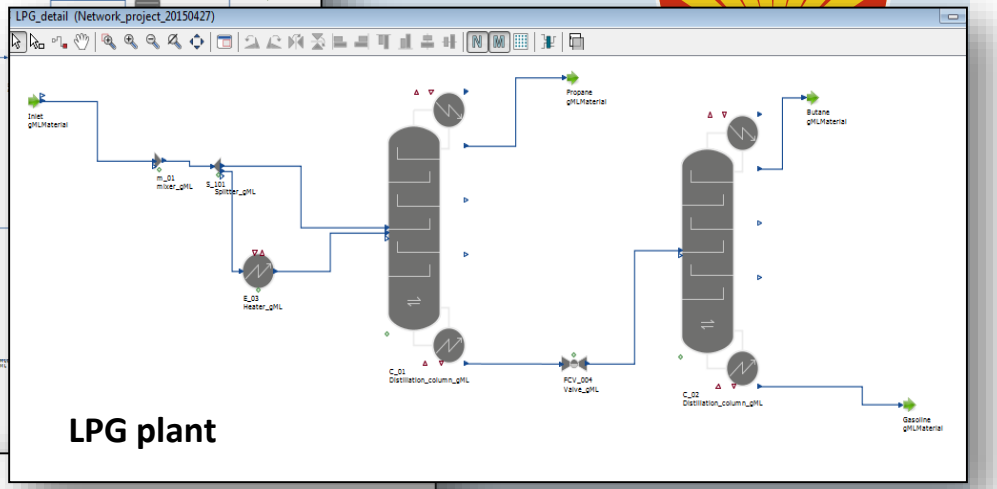
- Multiple compressor stations, NGL / LNG plants and other facilities spread over a wide geographical area
- How to make optimal use of capacity and reduce flaring?

APM Proof of Concept study: Shell/Basrah Gas Company

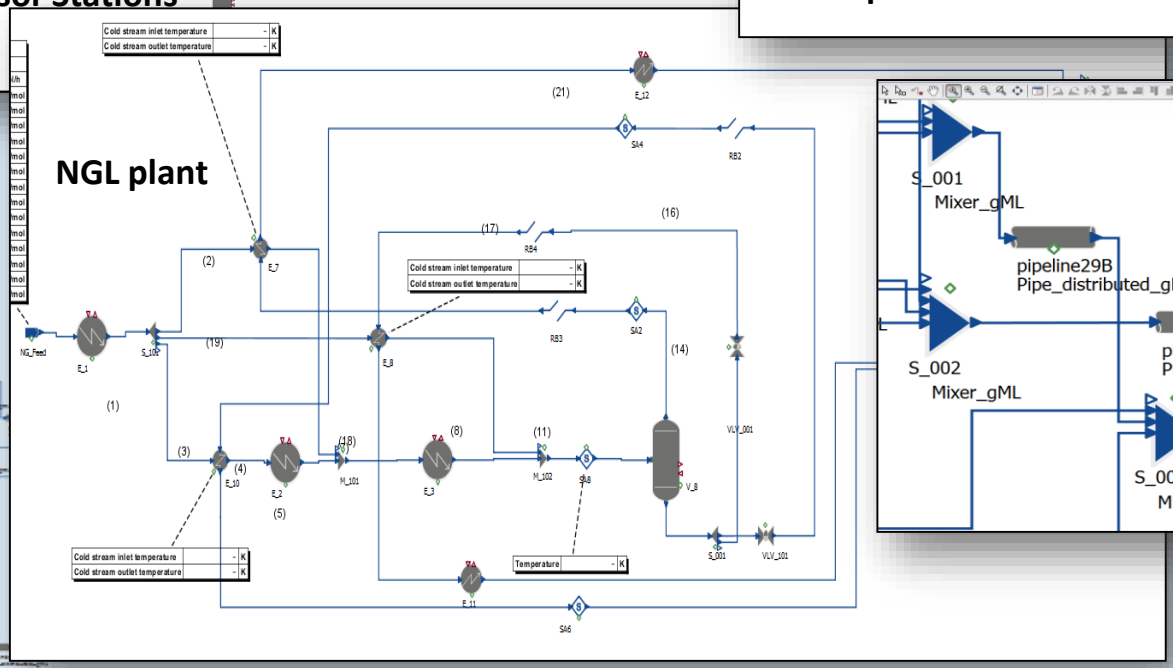
Integrated gas production & processing networks



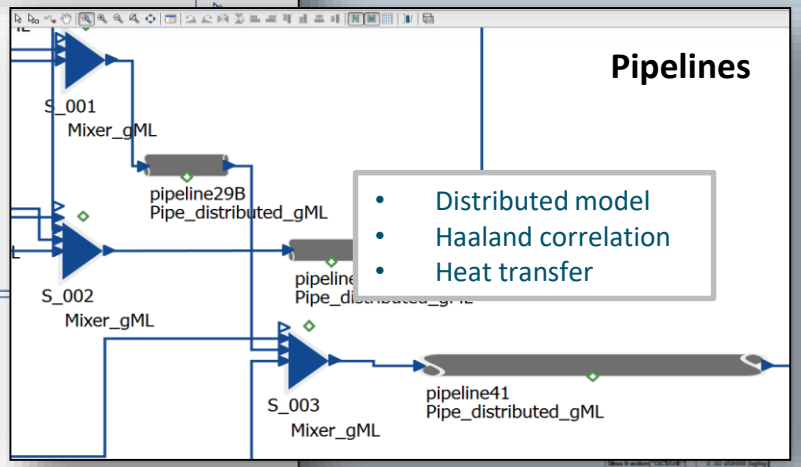
Compressor Stations (*n* trains)



LPG plant



NGL plant



Pipelines

- Distributed model
- Haaland correlation
- Heat transfer

Integrated gas production & processing network

Day-to-day optimisation: the benefits of a rigorous approach

Objective functions

- **Normal operation**
  - Maximise profit
  - Maximise total production
  - Maximise yields of specific products
  - Minimise flaring
- **Abnormal operation**
  - Maximise production under equipment failure scenario
  - Maximise production under field decline scenario

OBJECTIVE: Optimisation of day-to-day operations

- 77 decision variables
- 32 constraints
- ~300,000 model equations

BENEFITS over base case

- 4.9% improvement in profit
- 3.5% increase in total production
- 48% increase in propane production
- 87% reduction in flaring
- O($100m pa)

“Capture all important interactions”

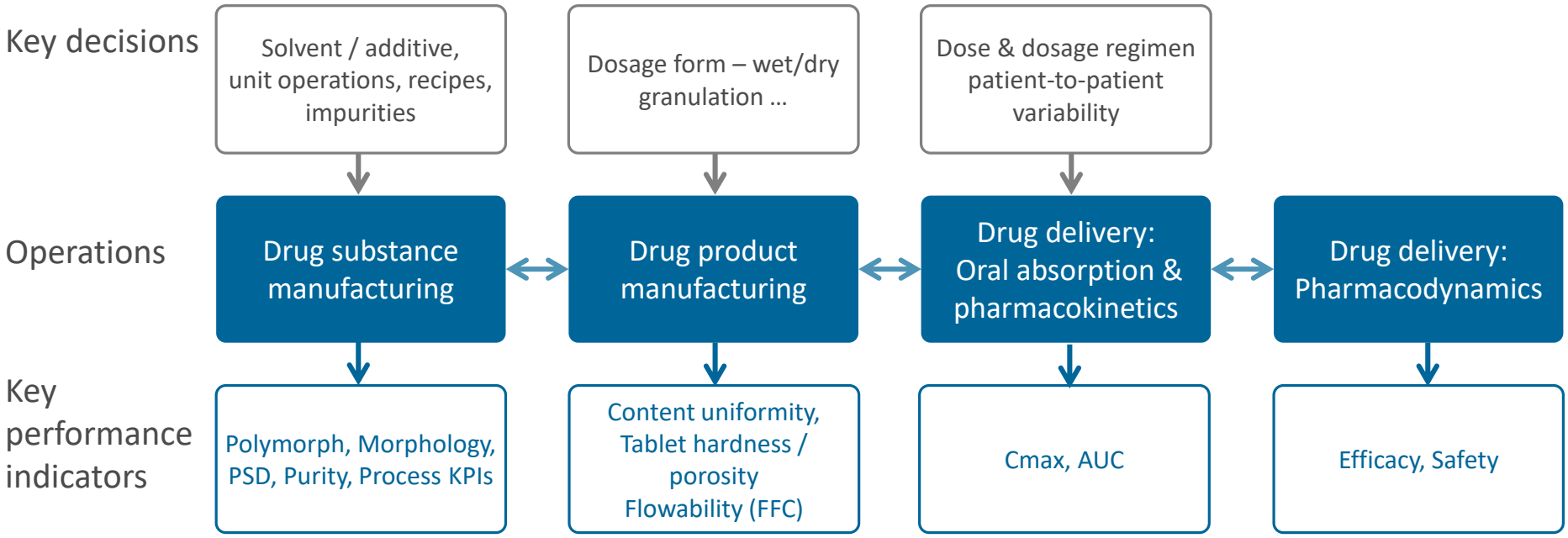
Systems-based Pharmaceutics
A holistic approach to drug design & manufacturing

