

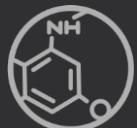


ADVANCED PROCESS MODELLING FORUM

22-23 APRIL 2015

The gPROMS Platform
Advancing the science of modelling

Costas Pantelides – Managing Director



gPROMS product family – 2015



General mathematical modelling



gPROMS ModelBuilder
Advanced process
modelling environment

Sector-focused modelling tools

Chemicals & Petrochemicals



gPROMS ProcessBuilder
Advanced process
simulation

Life Sciences, Consumer, Food, Spec & Agrochem



Solids process
optimisation



Crystallization
process optimisation



Oral absorption

Power & CCS



CCS system modelling

Oil & Gas



Flare networks &
depressurisation

Wastewater Treatment



Wastewater systems
optimisation

Fuel Cells & Batteries



Fuel cell stack &
system design



The gPROMS platform

Equation-oriented modelling & solution engine

Materials modelling



Model deployment tools

Enterprise Objects



Deploy models in common engineering software

gPROMS product family – 2015



General
mathematical
modelling



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Advanced process
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Sector-focused modelling tools

Chemicals &
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Life Sciences,
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Treatment



Wastewater systems
optimisation

Fuel Cells &
Batteries



Fuel cell stack &
system design



The gPROMS platform

Equation-oriented modelling & solution engine

~2 million lines of code
~25-strong development team

Materials
modelling

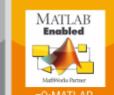


INFOCHEM
Multiflash



Model
deployment
tools

Enterprise Objects



Deploy models in common engineering software

Usability

Units of Measurement

Stream tables

Trajectories

Time Units support ; UoMs for domains

Public Model Attribute support throughout

Results: plots and value-tables

Unit Spacing

Expression evaluation

Vertical orientation

Protected Models

Improved diagnostics

GUI

Performance and memory improvements

Modelling & solution power

Flowsheet-Level Initialisation Procedures

Iteration

-25% run activity

As seen in
presentations, demos & workshops
throughout this APMF

Materials Modelling

Unified physical properties framework

Multiflash enhancements

gSAFT developments

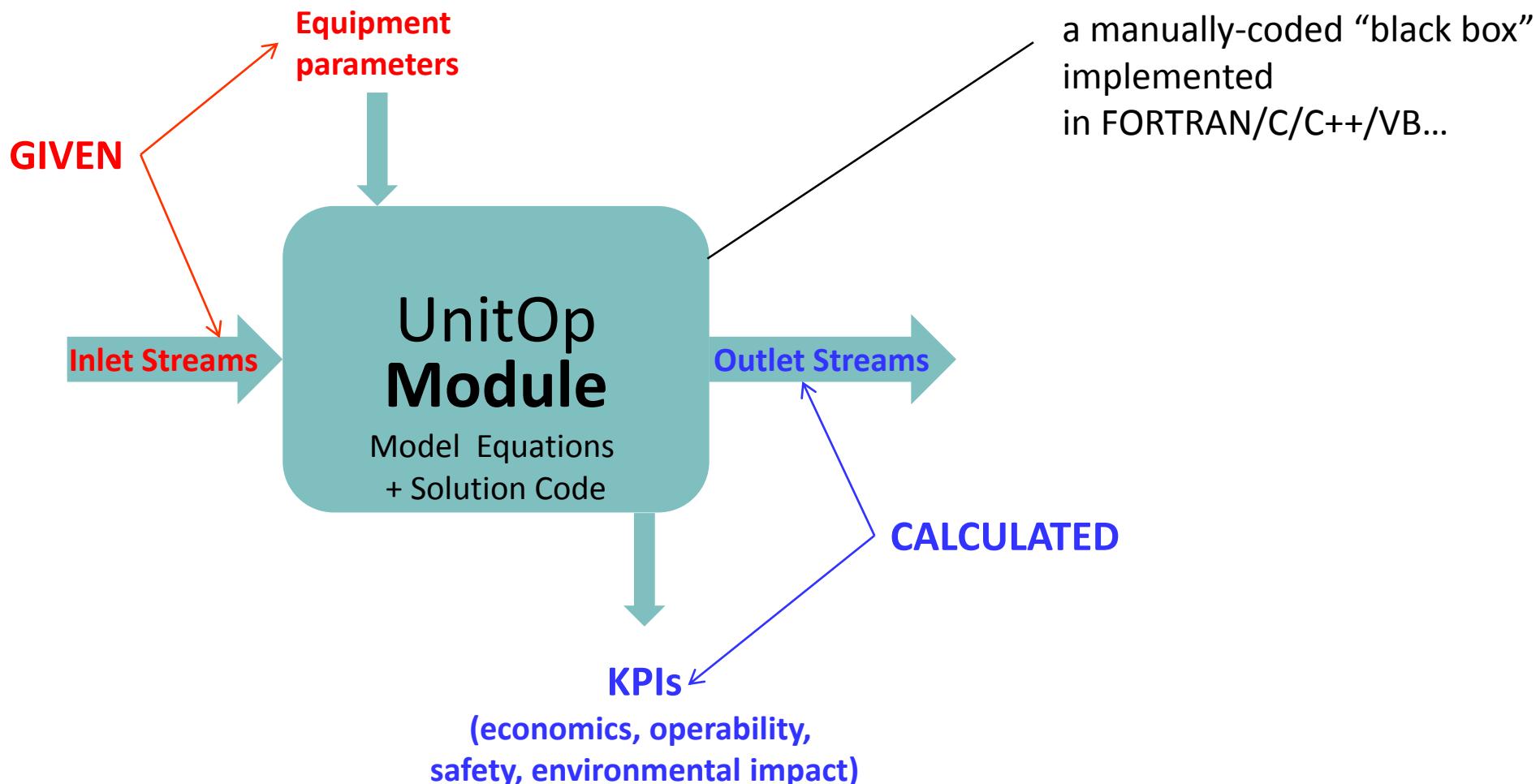
Software architecture & infrastructure

New modular licensing structure
(fully backward compatible)

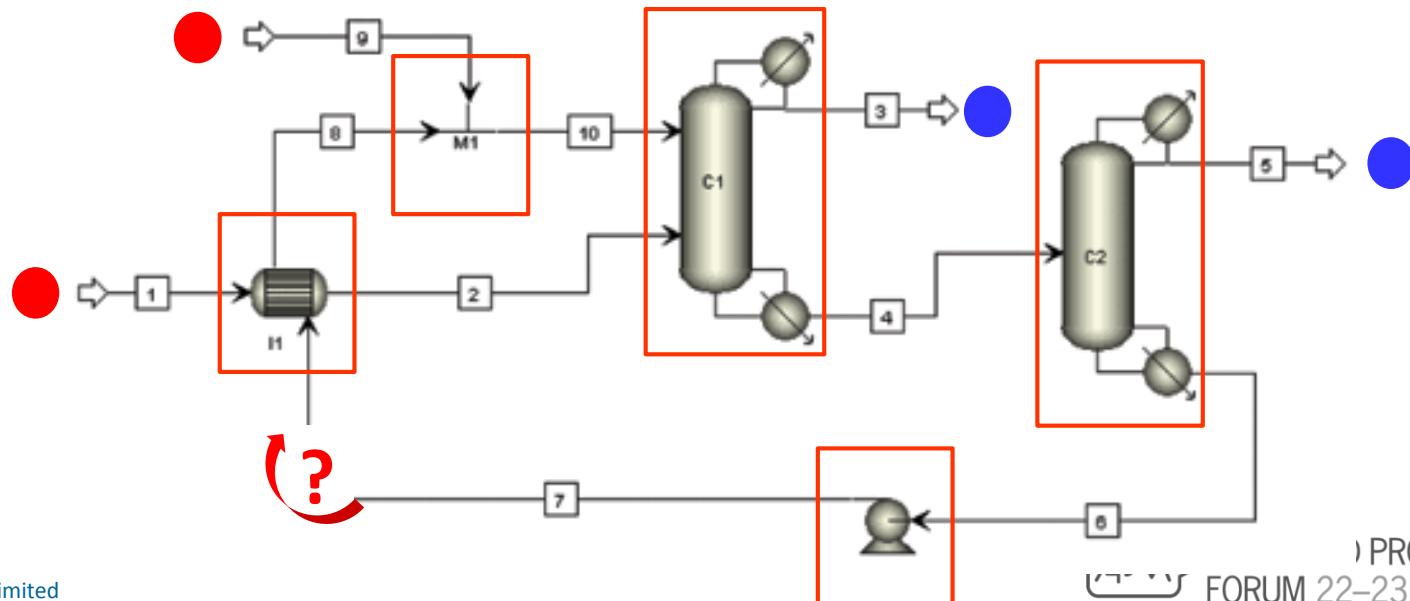
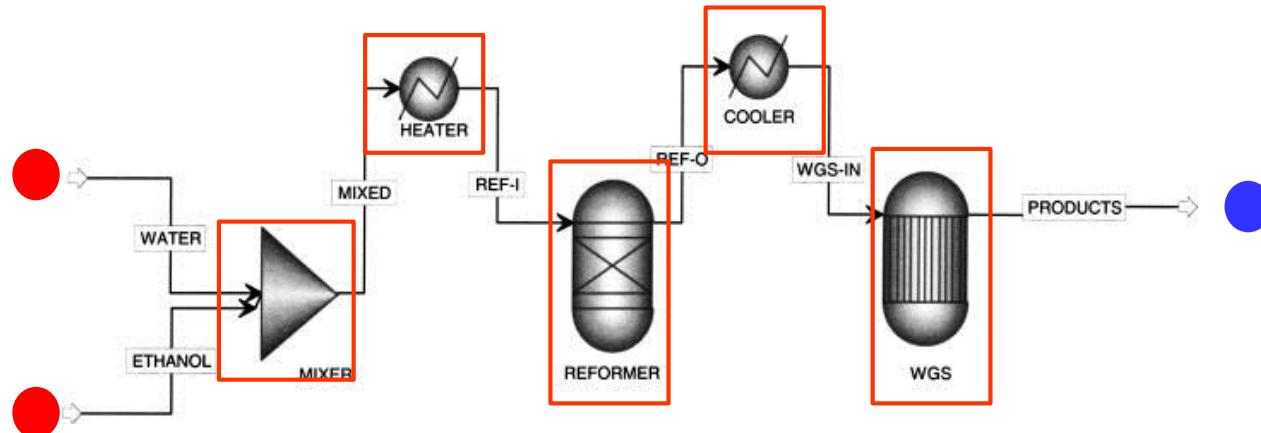
Sequential Modular vs. Equation Oriented Process Modelling

A thirty-year consensus...

The Sequential Modular (SM) approach



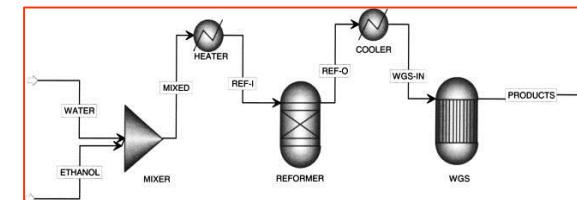
The Sequential Modular (SM) approach



The Sequential Modular (SM) approach

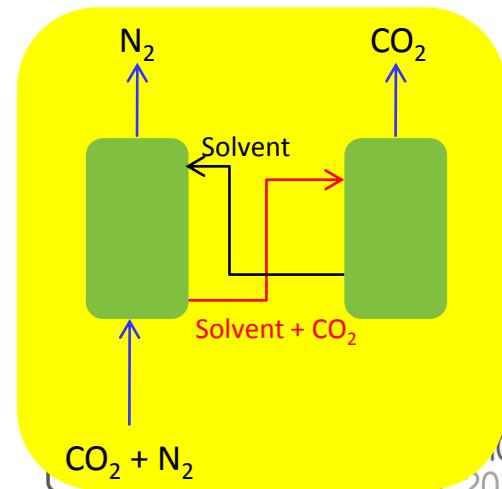
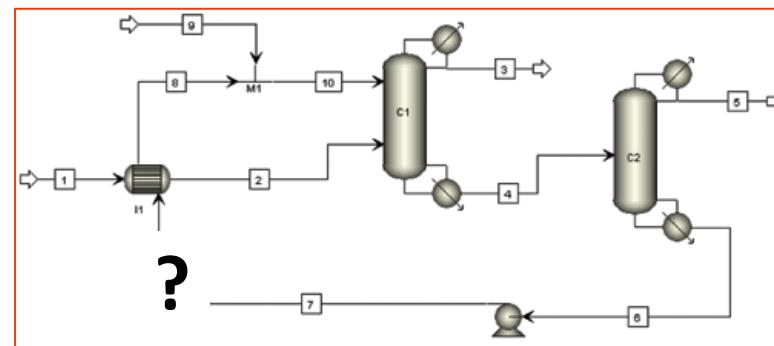
■ Advantages: manually-coded modules

- very quick for doing simple calculations
 - especially single-unit ones
- (should) rarely fail
 - and even then, can usually issue a meaningful message to the user
- user interface for each module can also be hand-coded
 - easy to use, can handle any number of “special” features

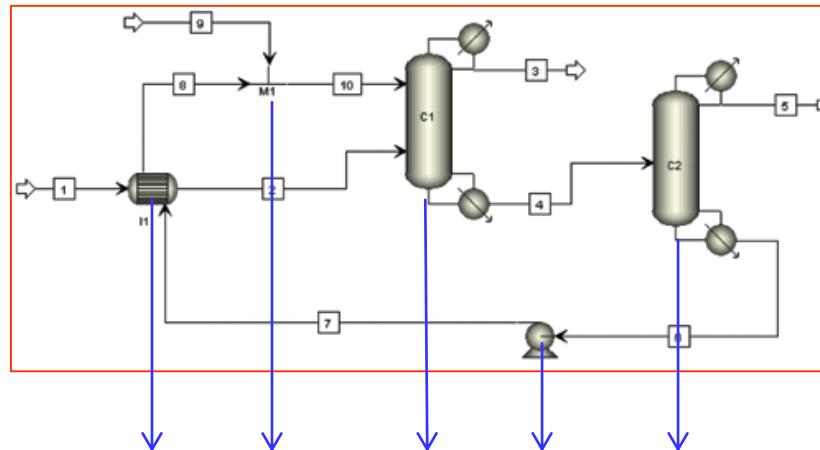


■ Disadvantages: manually-coded modules...