An APM vision

Pharmaceutical systems – a high-level view

Decisions & Disturbances

Critical Process Parameters

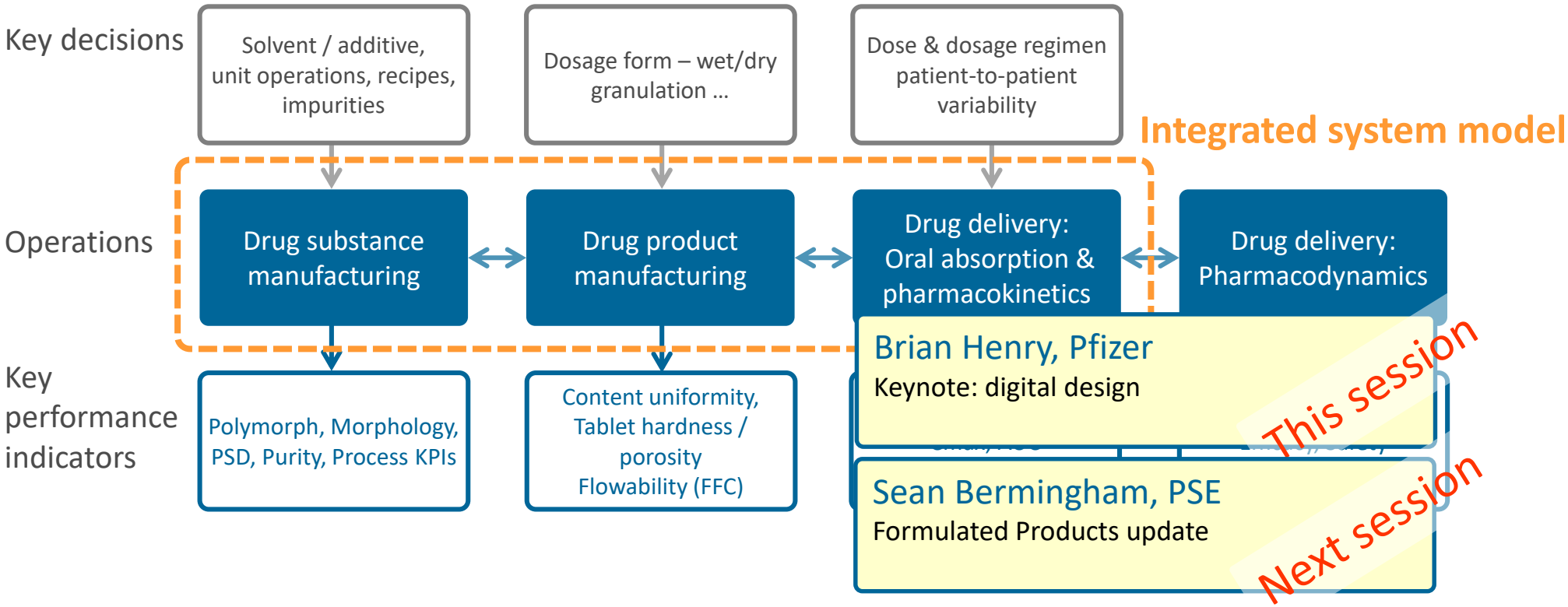


Objectives & Constraints

Product KPIs: Critical Quality Attributes

Process KPIs: Economics, Safety, Operability, Environmental Impact

Pharmaceutical systems – a high-level view



- Use an integrated system model
  - to quantify effects of critical parameters & disturbances
  - on critical quality attributes, process economics, operability, safety

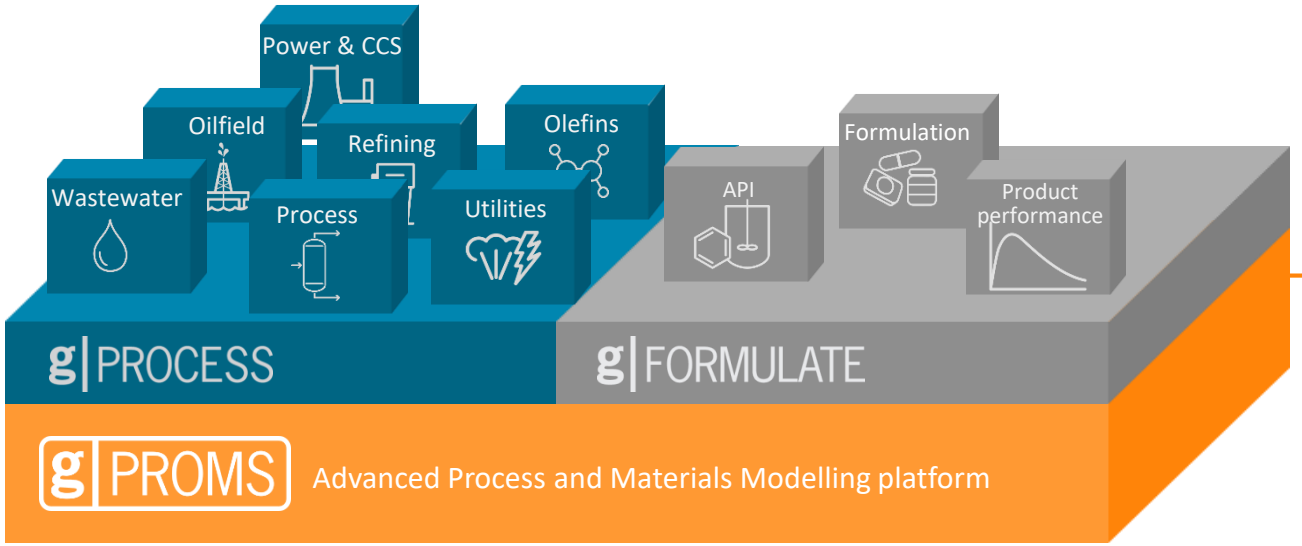
Advanced Process Modelling: from vision to realisation

The gPROMS software suite – 2017

Platform Environments Packages/Libraries

"Simple" products
gPROMS ProcessBuilder

Formulated products
gPROMS FormulatedProducts



Platform functionality

Process modelling
- Equation-oriented solution power
- Custom model construction
- Steady-state and dynamic simulation and optimisation
- Advanced parameter estimation
- Powerful dynamic and mixed-integer optimisation
- Global system analysis
- High-performance computing

Materials modelling
- Molecular & ionic species
- Complex species & mixtures
- Fluid, solid phases
- Phase & reaction equilibrium

A single powerful software platform
serving *diverse s*
via high-value app

Efficient software development & maintenance

Various presentations
gPROMS platform, gPROMS ProcessBuilder
gPROMS FormulatedProducts
Wed am