- have in-built directionality from inlets to outlets
 - can't easily specify an *outlet* stream variable and calculate the input
- handling recycles far from straightforward
 - may be (very) slow to converge
 - ...or even fail to converge
 - although this may not be apparent to the user
- difficult to add new “custom” models
 - user needs to code the solution method too
- difficult to use for optimisation
- difficult to



■ *Conceptually much simpler*



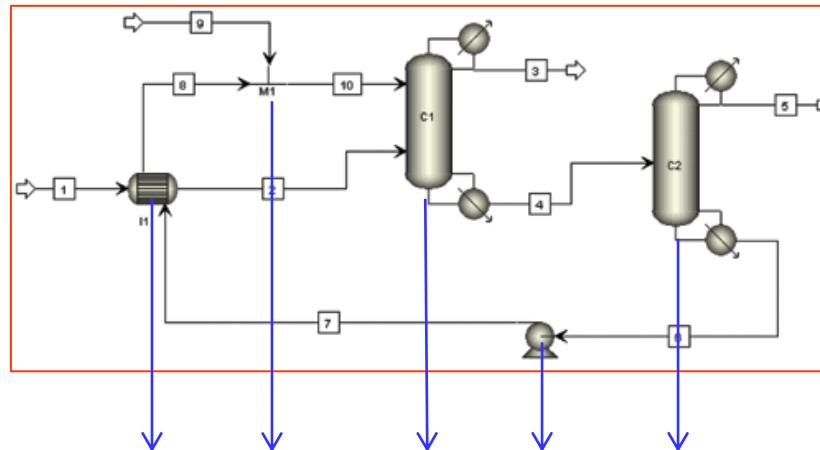
$$f(x) = 0$$

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

■ **Advantages**

- No inherent directionality of computation
 - can be solved with any valid degree-of-freedom specification
- Multiple recycles do not slow down convergence
- Optimisation straightforward with appropriate numerical solvers
- Custom modelling: model developer only needs to provide equations for new unit operations
 - solved automatically by the tool together with equations from all other modules

- *Technically much more complex*



$$f(x) = 0$$

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

- **Disadvantage: lack of robustness**

- Numerical solvers may fail to solve system $f(x) = 0$
- ...unless good initial guesses are provided for all key variables
- ...which may be problematic for very large systems – 10^4 to 10^6+ variables

Sequential Modular

- Robustness (real/perceived)

*Key
consideration*

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

Equation Oriented

- Efficient handling of tightly integrated plants with multiple recycles
- Handling of non-standard (e.g. design) specifications
- Optimisation
- Ease of custom modelling

*Well-understood
advantages*

SPEEDUP® → ACM®
gPROMS ModelBuilder®

Aspen Plus® (EO mode)
RomEO®



Sequential Modular vs. Equation Oriented Process Modelling

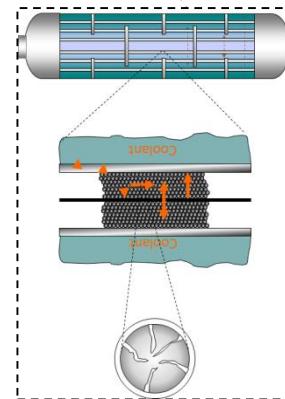
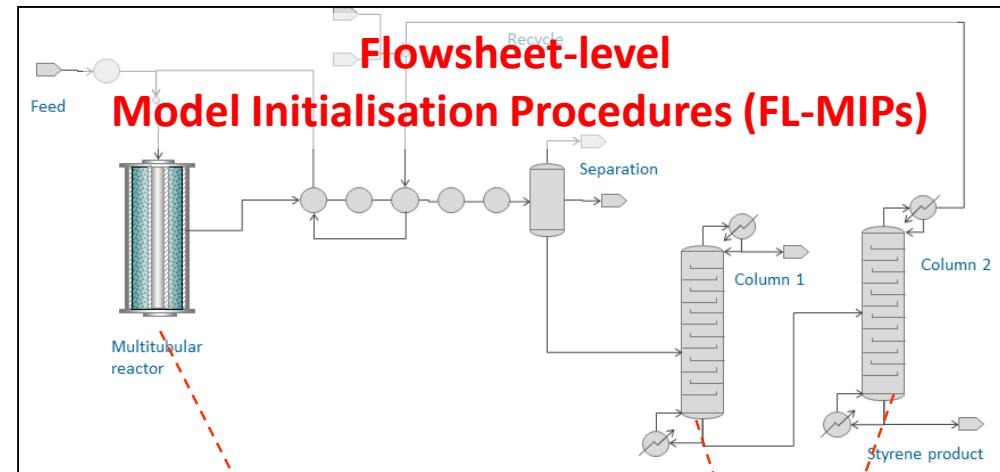
A thirty-year consensus... **and how to disrupt it**

- **Objective: comprehensively address robustness issues in EO flowsheeting technology**

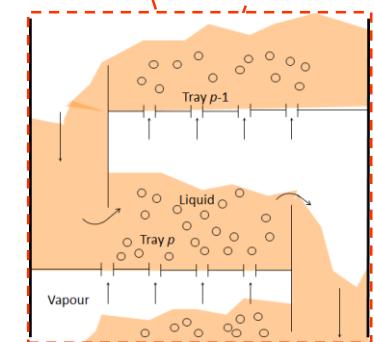
- a long-term fundamental R&D project at PSE

- 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

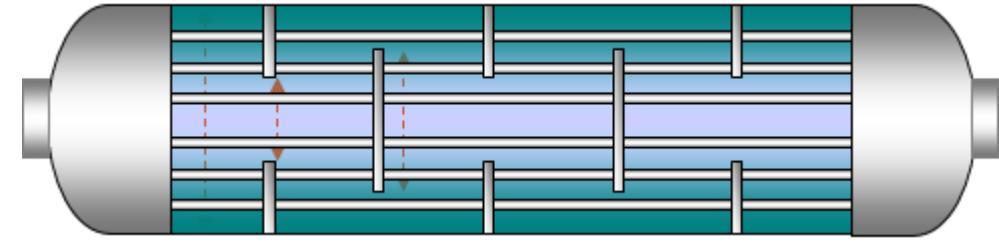


Unit-level Model Initialisation Procedures (UL-MIPs)



Example: Initialisation of tubular reactor model

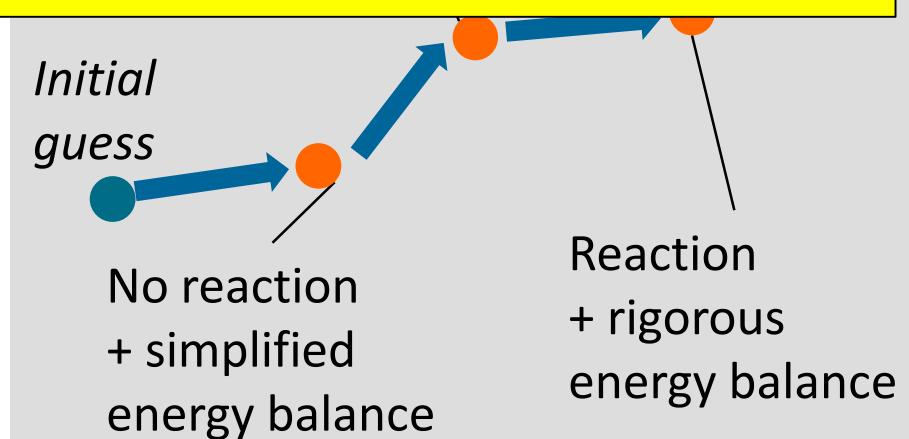
- Complex 3-dimensional model
 - axial, radial, intra-particle variations
 - Maxwell-Stefan multicomponent mass & energy transfer

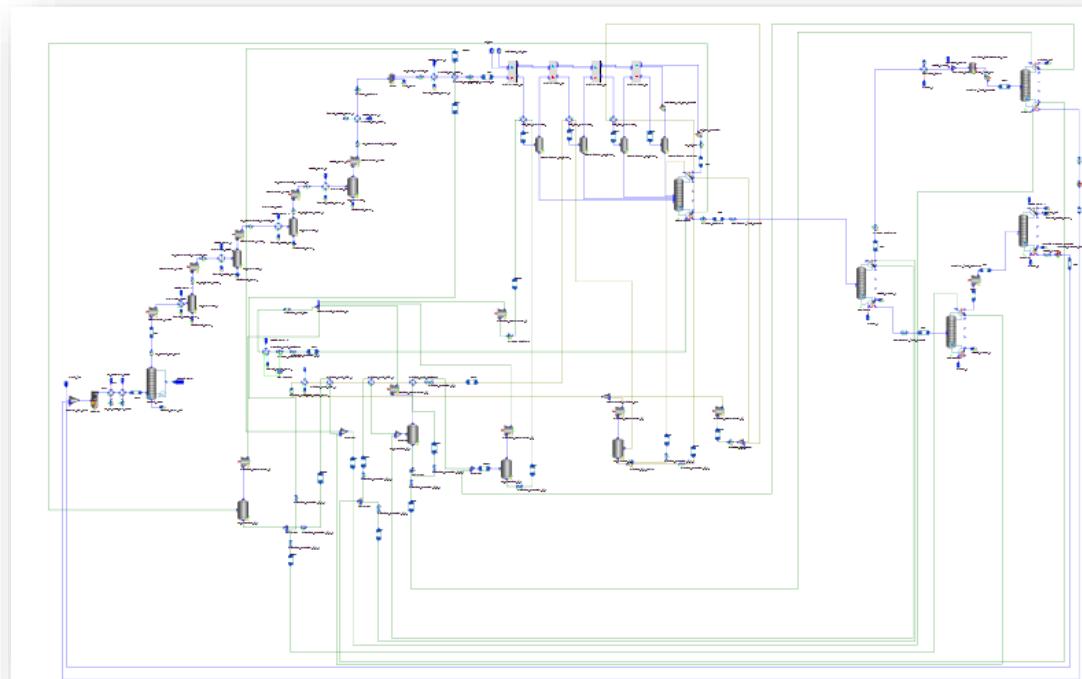


- Unit-level Model Initialisation Procedures
 - capture model developer's knowledge & insight
 - described formally via high-level mechanisms in gPROMS Platform

- Now used throughout gPROMS-family products

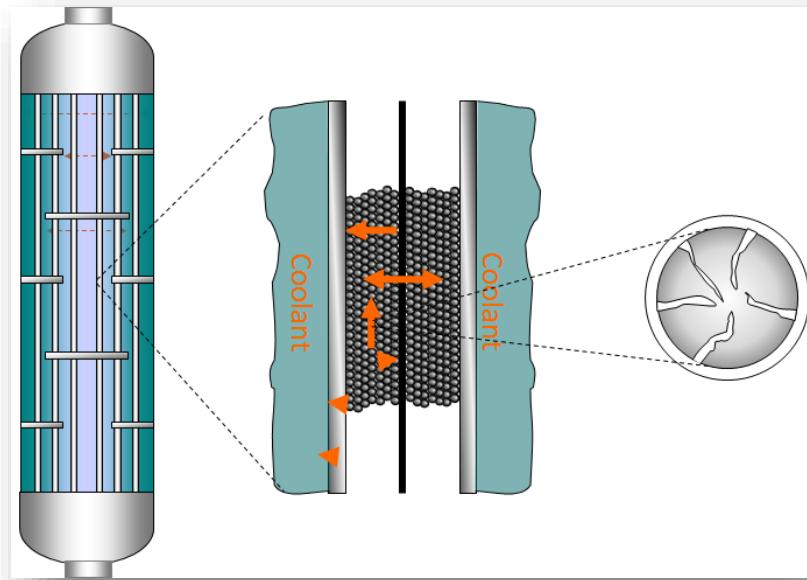
1. Switch off reaction,
use simplified energy balance
2. Switch reaction back on,
keep simplified energy balance
3. Switch to rigorous energy balance



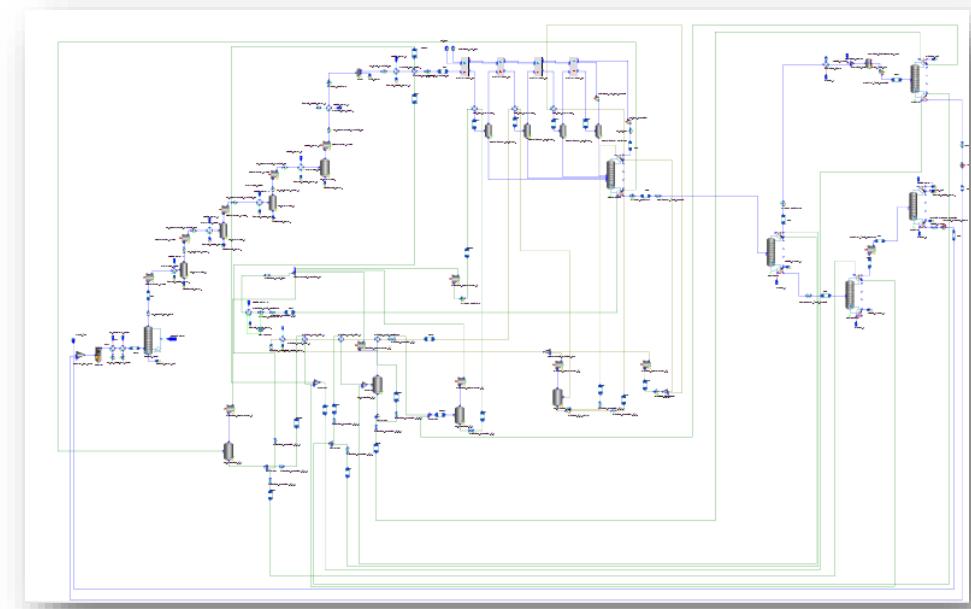


- FL-MIPs based on material & energy coupling within the flowsheet
 - Manage execution of individual UL-MIPs
 - Apply sophisticated convergence algorithms at flowsheet level
- Executed automatically by gPROMS Platform (v4.1+)
 - Largely transparent to the user

UL-MIPs



FL-MIPs



Model Initialisation Procedures (MIPs)
can potentially bring a radical change in the balance between
Sequential Modular and Equation Oriented
process flowsheeting technologies

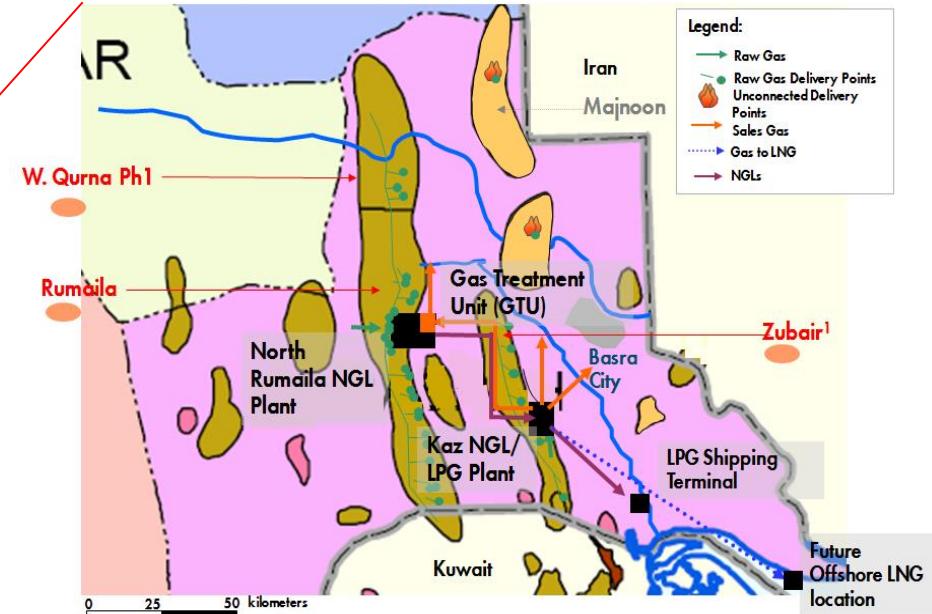


What next?

Key drivers for process modelling

I. A world of complex systems

Example #1: integration across geographical boundaries Integrated natural gas production & processing networks



~20 mmSCM/d of gas (170,000 boe/d)
currently being flared

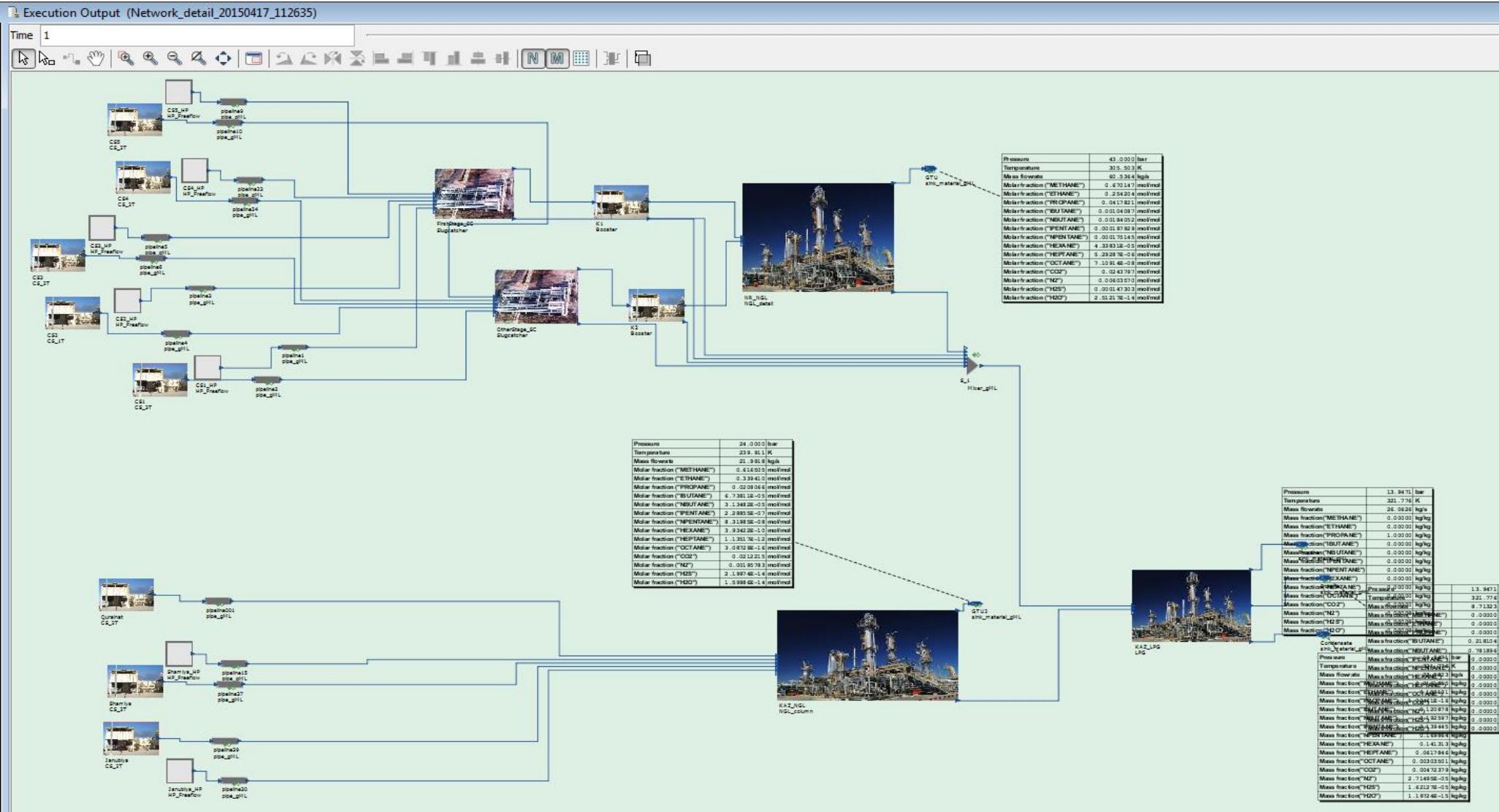


Acknowledgement: Daniel Aluma

- Basrah Gas Company (Iraq) – a Shell Joint Venture
- PhD project at Imperial College London

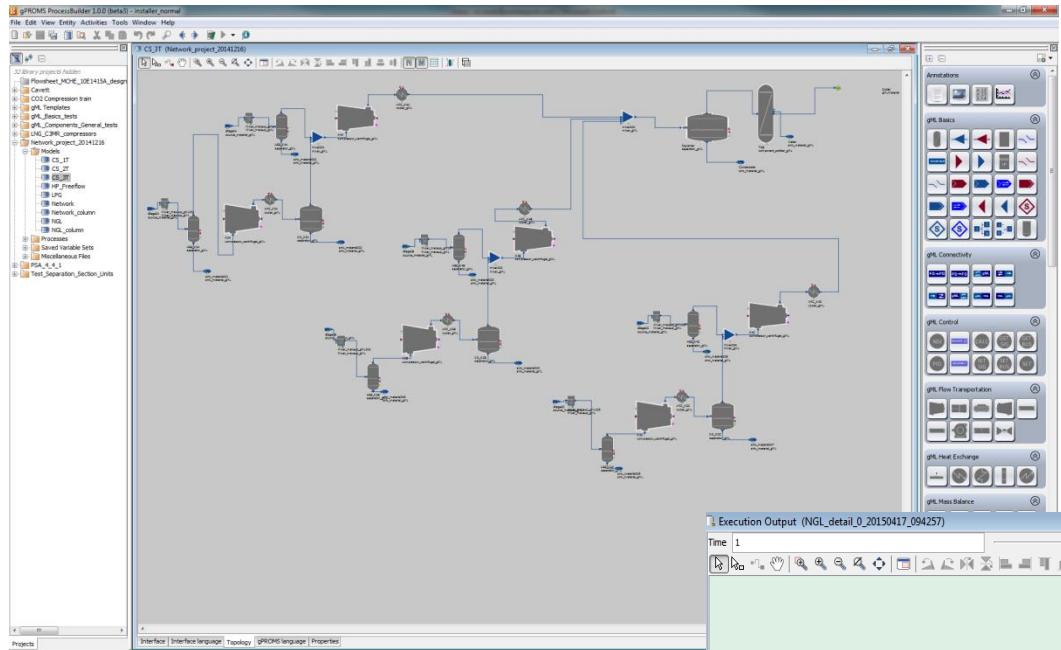
Example #1: integration across geographical boundaries

Integrated natural gas production & processing networks

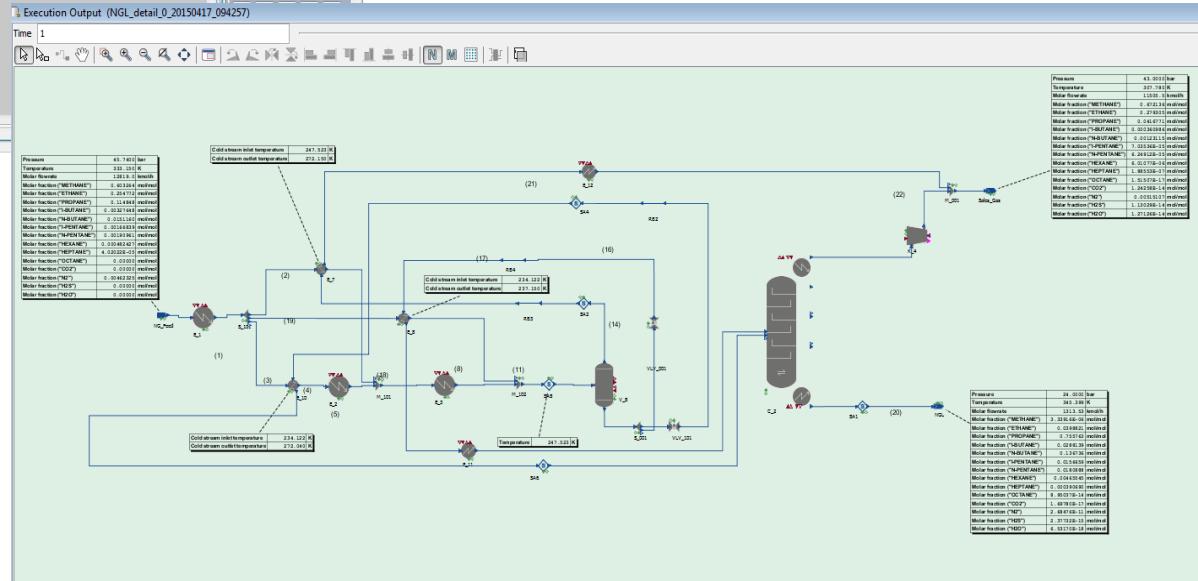


Acknowledgement: Daniel Aluma

Example #1: integration across geographical boundaries Integrated natural gas production & processing networks