gPROMS ProcessBuilder

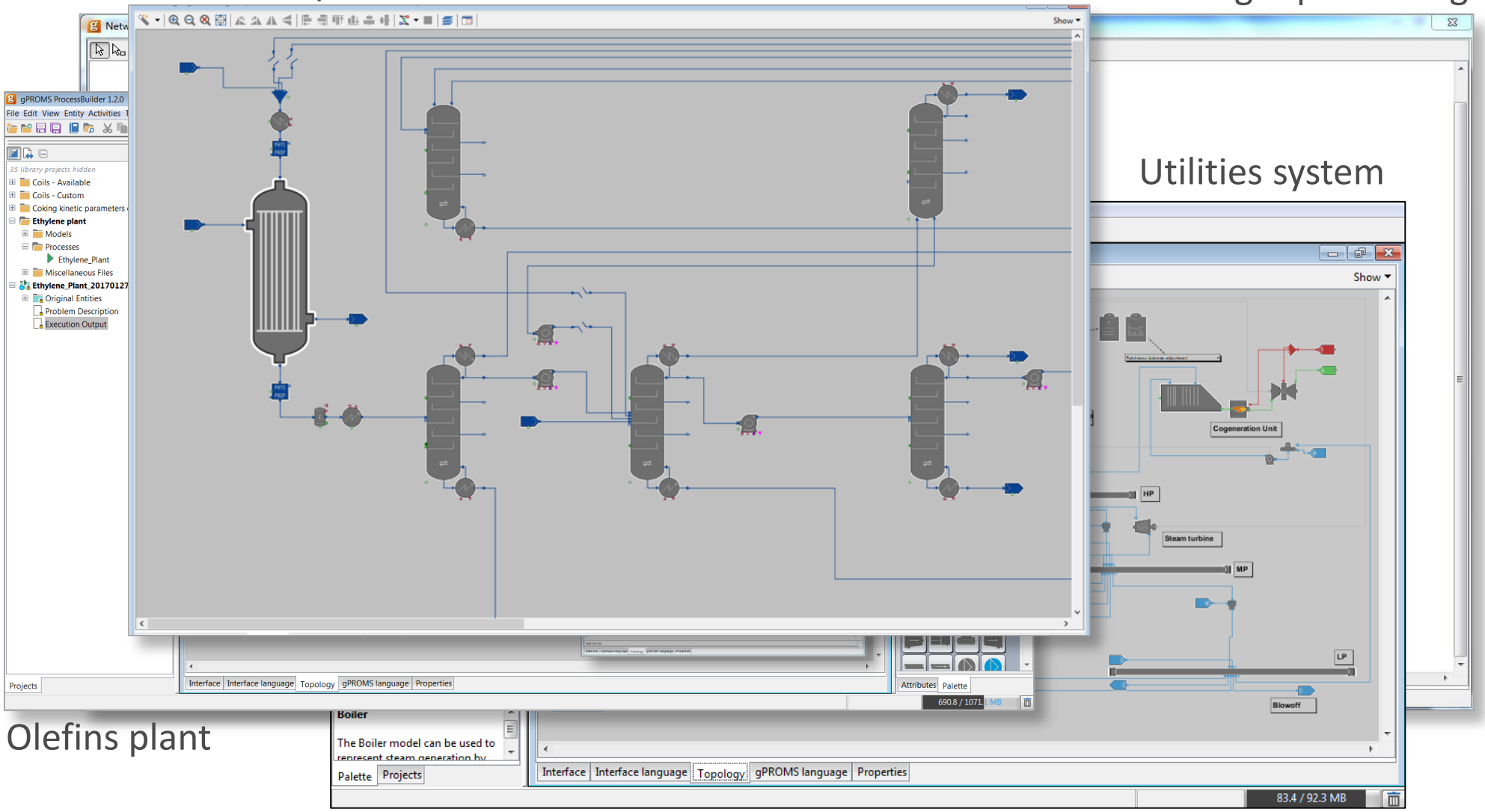
Unified system for process flowsheeting

Petrochemical process with detailed reactor

Multi-site gas processing

Utilities system

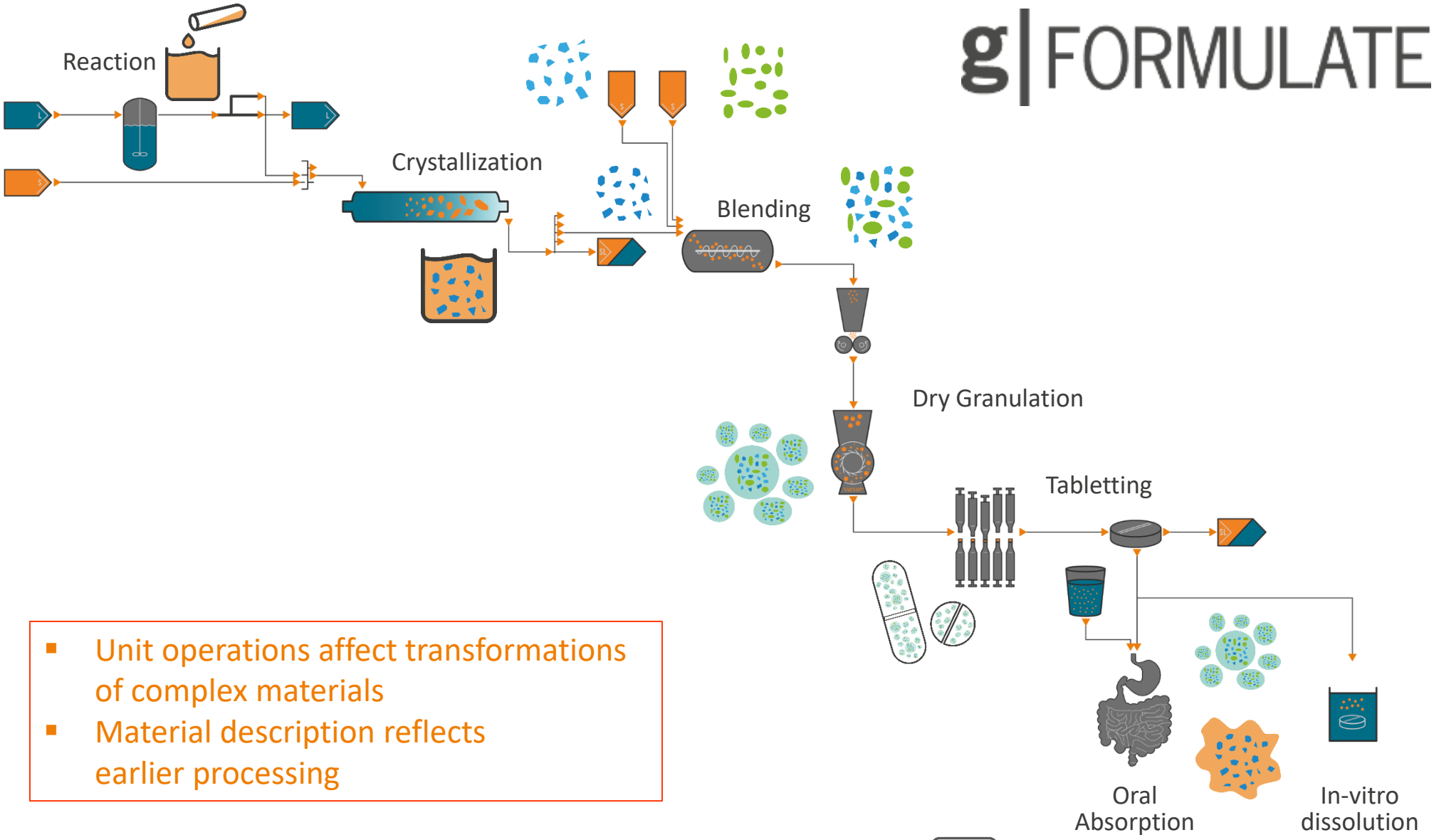
Olefins plant



Multi-level flowsheets; multi-scale; process, utilities, …

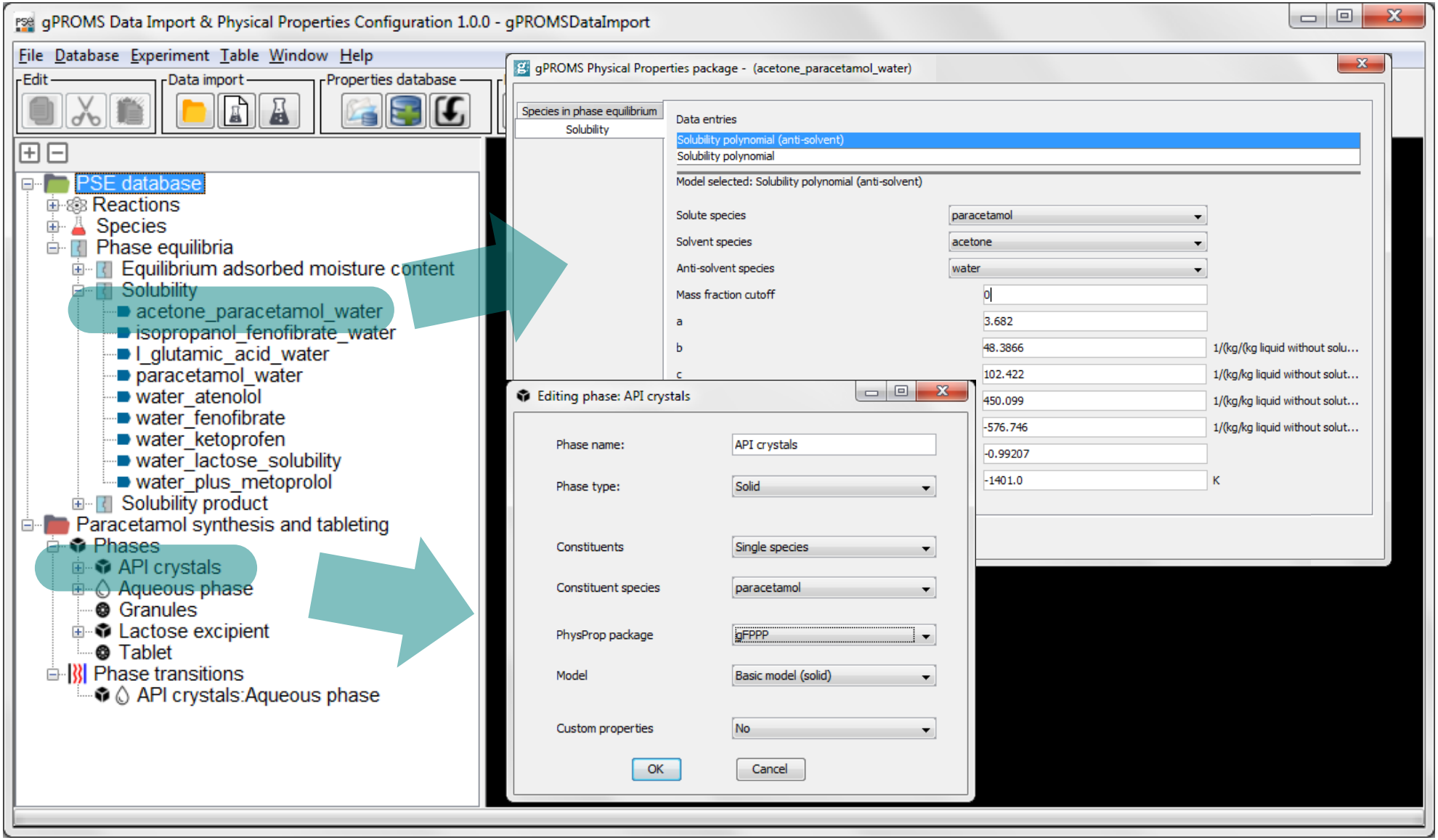
Linking manufacture directly to product performance

g|FORMULATE



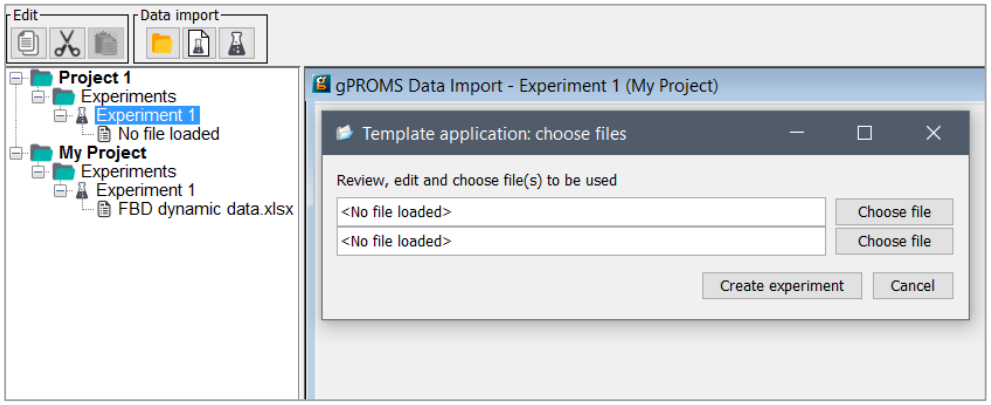
- Unit operations affect transformations of complex materials
- Material description reflects earlier processing

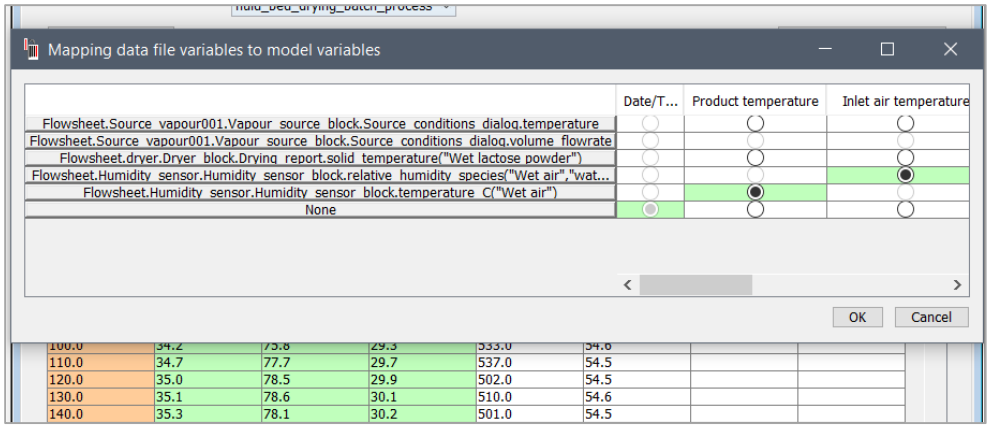
Consistent model configuration – S/L/V properties package



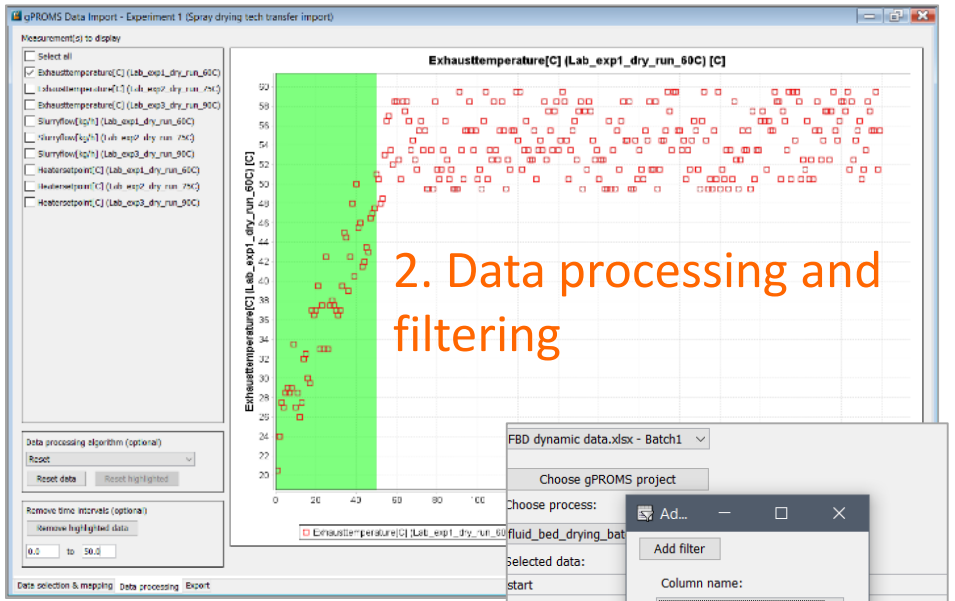
gPROMS FormulatedProducts

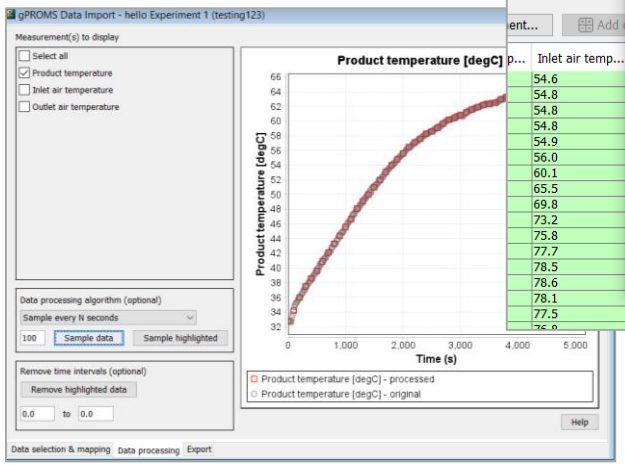
Model validation workflows – data import and processing