Compressor station sub-model



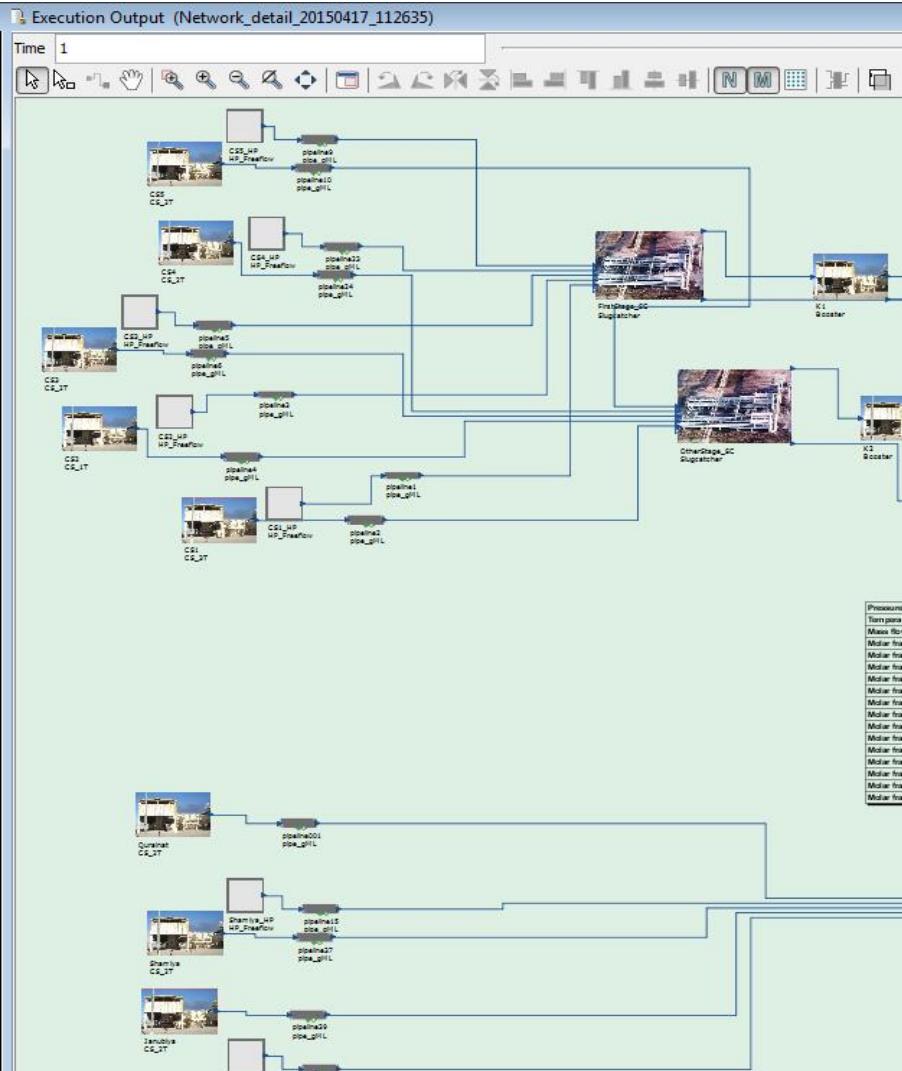
NGL plant sub-model



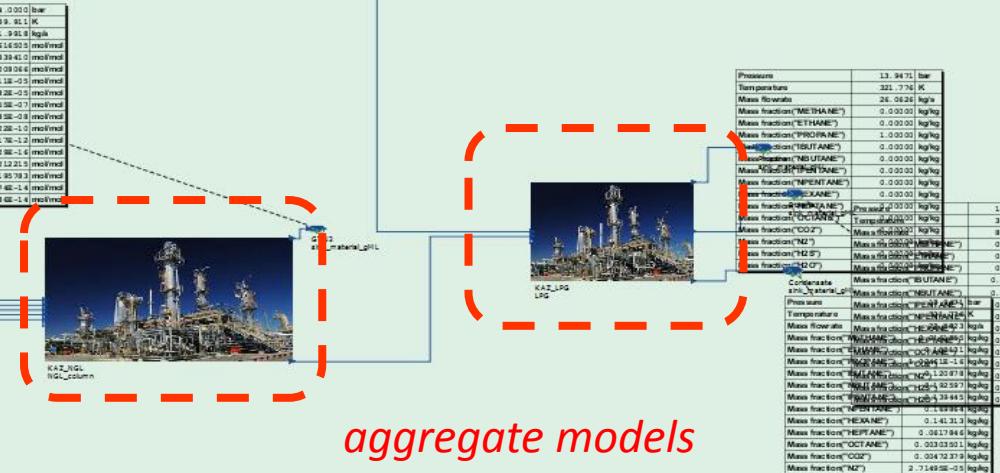
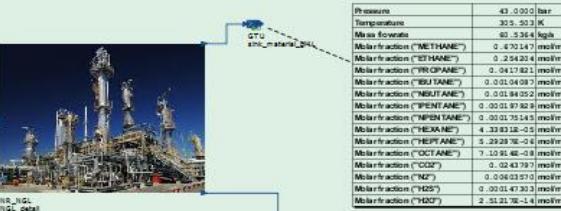
Acknowledgement: Daniel Aluma

Example #1: integration across geographical boundaries

Integrated natural gas production & processing networks



Model equations : 68,772
 "Cold start" simulation : 712s

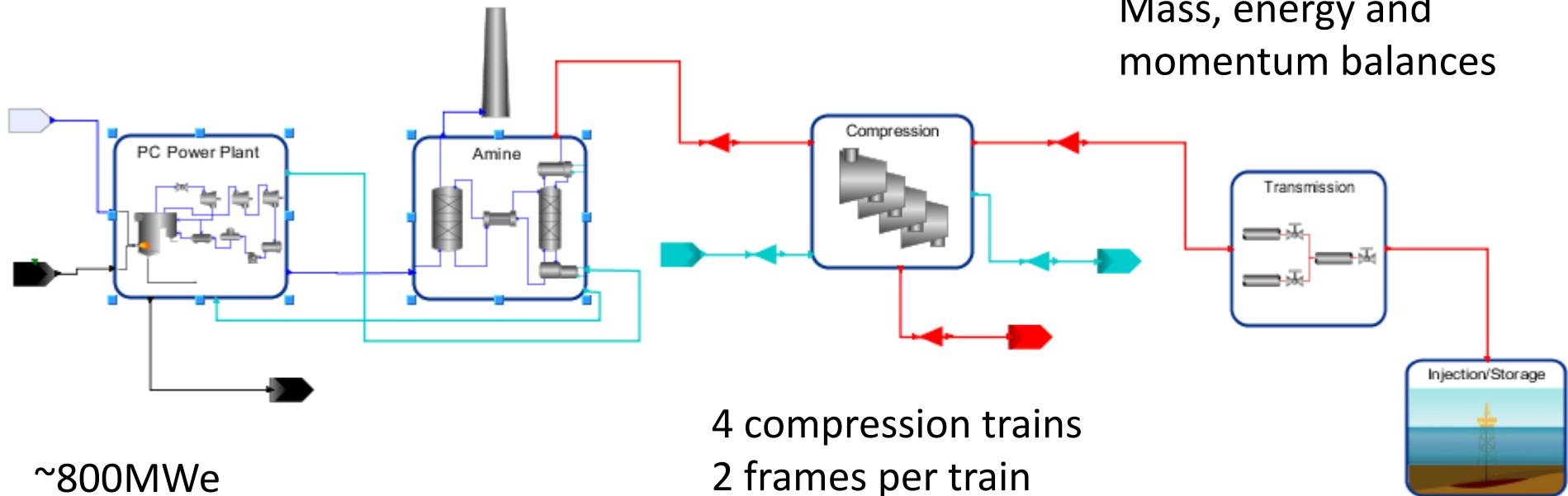


Acknowledgement: Daniel Aluma

Integrated carbon capture & storage chains

Chemical absorption
MEA solvent
90% CO₂ capture

220km of pipeline
Onshore and Offshore
Mass, energy and
momentum balances



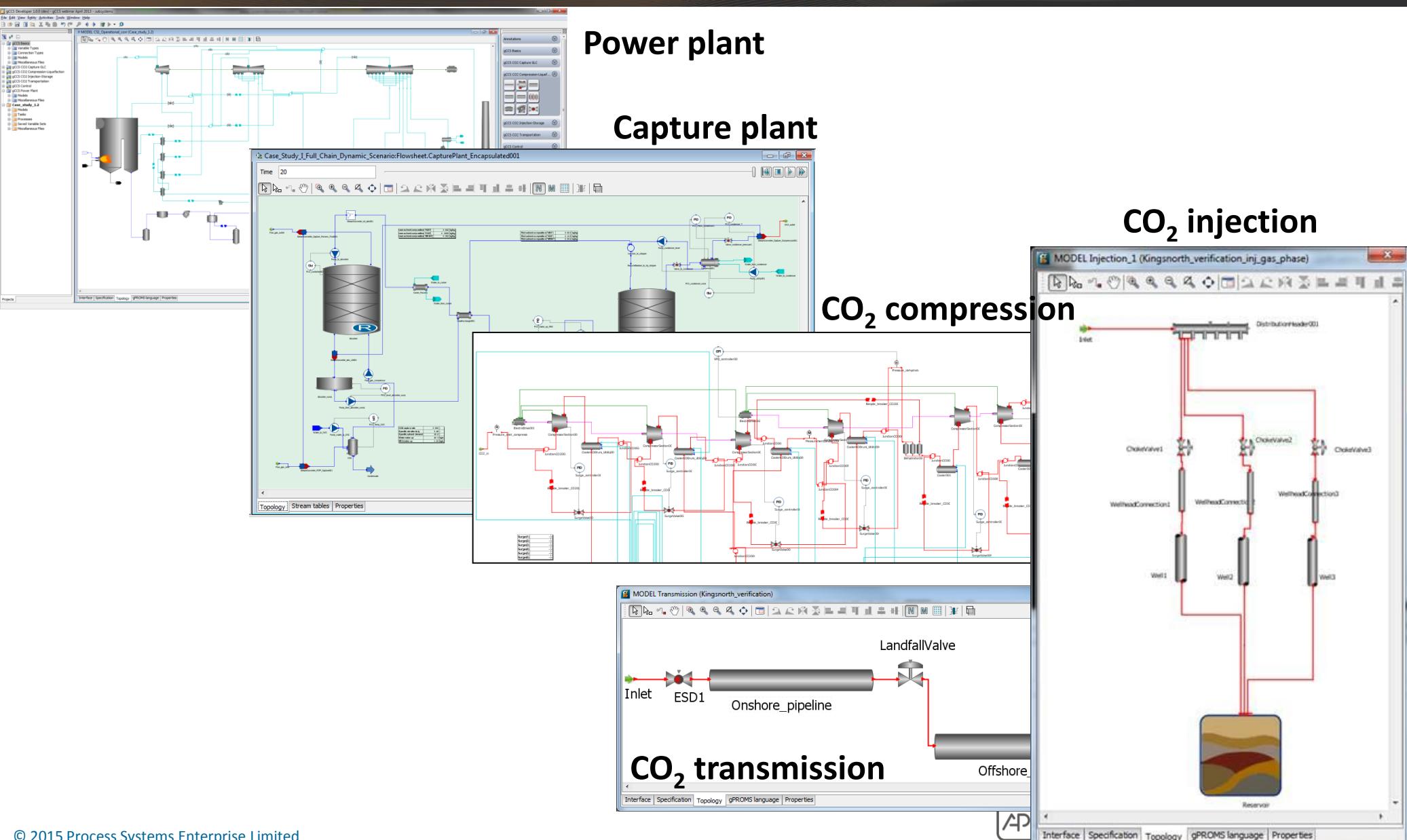
~800MWe
Supercritical
Pulverized coal
Developed with
E.ON

4 compression trains
2 frames per train
Surge control
Developed with
Rolls Royce

Offshore injection
Dense phase injection
4 injection wells
~2km reservoir depth

Example #2: integration across organisational boundaries

Integrated carbon capture & storage chains



Example #3: integration across discipline boundaries

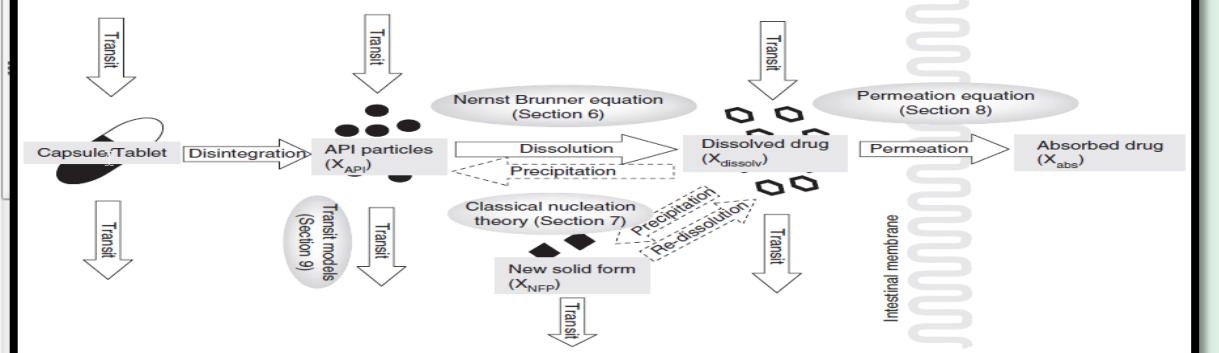
Systems-based Pharmaceutics

gPROMS ModelBuilder 4.0.0

File Edit View Activities Tools Window Help

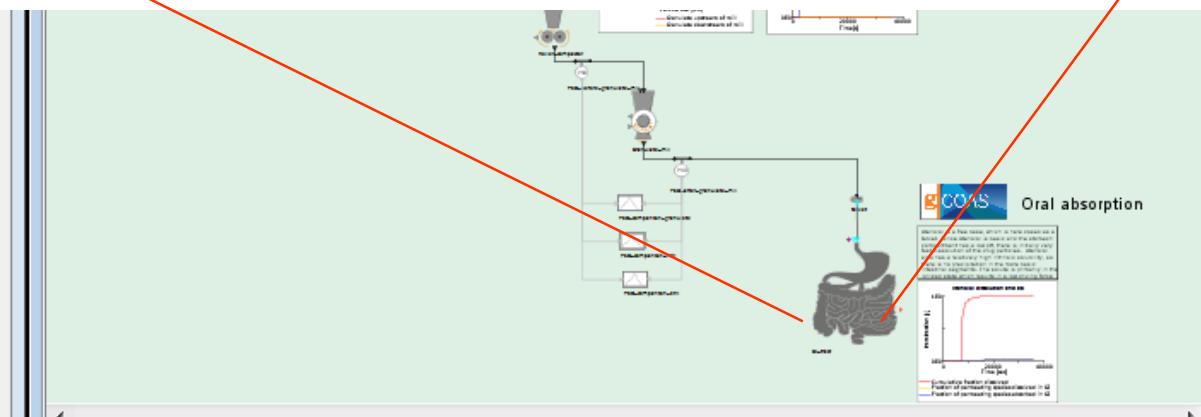
Projects

- SbP - Atenolol
 - Original Entities
 - Variable Types
 - Stream Types
 - Connection Types
 - Models
 - Tasks
 - Processes
 - Saved Variable Sets
 - Miscellaneous Files
 - Results
 - Trajectories
 - Flowsheet
 - Content_uniformity_sensor001
 - crystalliser
 - holdup
 - Variables
 - ic
 - csd
 - sp
 - Variables
 - Ordered_sets_gCR
 - zone
 - evaporation_rate_measurement
 - Variables
 - evap_rate_measured_va
 - feed_point
 - fmc
 - heat_input



K. Sugano, *Expert Opin. Drug Metab. Toxicol.* (2009) 5, pp. 259-293.

K. Sugano, *Biopharmaceutics Modeling & Simulations: Theory, Practice, Methods and Application*, (2012)

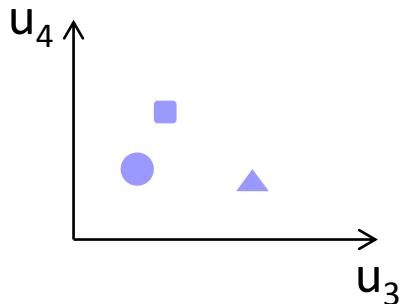




What next?

Key drivers for process modelling

- I. A world of complex systems
- II. Understanding global system behaviour**



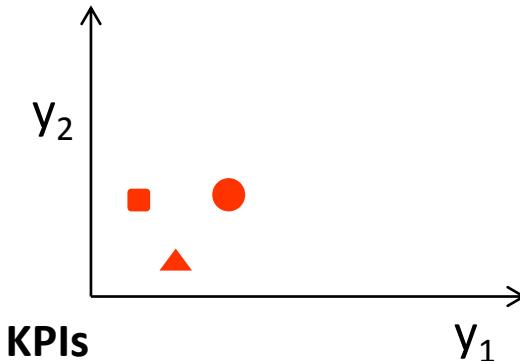
Environmental inputs

- External disturbances
- Commercial environment

Decisions

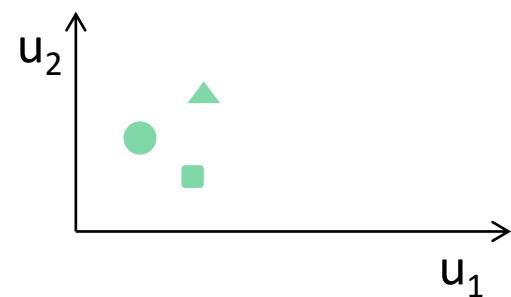
- Design
- Operational

System



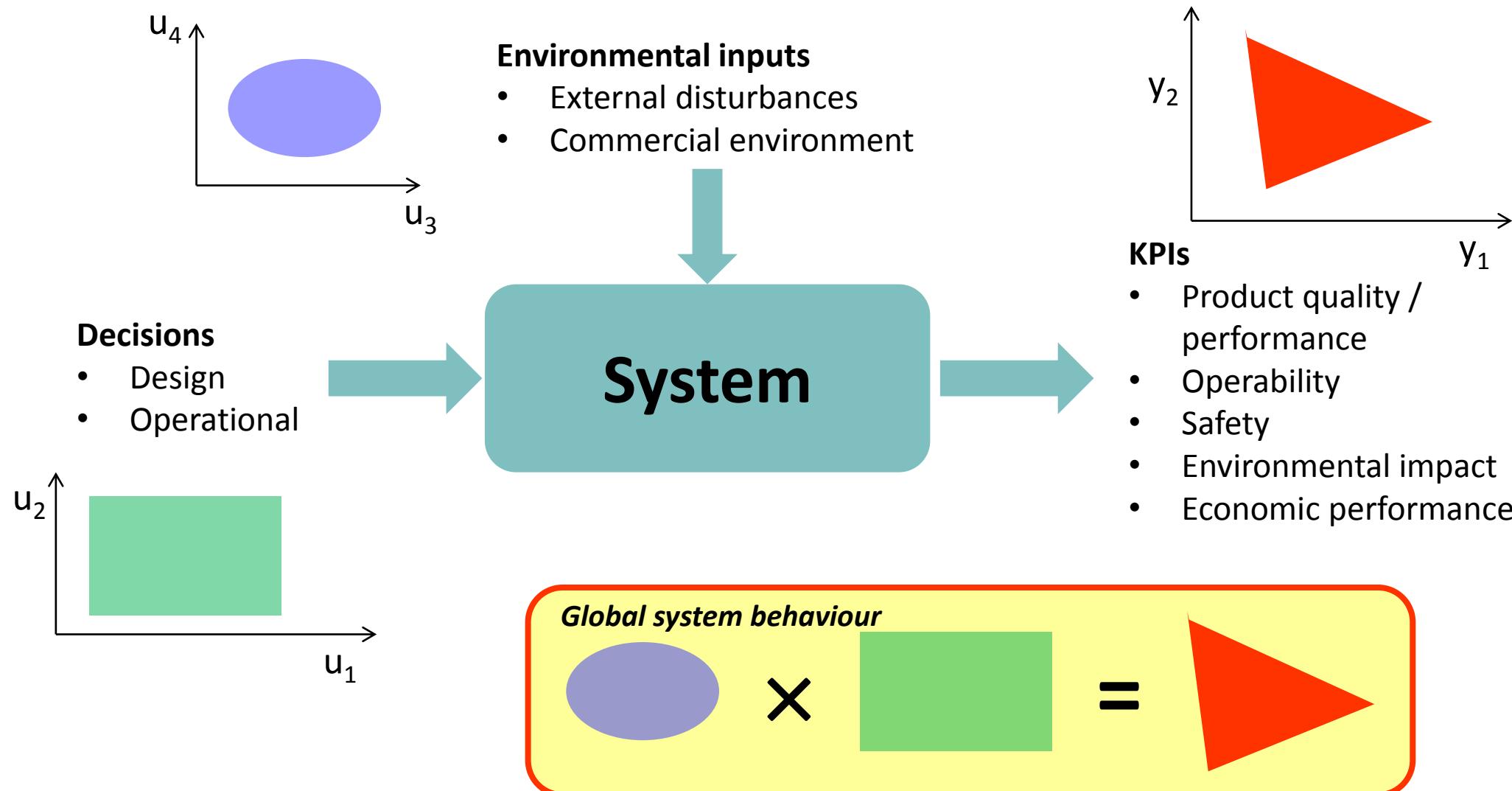
KPIs

- Product quality / performance
- Operability
- Safety
- Environmental impact
- Economic performance