1. Data file import and link to gPROMS variables



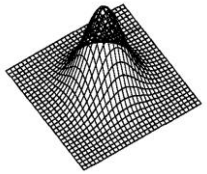


3. Export to gPROMS

Manage risk – quantify impact of uncertainty & variability

Environmental inputs
- External disturbances
- Commercial environment

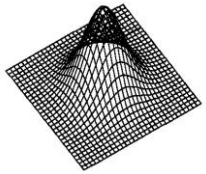
Innovate UK collaborative R&D project on Global Systems Analysis
AstraZeneca, Britest, GSK, Pfizer, PSE
2014/06 – 2016/05



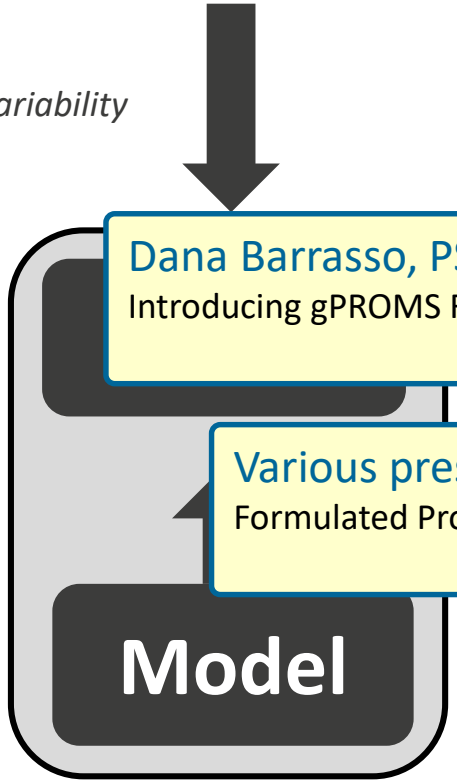
Variability

Decisions
- Design
- Operational

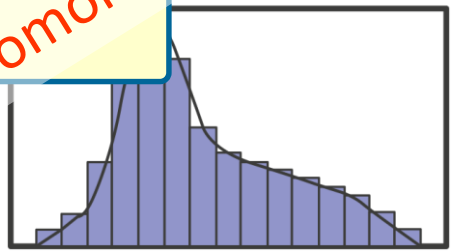
Model parameters



Uncertainty



KPIs
- Process operability
- Process safety
- Environmental impact
- Economic performance



Risk associated with model-based decisions

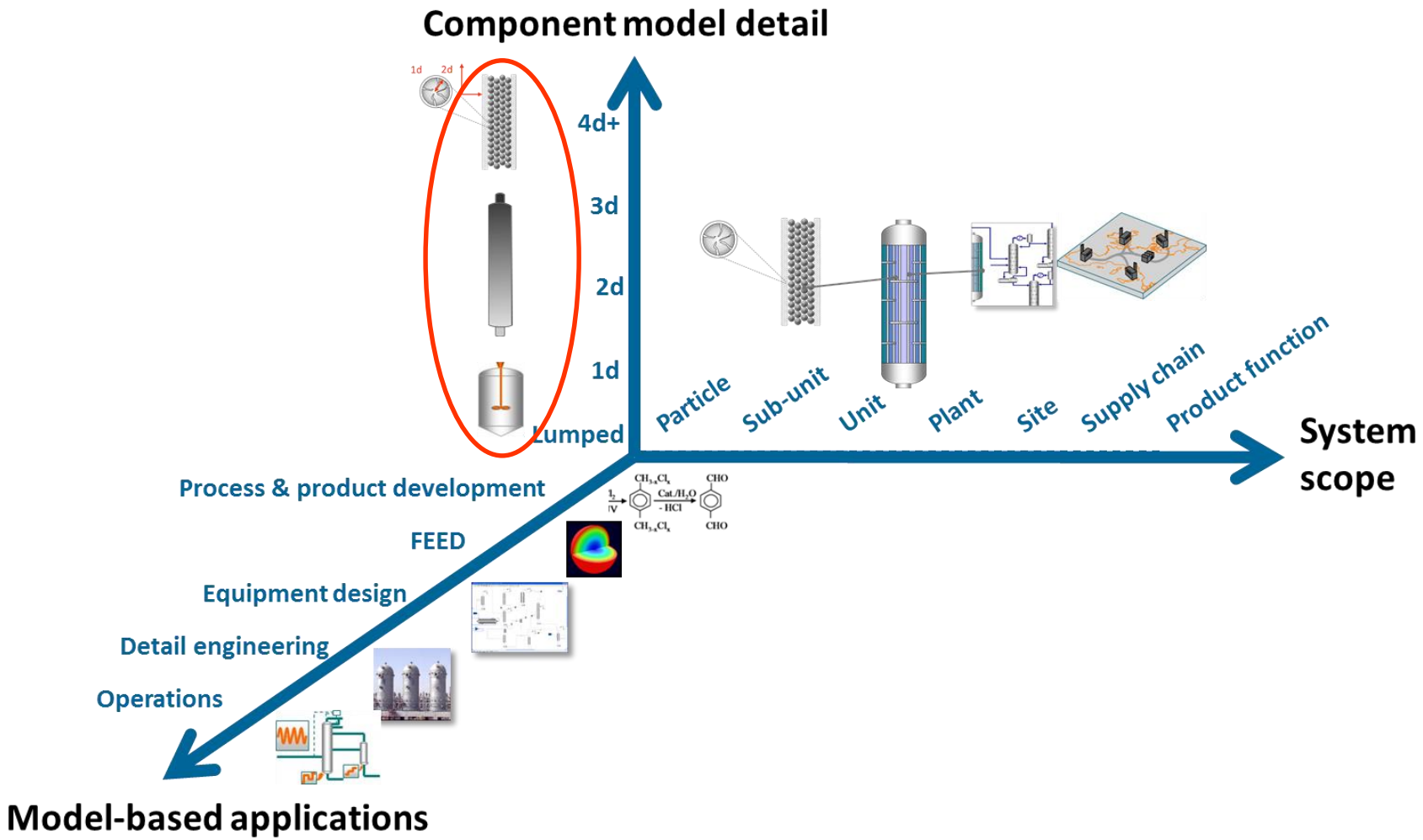
Dana Barrasso, PSE
Introducing gPROMS FormulatedProducts
Tomorrow am

Various presentations
Formulated Products sessions
Tomorrow

Process Modelling – where to next?

Improving the efficiency & quality of process modelling

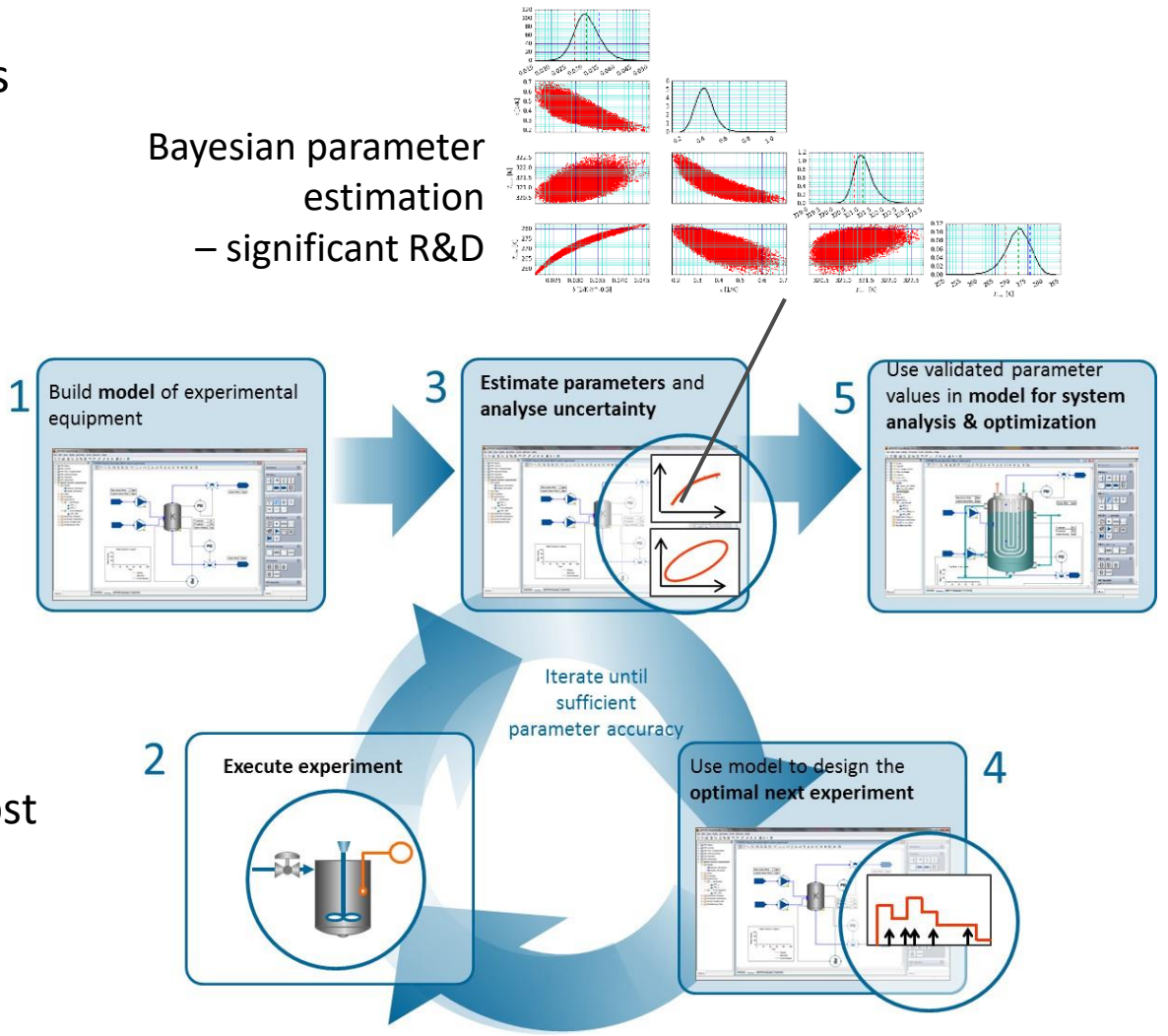
Improving the efficiency of component model construction & validation