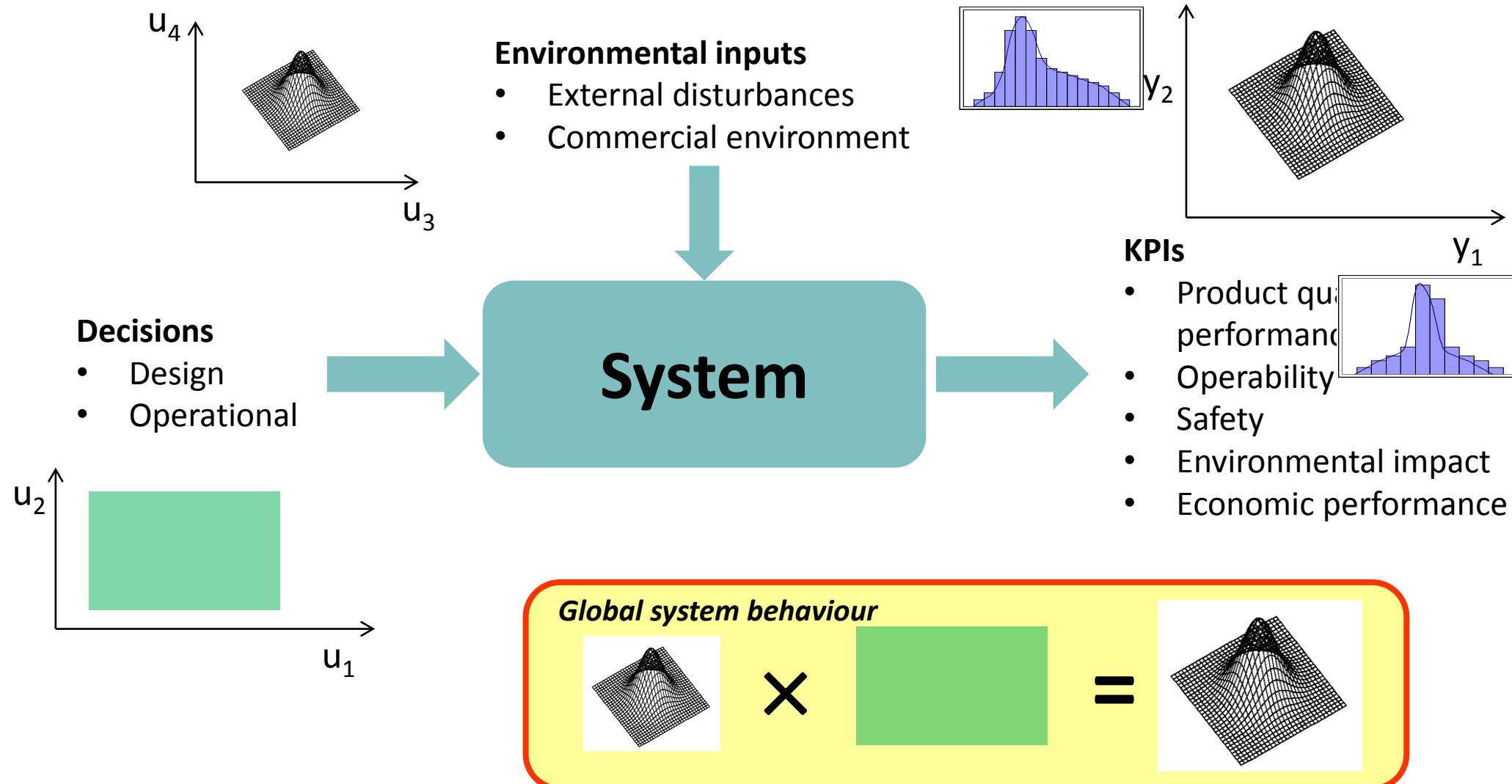


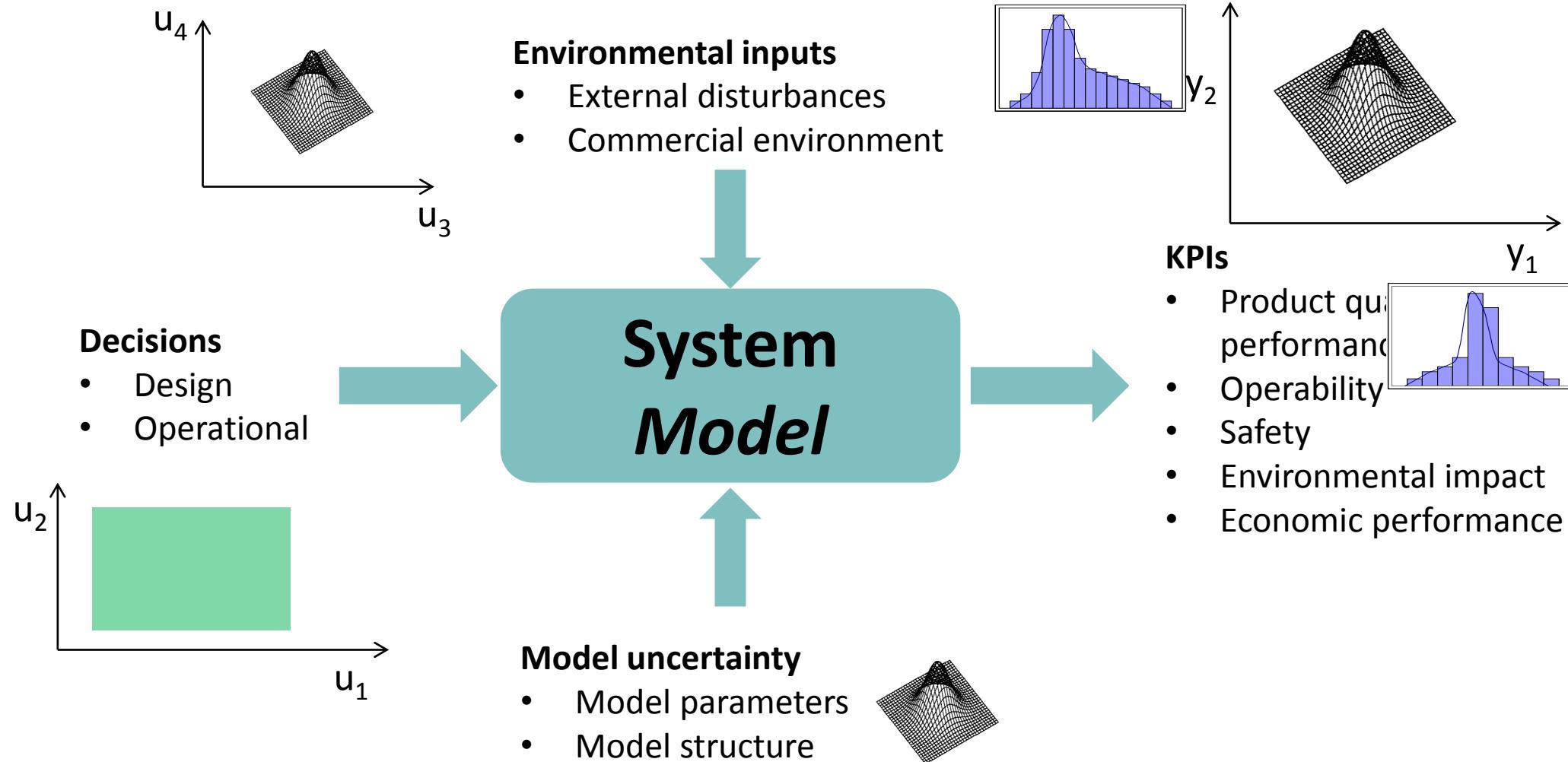
System analysis

$$\bullet \times \circ = \bullet$$

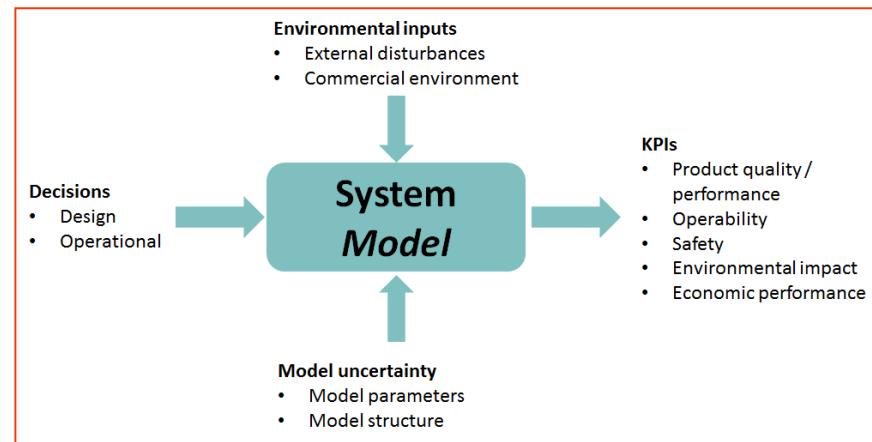


Global system behaviour in an uncertain world





Model-based global system analysis in an uncertain world



Key objectives

■ Probability distribution of KPIs

- taking account of variability/uncertainty in all system inputs

■ Global sensitivities of KPIs with respect to...

- decisions: process controllability
- disturbances: process robustness
- model parameters: model reliability

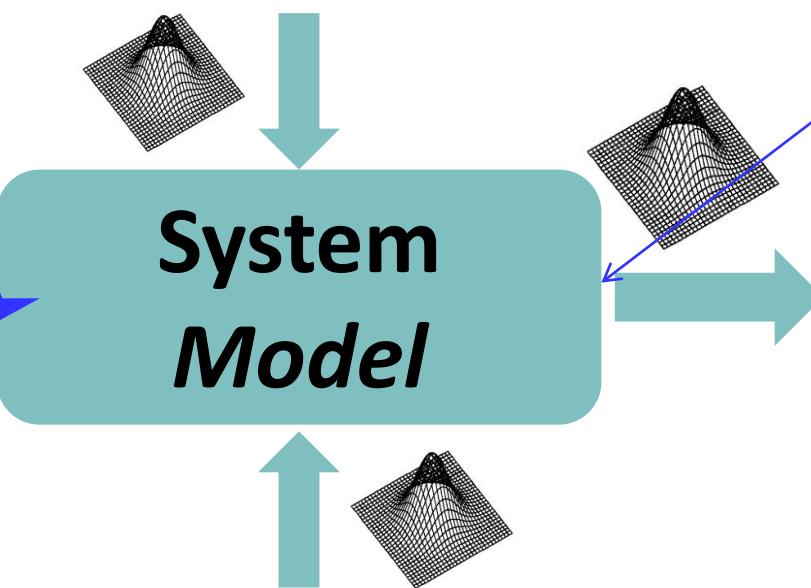
over entire space of interest

2. Reduce variability in environmental inputs

as indicated by Global Sensitivity Indices

Environmental inputs

- External disturbances
- Commercial environment



3. Revise decisions to improve system robustness

Robust Optimization technology

Model uncertainty

- Model parameters
- Model structure

1. Improve model, reduce parameter uncertainty

R&D focus guided by
Global Sensitivity Indices

4. Modify system

e.g. allow operational
decisions to be manipulated
by control system

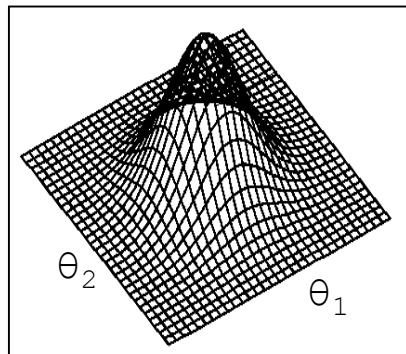
KPIs

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- Operability
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- Economic performance

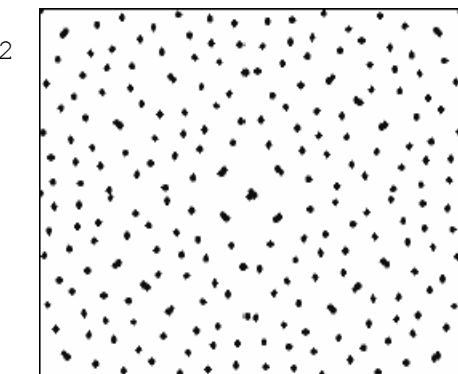
Global System Analysis

A general tool for the gPROMS platform

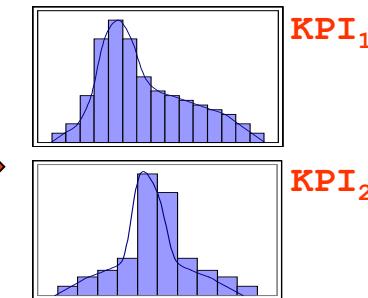
I. Inputs



II. Sampling



III. Outputs



A collaborative R&D project (June 2014-May 2016)

- Project leader : PSE
- Consortium : AstraZeneca, Britest, GSK, Pfizer
- Funding (partial) : £988k ($\sim \$1.5m$) by InnovateUK

A fundamental capability within the gPROMS platform

- directly applicable to any gPROMS model in any gPRODUCT



What next?

Key drivers for process modelling

- I. A world of complex systems
- II. Understanding global system behaviour
- III. The Ubiquitous Model**

Modelling across the process lifecycle

R & D

Laboratory data analysis

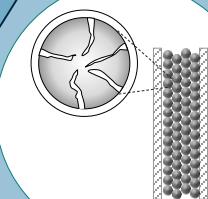


Optimal experiment design

Conceptual process design

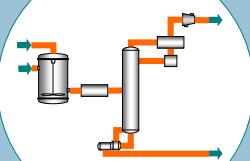


Catalyst design and analysis

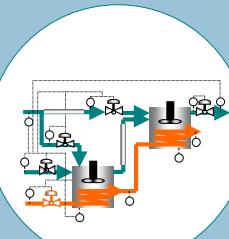


Engineering design

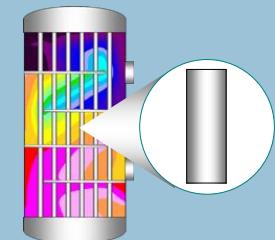
Process front-end design (FEED)



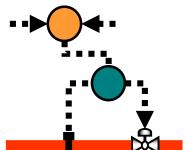
Process and equipment design optimisation



Detailed design of key units

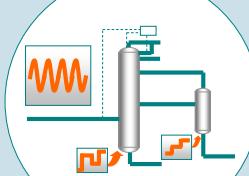


Control design and verification

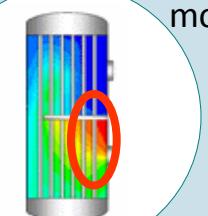


Operations

Design of optimal operating procedures



Troubleshooting with detailed predictive models

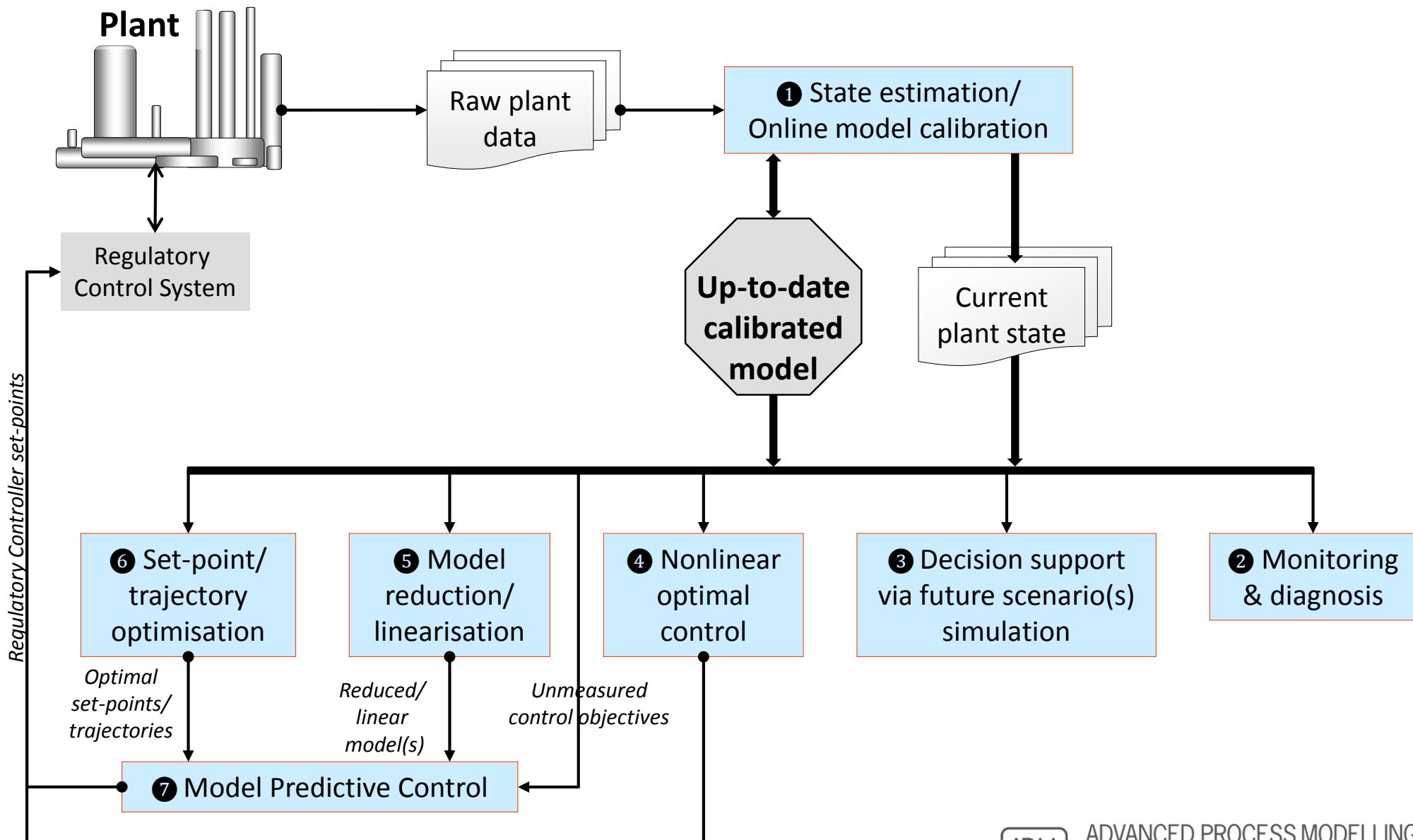


Online Model-Based Applications



Online Model-Based Applications

An integrated framework



Online Model-Based Applications Advanced Real-time Refinery Monitoring & Optimisation



Main FCO website

Foreign & Commonwealth Office

Blogs home | About our blogs | All bloggers | About the team | A

FCO Blogs > Science & Innovation Network, India > Health and disease > Deputy Prime Minister announces new UK-India partnerships to tackle some of the world's biggest problems

Deputy Prime Minister announces new UK-India partnerships to tackle some of the world's biggest problems

August 27, 2014

During a trade mission to India this week Nick Clegg, announced a series of new and Indian scientists which will look to issues facing the two countries. From the weather, the new partnerships will cement the position of both countries in the vanguard of scientific research. You can see more photos from the visit on Flickr.



He announced four projects that have won a share of over £1.7 million funding from the UK's innovation agency, the Technology Strategy Board and the Indian Department of Science and Technology to create new commercial technology in the health and energy sectors. The four projects successfully bid for funding from the UK-India Joint Industrial Research and Development Programme.

Mr Cleo also met PM Modi in Delhi

The successful partnerships are:

- GBIT in India and Oxitec Ltd in the UK: Research on sustainable prevention of dengue fever, a mosquito-born disease which threatens 40% of the world's population.
- Lifecare Innovations in India and Wockhardt Ltd/University of Central Lancashire in the UK: improving the treatment for the life-threatening tropical disease Leishmaniasis.
- Chogen Powers Ltd in India and GeoCapita Ltd/University of Glasgow in the UK: research into improving the process for generating power from biofuels.
- Bharat Petroleum Corporation/Gyan Data in India and Process Systems Enterprise Ltd in the UK: to improve efficiency and yields in oil refineries.

We, the UK Science and Innovation Network-India are very pleased to

• Bharat Petroleum Corporation/Gyan Data in India and Process Systems Enterprise Ltd in the UK: to improve efficiency and yields in oil refineries.

partnership between both TSB and DSTI that led to the announcement of the UK-India Collaborative Industrial R&D Programme. We have been working closely with the TSB to establish opportunities for UK-India Innovation collaboration and this call is the first step in that direction.

- <http://blogs.fco.gov.uk/science-innovation-network-india/2014/08/27/deputy-prime-minister-announces-new-uk-india-partnerships-to-tackle-some-of-the-worlds-biggest-problems/>



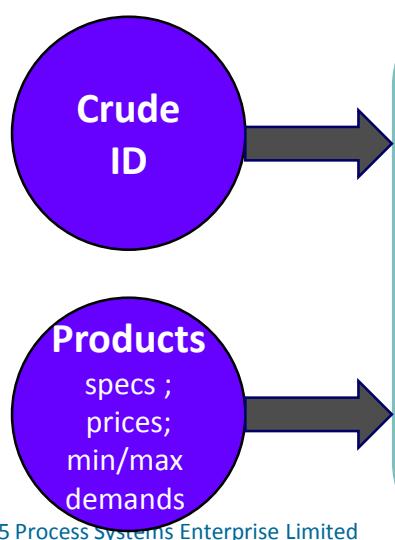
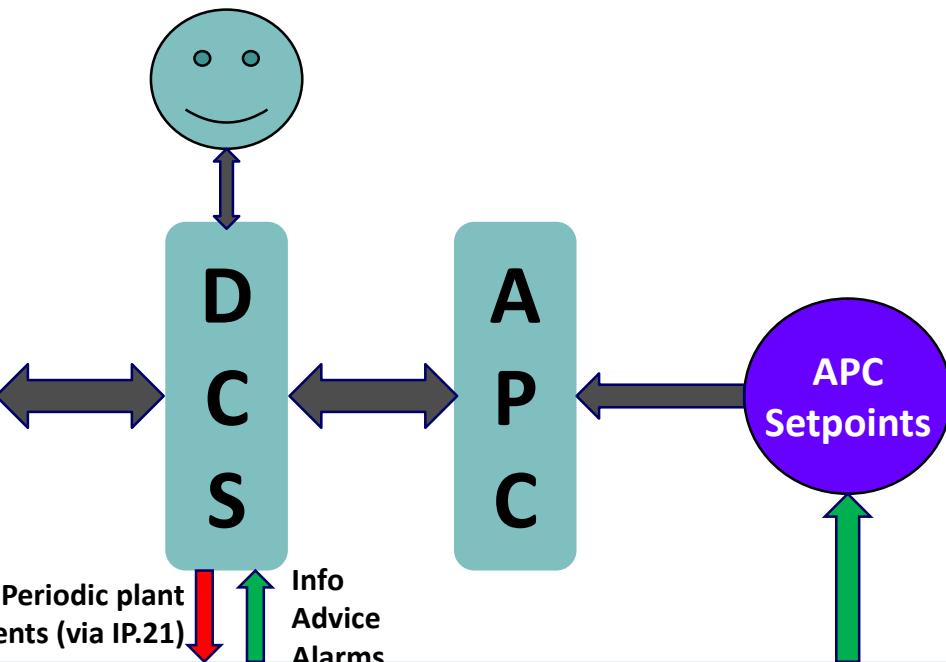
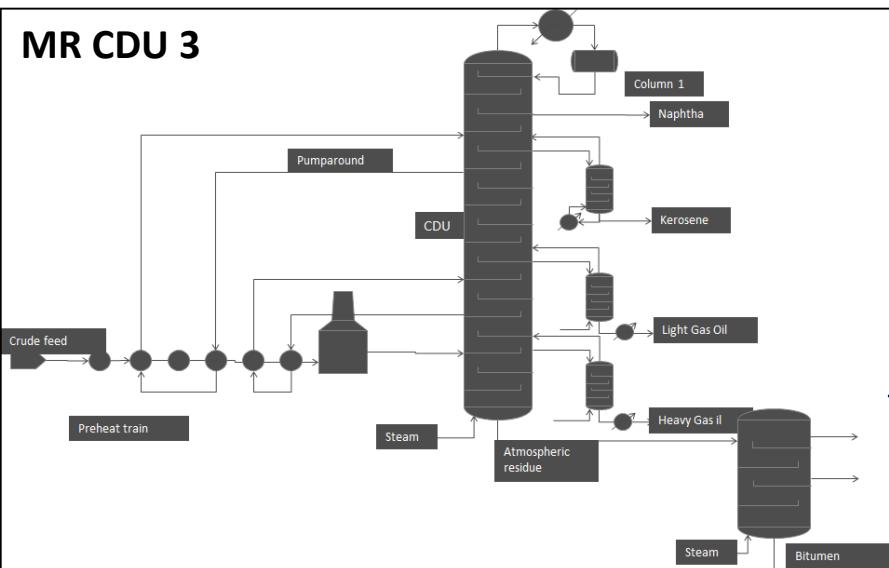
ADVANCED PROCESS MODELLING
FORUM 22-23 APRIL 2015

Advanced Real-time Refinery Monitoring & Optimisation

Overview



MR CDU 3



ARRMO

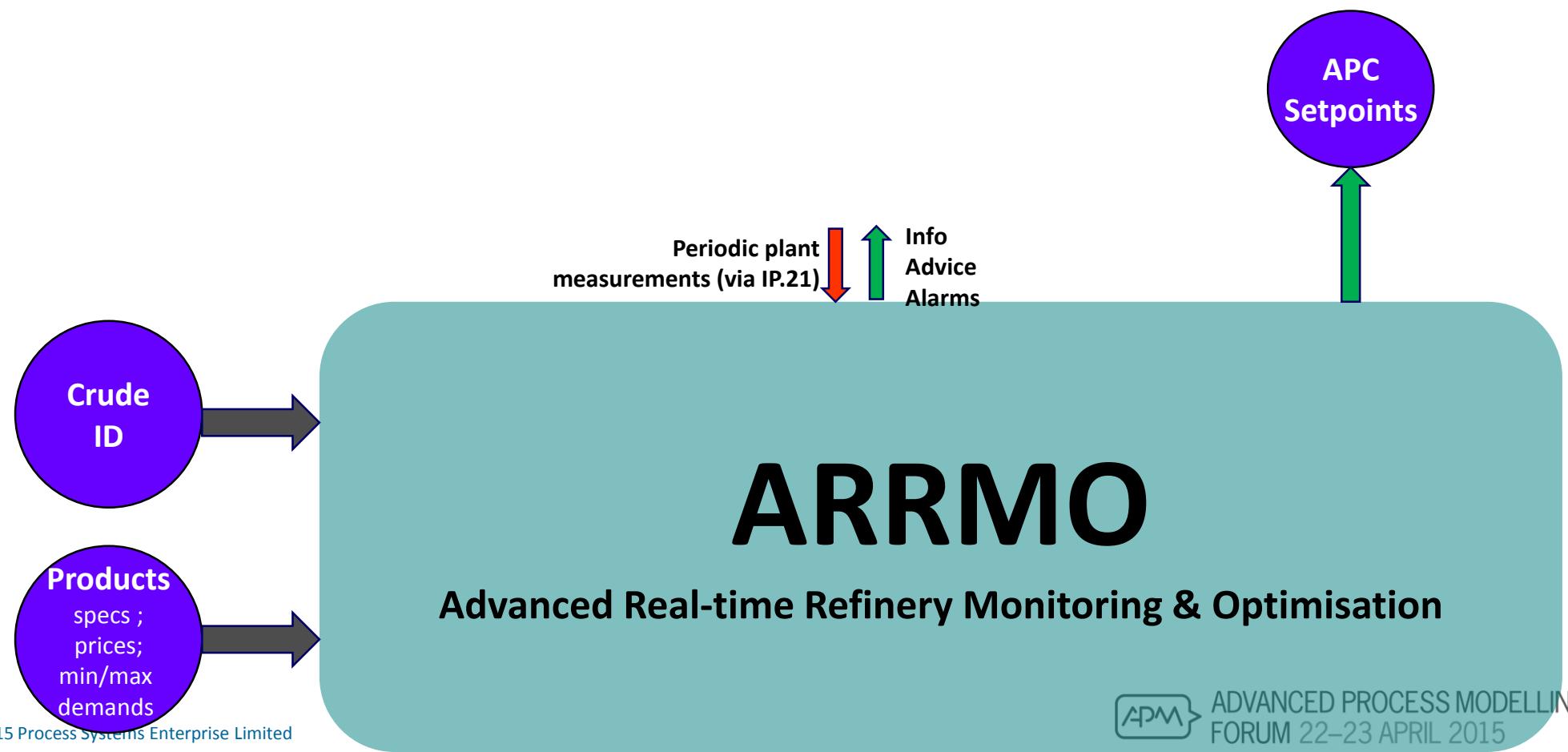
Advanced Real-Time Refinery Monitoring & Optimisation



ADVANCED PROCESS MODELLING
FORUM 22-23 APRIL 2015

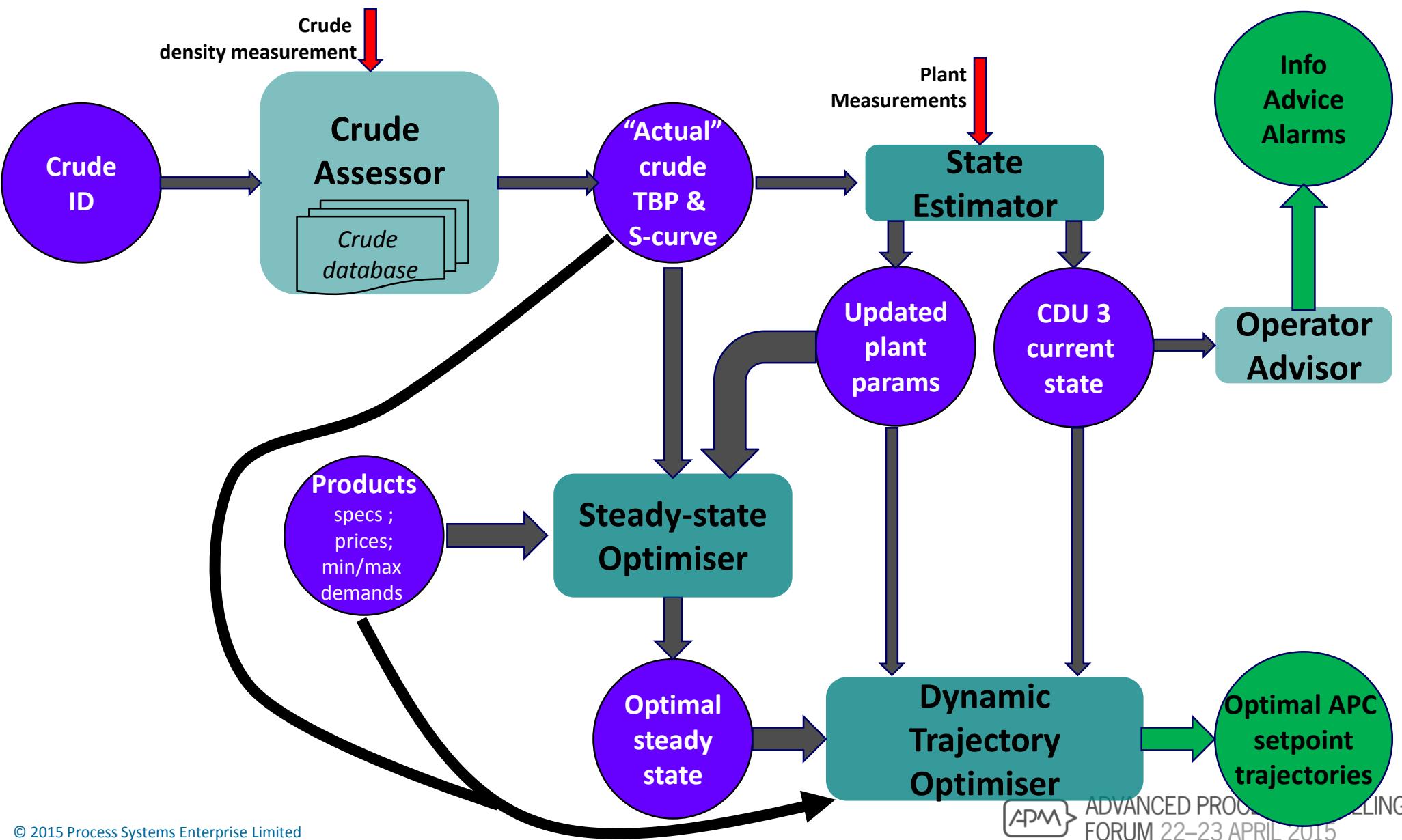
Advanced Real-time Refinery Monitoring & Optimisation