Component model parameterisation

- Most component process models contain parameters that are not known *a priori*
  - thermodynamics
  - heat & mass transfer
  - hydrodynamics
  - reaction & other kinetics
  - . . . . . .
- Typically estimated based on experimental data
  - experimentation often the bottleneck in terms of time & cost
  - ➔ need carefully designed experimental programs

Bayesian parameter estimation – significant R&D



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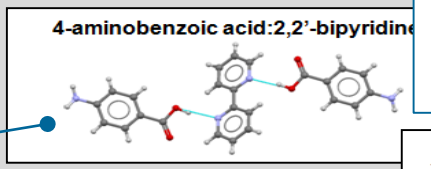
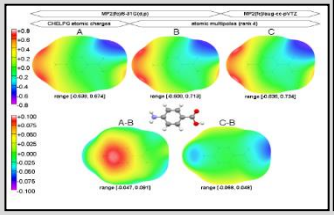
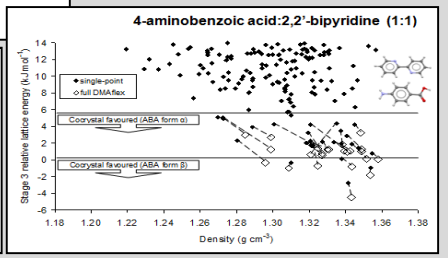
  - ➔ need carefully designed experimental programs
- ALTERNATIVE:

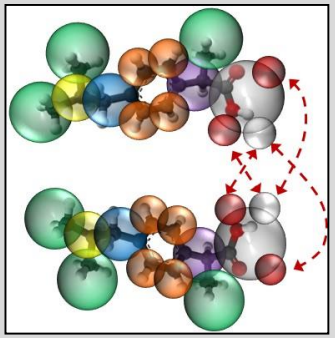
  multiscale modelling



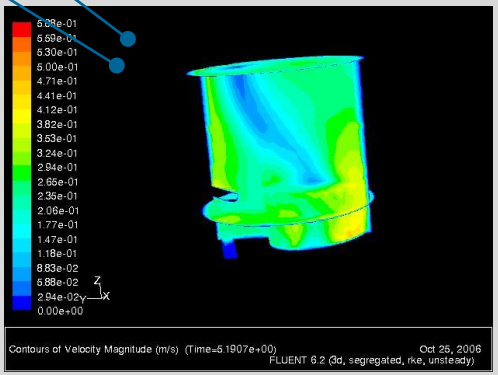




Cocrystal lattice energy landscape in CrystalPredictor/ CrystalOptimizer



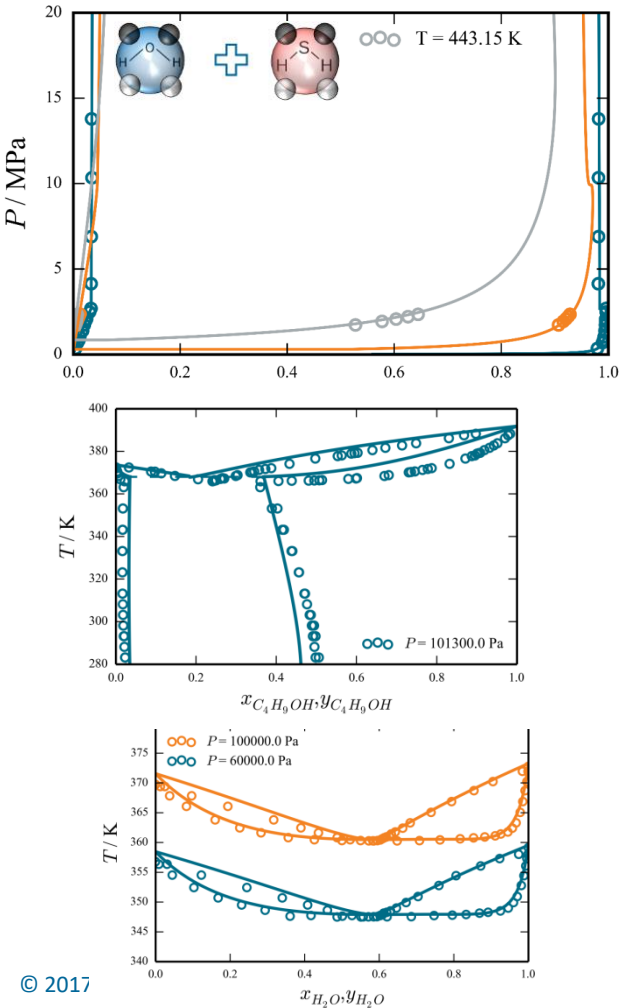
Ibuprofen model in SAFT-γ Mie



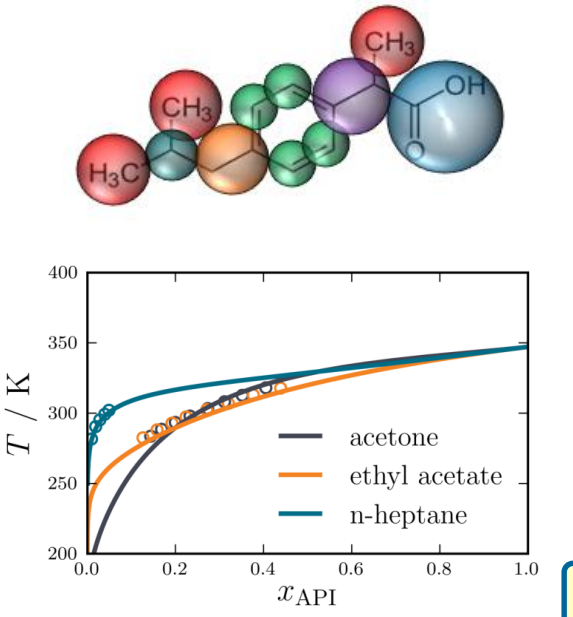
CFD model of agitated solid/liquid reactor for drug substance manufacturing

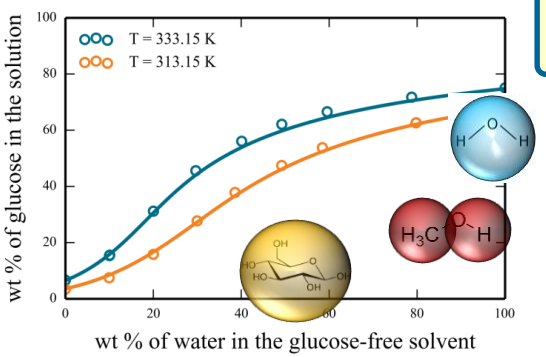
gSAFT: unified platform for modelling material behavior

Vapor/liquid equilibria of complex mixtures

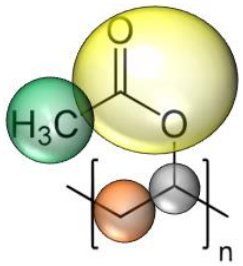


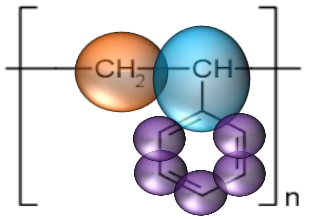
Solubility prediction

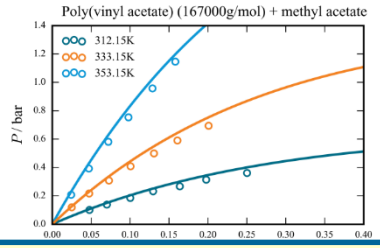


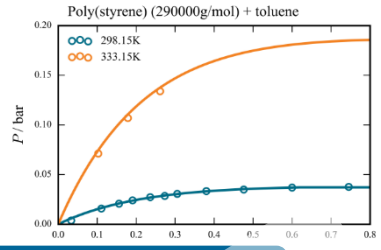


Polymeric system prediction





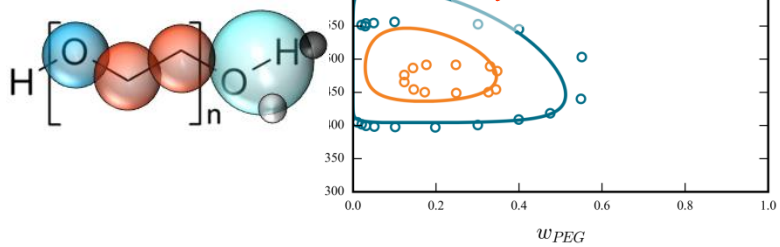




Tom Lafitte

"gSAFT: predicting reaction equilibrium and other advances in thermodynamic modelling"

Wed am



Process Modelling – where to next?

Incorporating molecular structure decisions in process development & design

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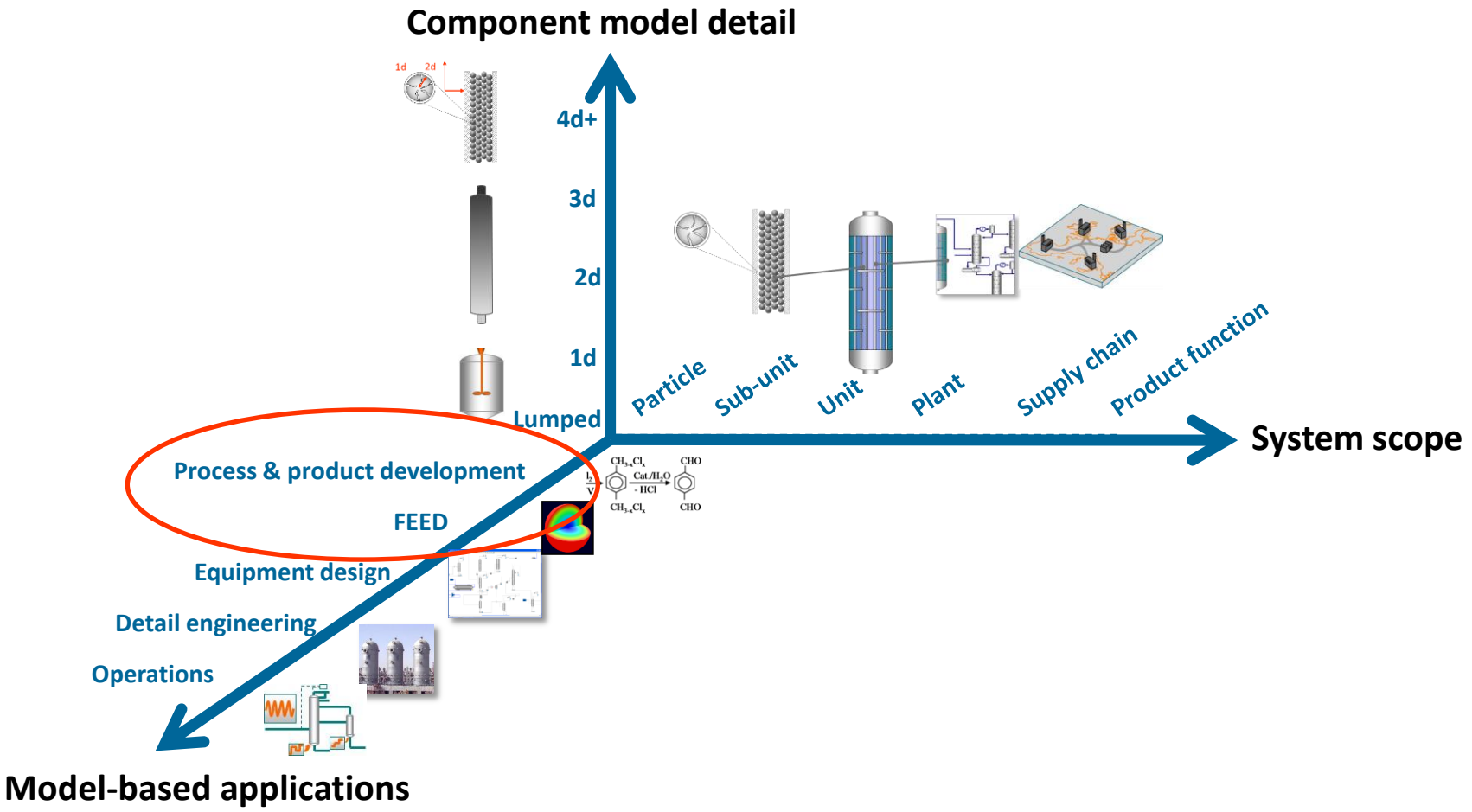


Computer-aided molecular design (CAMD)

- Aim: include molecular design decisions within overall process development & design optimisation

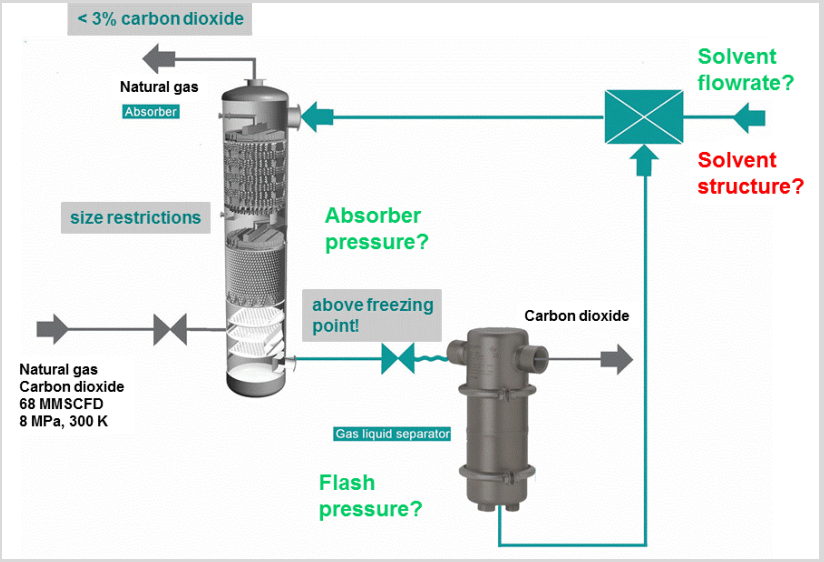
- Focus: "auxiliary" process materials
  - solvents, entrainers, working fluids
  - co-crystallizing agents, homogeneous/ heterogeneous catalysts

- Requirements

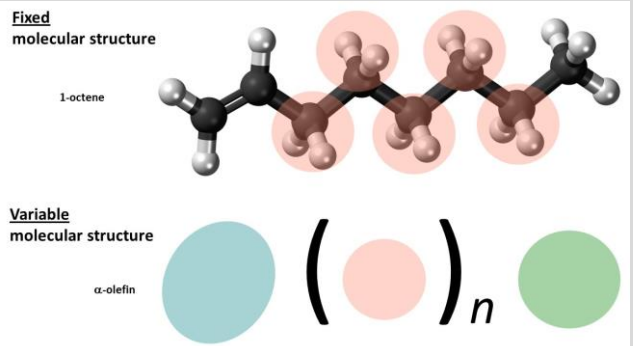
1. **Predictive models:**
   molecular structure →
   material behaviour within the process
2. **Appropriate molecular super-structures**

→handle molecular structure decisions directly within overall optimisation calculations

→efficient search of molecular design space



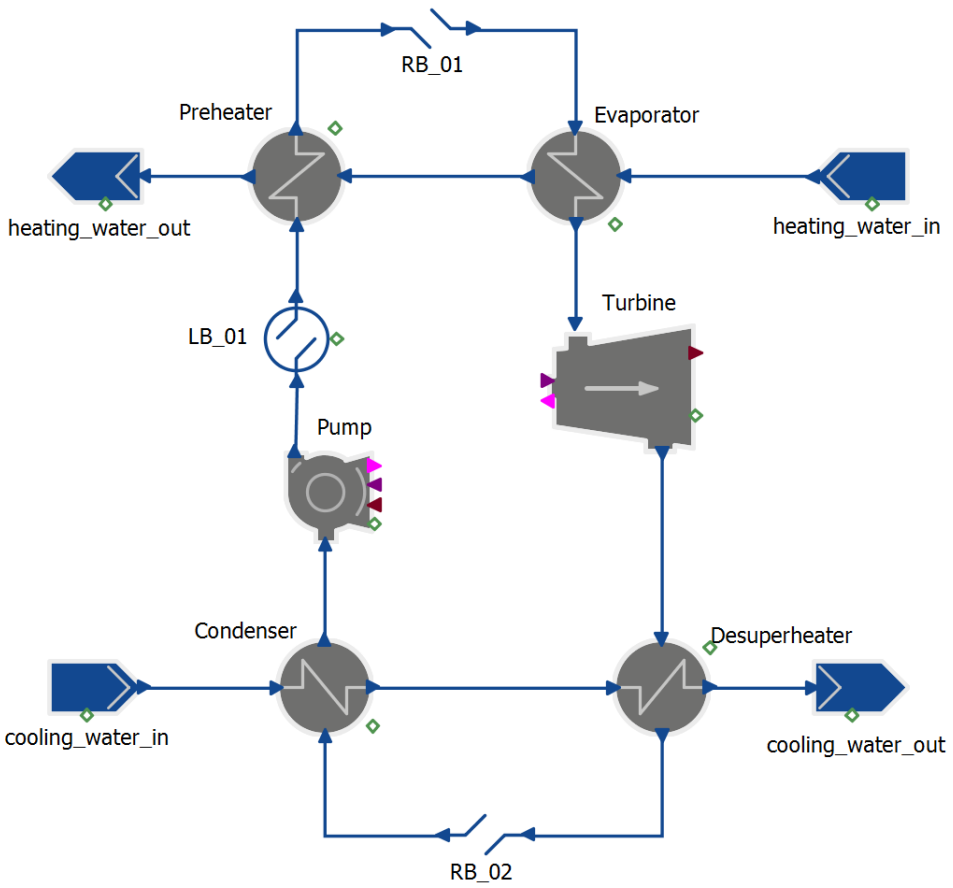
Burger, Papaioannou, Gopinath, Jackson, Galindo, Adjiman, *AIChE J.* doi: 10.1002/aic.14838 (2015)