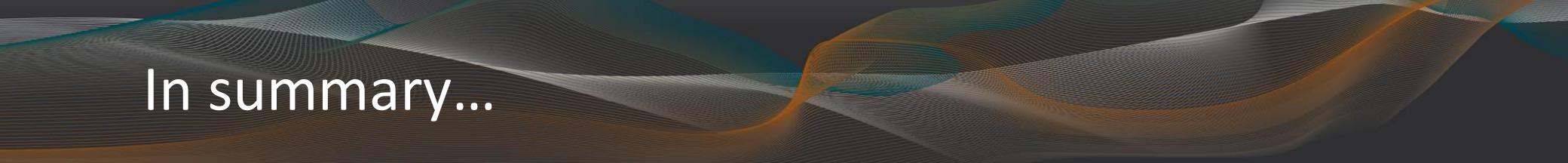
Overview



Advanced Real-time Refinery Monitoring & Optimisation

Overview





In summary...

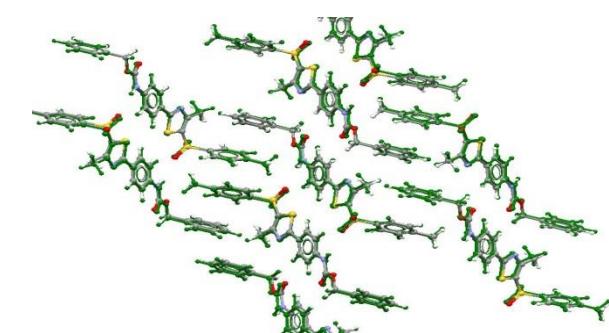
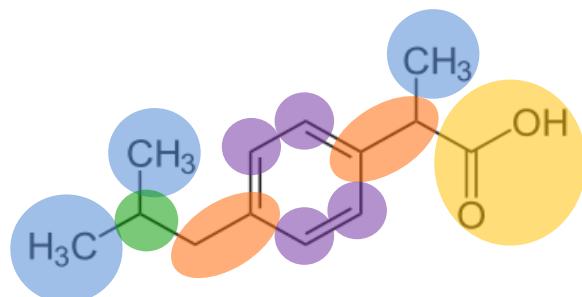
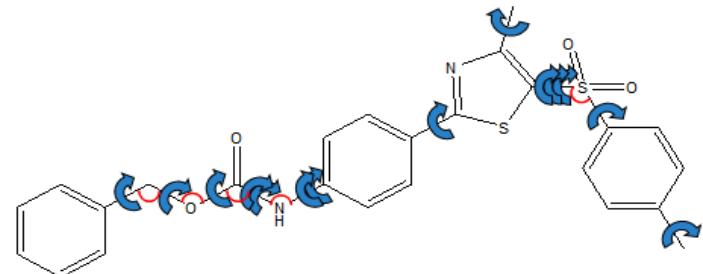
An era of change for process modelling

■ Current drivers

- a world of complex systems
- understanding global system behaviour
- the Ubiquitous Model
-

■ ...have serious technological implications

- modelling of processing equipment behaviour
- modelling of material behaviour
- integration of modelling with experimental R&D



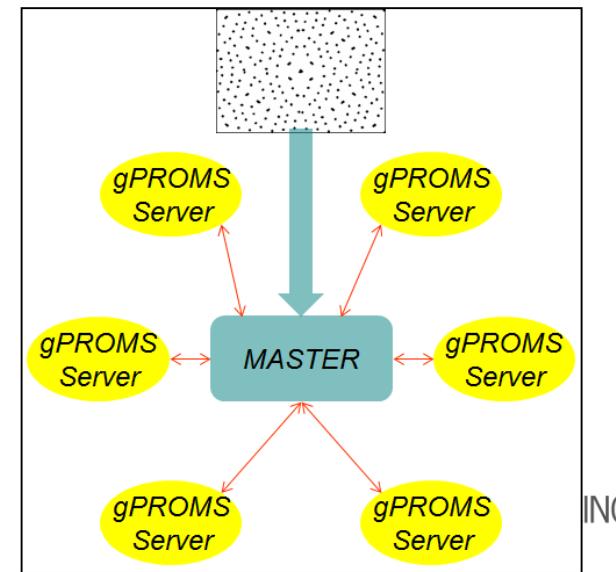
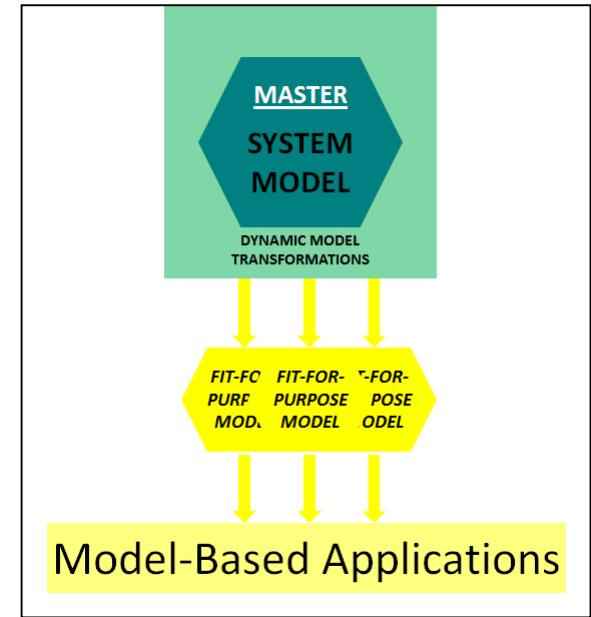
An era of major change for process modelling

■ Current drivers

- a world of complex systems
- understanding global system behaviour
- the Ubiquitous Model
-

■ ...have serious technological implications

- modelling of processing equipment behaviour
- modelling of material behaviour
- integration of modelling with experimental R&D
- **software architectures for process modelling**
- **exploitation of advanced computing hardware**



General mathematical modelling



gPROMS ModelBuilder
Advanced process modelling environment

Sector-focused modelling tools

Chemicals & Petrochemicals



gPROMS ProcessBuilder
Advanced process simulation

Life Sciences,
Consumer, Food,
Spec & Agrochem



Solids process optimisation



Crystallization process optimisation



Oral absorption

Power & CCS



CCS system modelling

Oil & Gas



Flare networks & depressurisation

Wastewater Treatment



Wastewater systems optimisation

Fuel Cells & Batteries



Fuel cell stack & system design



The gPROMS platform

Equation-oriented modelling & solution engine

Materials modelling



INFOCHEM
Multiflash



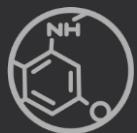
Model deployment tools

Enterprise Objects



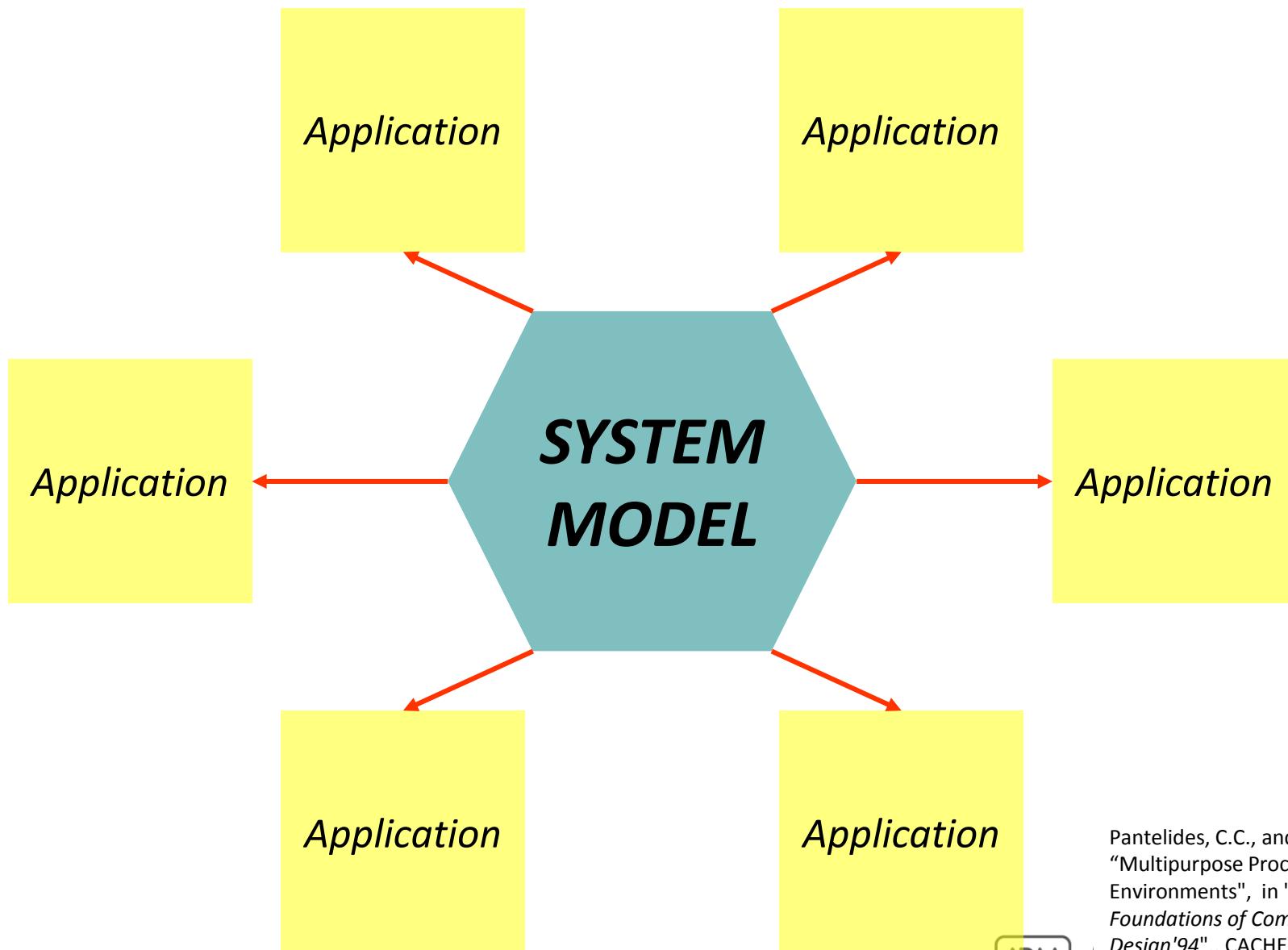
Deploy models in common engineering software

Thank you



Process Modelling Environments

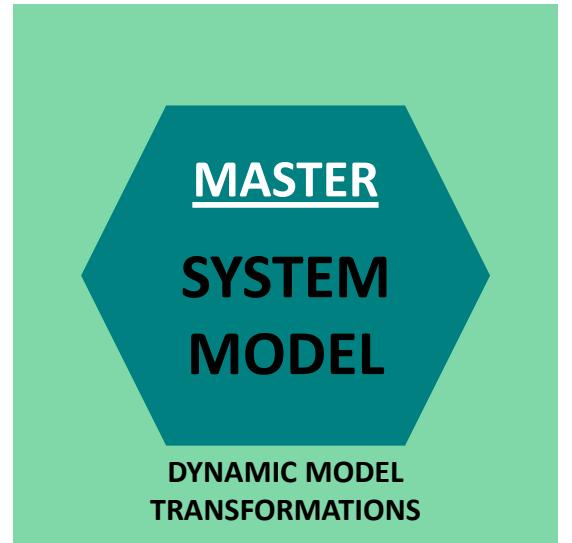
The Original Vision (~1990s)



Pantelides, C.C., and Britt, H.
"Multipurpose Process Modeling
Environments", in "Proc. Conf. on
*Foundations of Computer-Aided Process
Design'94*", CACHE Publications (1995),
128-141.

Process Modelling Environments

A New Paradigm



Model optimized
for each specific application
...generated automatically
from Master Model

...incorporating
multi-level component
models

...and changing dynamically
over time

Model-Based Applications