Variable molecular structures in gSAFT

Example: Design of Organic Rankine Cycles

J. Schilling, A. Bardow, (RWTH Aachen), J. Gross (U. Stuttgart)



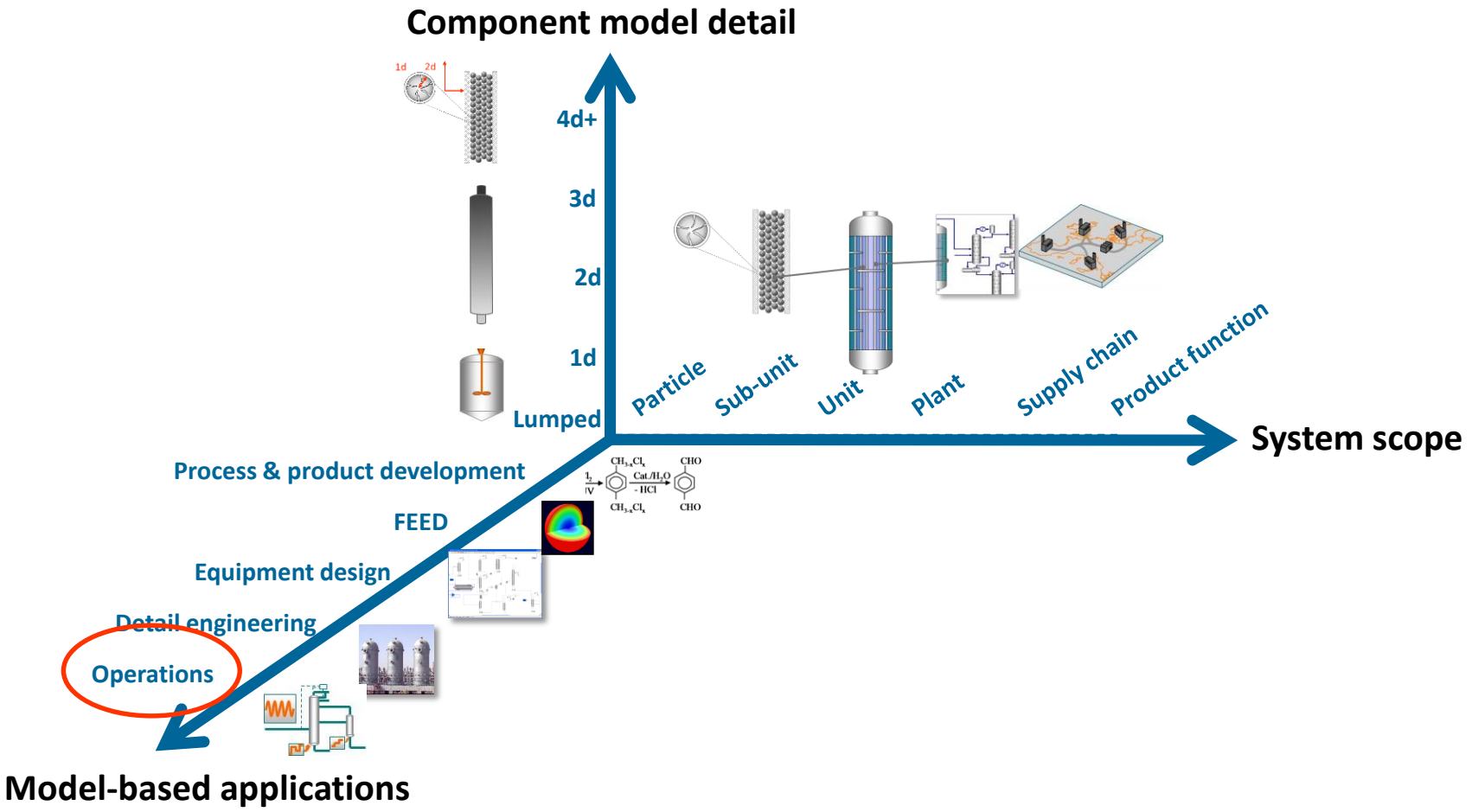
Implemented in gPROMS ProcessBuilder

- Objective: Simultaneous determination of optimal
  - ORC operating conditions
  - **working fluid**
- **Approach I: Targetting**
  - *Step 1*: Determine EoS parameters for optimal "theoretical" working fluid
    - Use "standard" EoS
  - *Step 2*: Use a database of real fluids to identify the one that most closely matches parameters' theoretical optimum
- **Approach 2: Direct Optimisation**
  - Determine molecular structure of working fluid by including number of functional groups of each kind as integer decision variables
    - Use group-contribution EoS

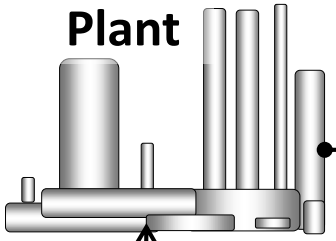
Process Modelling – where to next?

Online decision support tools for plant operations based on “first-principles” models

Online decision support tools for plant operations based on “first-principles” models



Online decision support tools for plant operations based on "first-principles" models



Plant

Plant Data

Data conditioning

State estimation/ Online model re-calibration

Regulatory Control System

Up-to-date (re-calibrated) model

Current plant state

Regulatory Controller set-points

Set-point/ trajectory optimisation

MPC model derivation

Economic MPC

Decision support via future scenario simulation

Monitoring & diagnosis

Optimal CV set-points/ trajectories

Reduced/ linear model(s)

Model Predictive Control
(Linear / Nonlinear)

Unmeasured CVs

Adapted from Pantelides, C.C. and Renfro, J.G., "The online use of first principles models in process operations: review, current status & future needs", *Comput. chem. Engng.*, (2012), **51**, 136-148

Online decision support tools for plant operations based on “first-principles” models

- Detailed models only now beginning to be used
- Huge economic benefits possible by operating closer to constraints
  - cf. recent Shell published case study

.

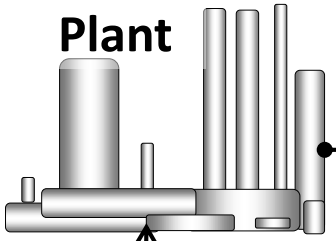
- Limited range of applications (e.g. RTO/scheduling)
- Key considerations:
  - model development, maintenance & validity
  - complex computations (e.g. large-scale dynamic optimisation)

- Mostly simple linear models derived from plant responses
- Key considerations:
  - system identification (80% of effort/cost)
  - maintaining the model over the plant’s lifecycle
  - accurate state estimation

- Rapidly becoming commodity
  - Current strong push towards standardisation ➔ lower costs to end users
  - **Open Process Automation™ Forum**

Online decision support tools

Model-based automation



Plant Data

Data conditioning

State estimation/ Online model re-calibration

Up-to-date (re-calibrated) model

Current plant state

Regulatory Control System

Regulatory Controller set-points

Set-point/ trajectory optimisation

MPC model derivation

Economic MPC

Decision support via future scenario simulation

Monitoring & diagnosis

Optimal CV set-points/ trajectories

Reduced/ linear model(s)

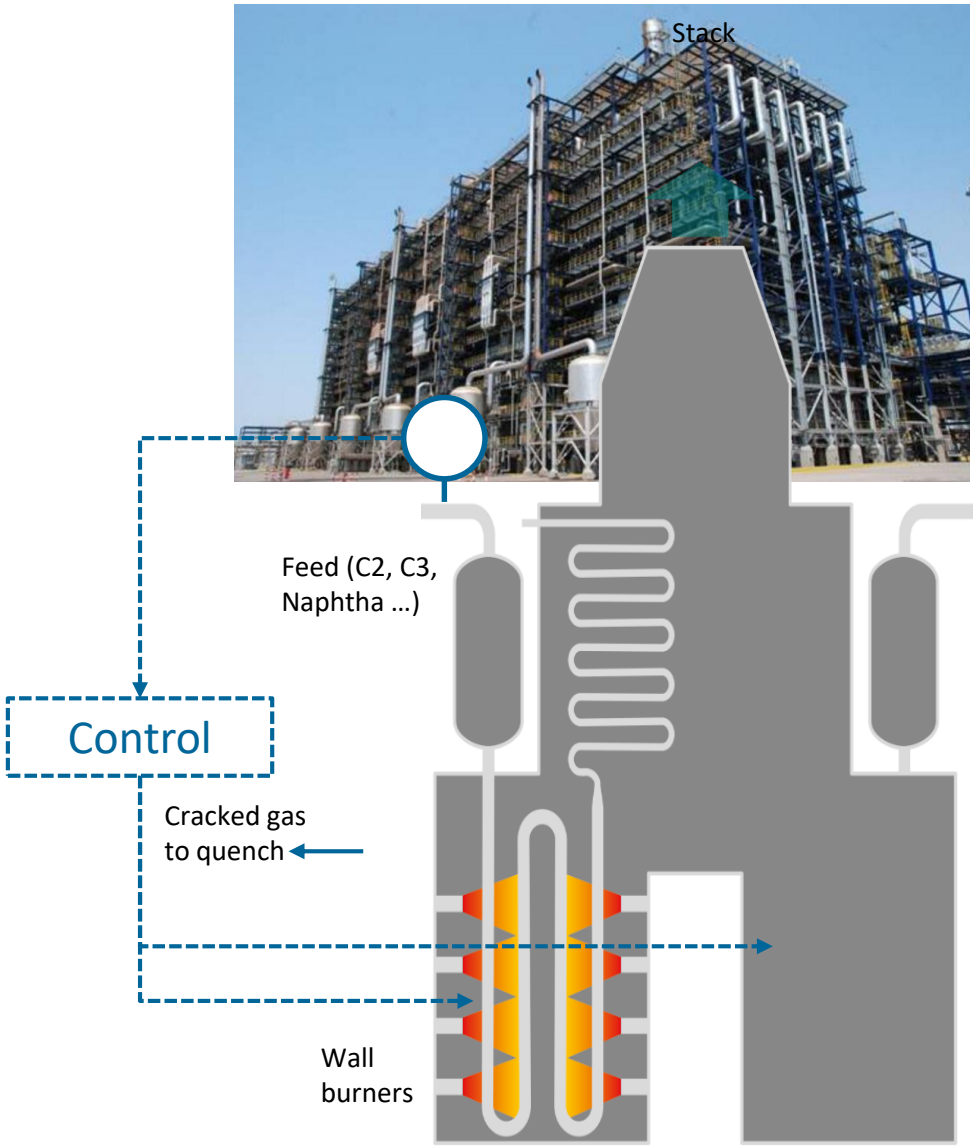
Model Predictive Control
(Linear / Nonlinear)

Unmeasured CVs

Adapted from Pantelides, C.C. and Renfro, J.G., "The online use of first principles models in process operations: review, current status & future needs", *Comput. chem. Engng.*, (2012), **51**, 136-148

Cracking furnace operation: product yields

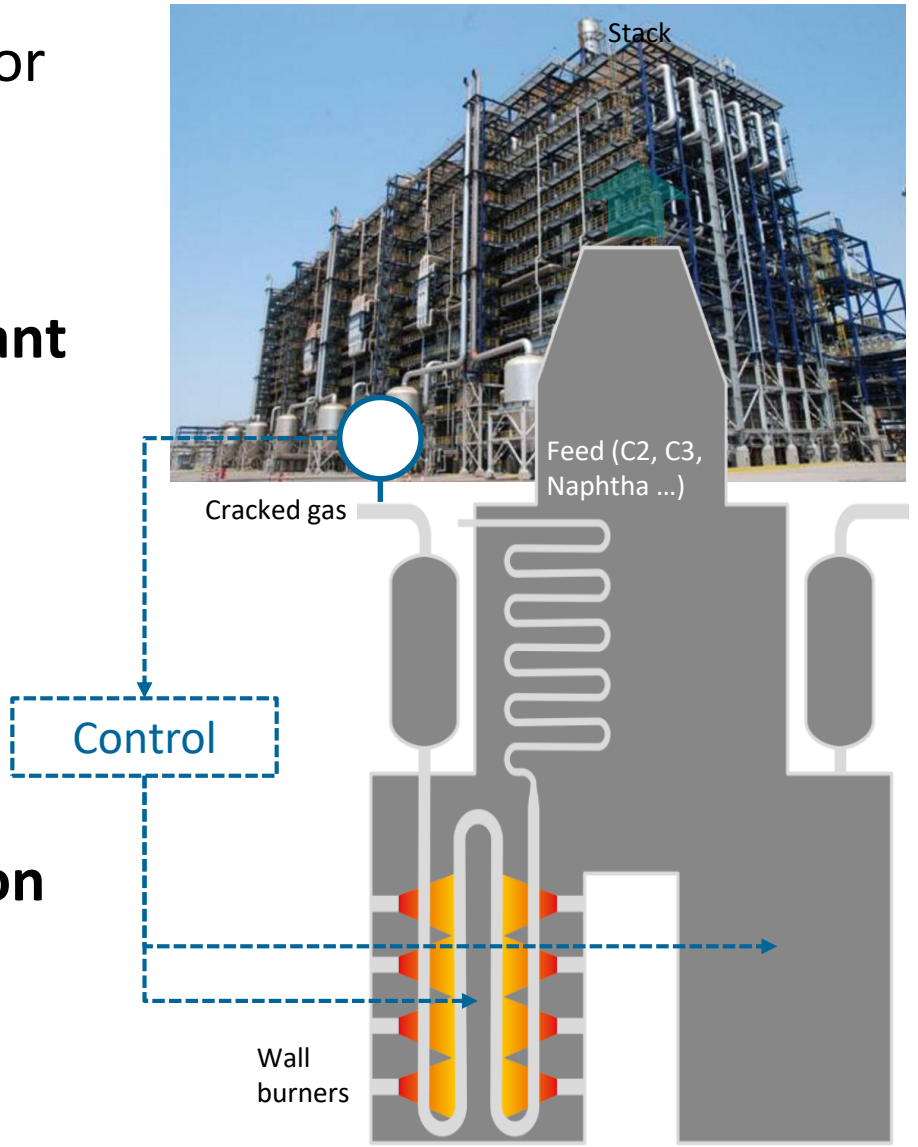
- Ethylene/propylene yields essential information for good control
- Challenge: very difficult to get reliable exit composition data
- Use high-fidelity model to provide high-accuracy Virtual Analyser
  - ethylene yield prediction
  - also predicts coke build-up



Cracking furnace operation: product yields

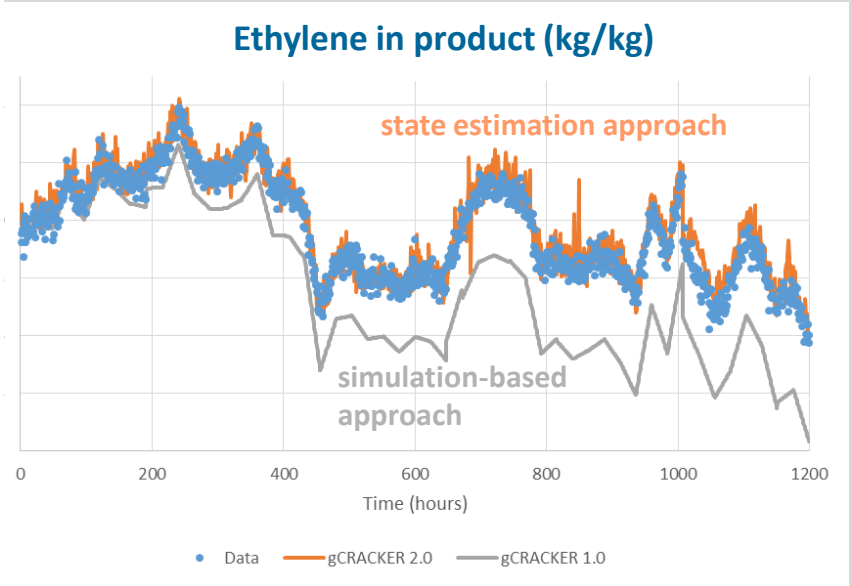
- gPROMS Olefins Cracking Monitor

- Couples
  1. detailed predictive **furnace/plant model**
     - including coil geometry, cracking kinetics, coking kinetics
  2. all available **plant data**
     - feed rate, composition, CIT, COT, etc.
- … using **dynamic state estimation** technology



Dynamic state estimation

- Concept
  - use all available plant measurements
    - exploit data redundancy
  - use Bayesian approach to reconcile
    - measurement error
    - model error
- Algorithms
  - Extended Kalman Filter
  - Unscented Kalman Filter
  - Ensemble Kalman Filter
  - Particle Filtering
  - Moving Horizon Estimation
- Challenge: correct characterisation & quantification of model uncertainty
  - requires good understanding of physical system



Extended Karman Filter

DAE model size	
Differential variables	260
Algebraic variables	44,240
Parameters recalibrated	6
Measurements	~120
Sampling frequency	60 s

Dynamic state estimation

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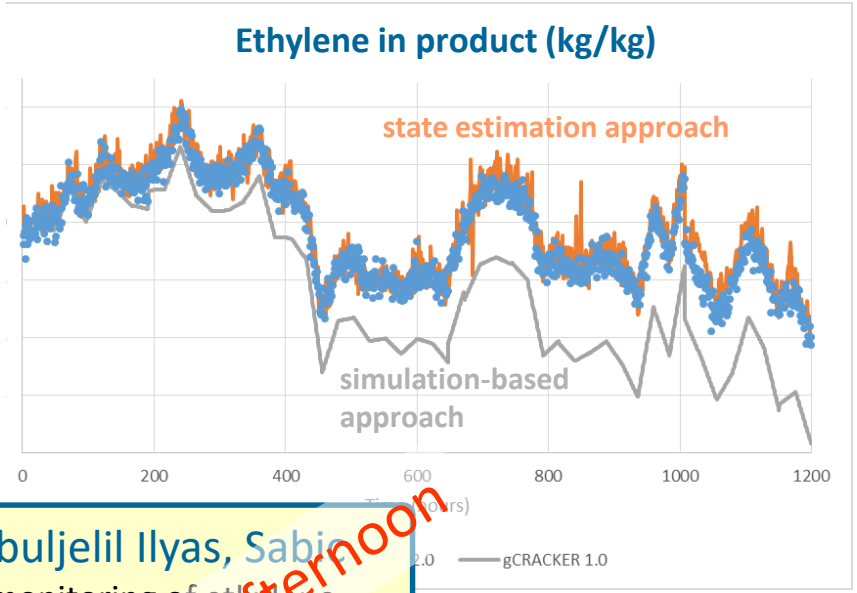
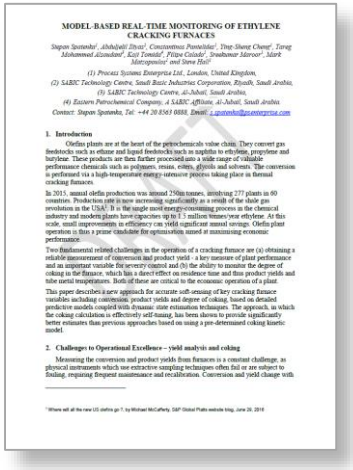


Steve Hall, PSE; Adbuljelil Ilyas, Sabic
Model-based real-time monitoring of ethylene cracking furnaces

This afternoon

17AIChE Spring Meeting, San Antonio, TX


MODEL-BASED REAL-TIME MONITORING OF ETHYLENE CRACKING FURNACES

gPROMS Process Operations Solutions
A key area

- Generic technologies for leveraging detailed models
  - Advanced Real-time Monitoring & Optimisation
  - Key activity in PSE
  - New groups for development and delivery (Frances Pereira, Steve Hall)
- Various presentations over next 2 days
  - Steve Hall:
    gPROMS Olefins Cracking Monitor
  - Dorus van der Linden, DSN:
    gPROMS Utilities Advisor
  - Steve Hall:
    Advanced refinery technologies

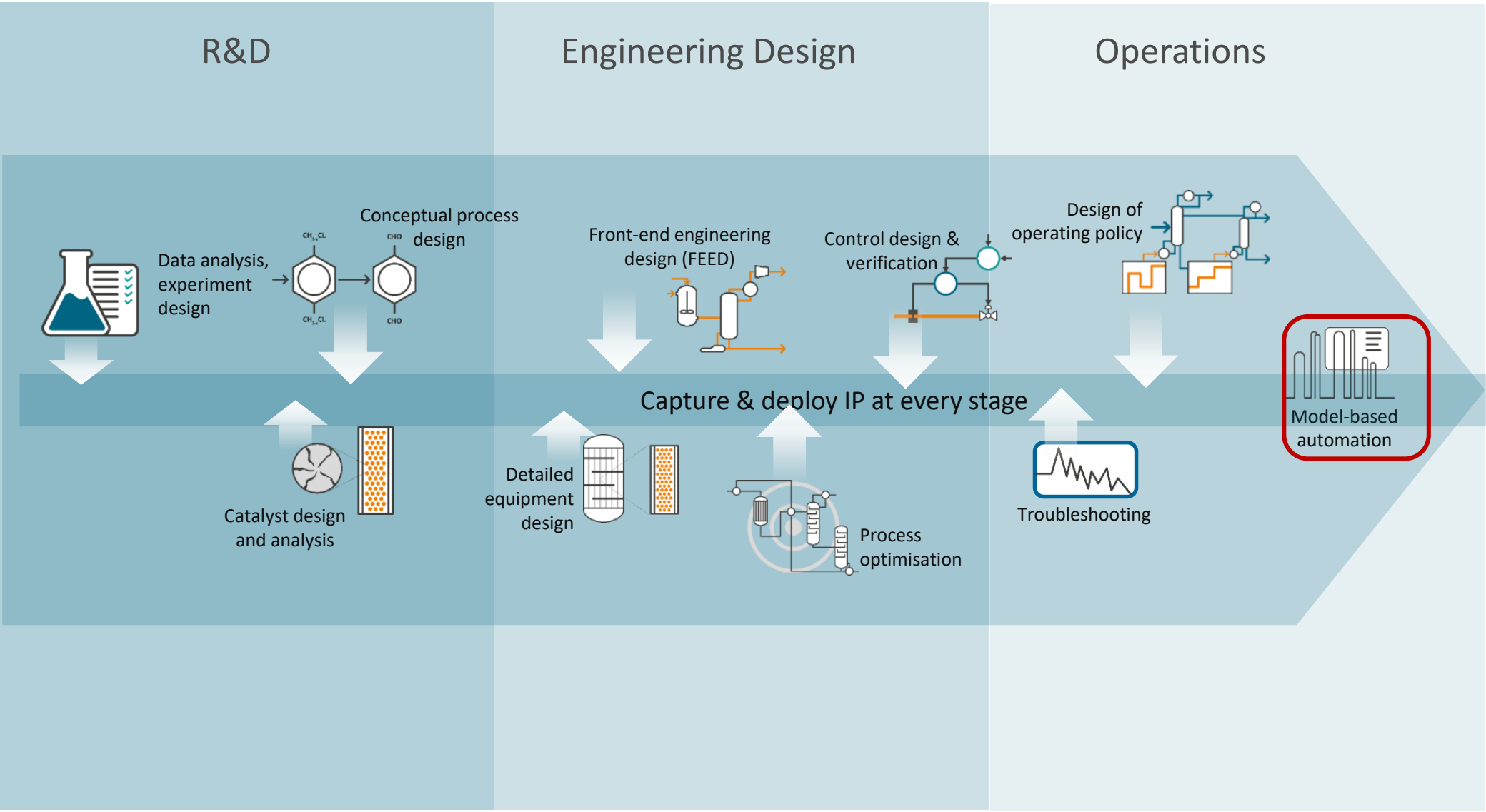
g | Process Operations Solutions

Jan van Schijndel, van Schijndel Strategic consulting
Keynote: Operational Excellence

This session

A unified system across the process lifecycle

PSE 5-year strategy



Thank you