Process Modelling

Current Perspectives, Future Visions

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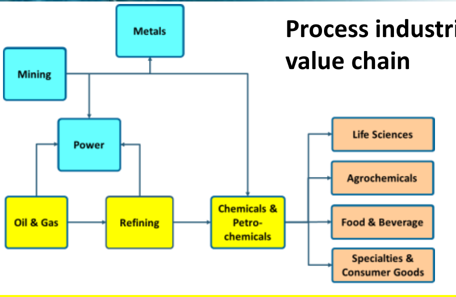
Modelica Jubilee Symposium
Lund, 30 September 2019

Process modelling technology

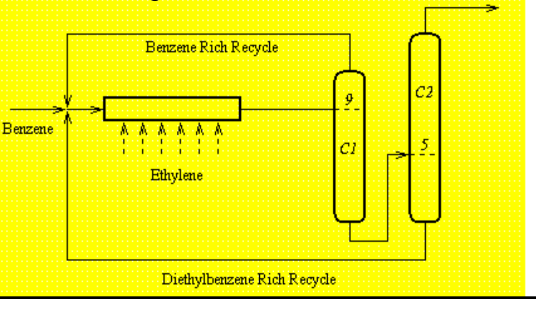
General methodologies & software systems for the effective & efficient

1. capture of available knowledge in the form of mathematical models
2. deployment of this knowledge for engineering throughout the process lifecycle
3. identification of significant limitations of/gaps in currently available knowledge

Process industries value chain



Process modelling ~1990s



Process modelling technology

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1. capture of available knowledge in the form of mathematical models
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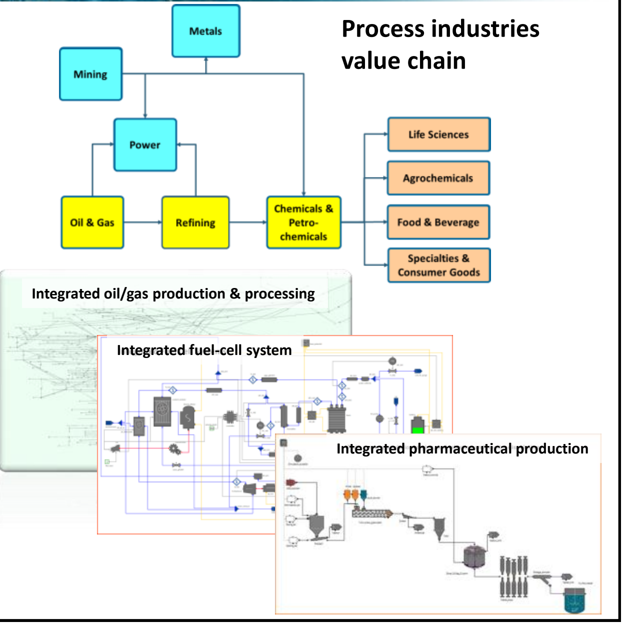
Challenge: **COMPLEXITY**

- conceptual
- computational

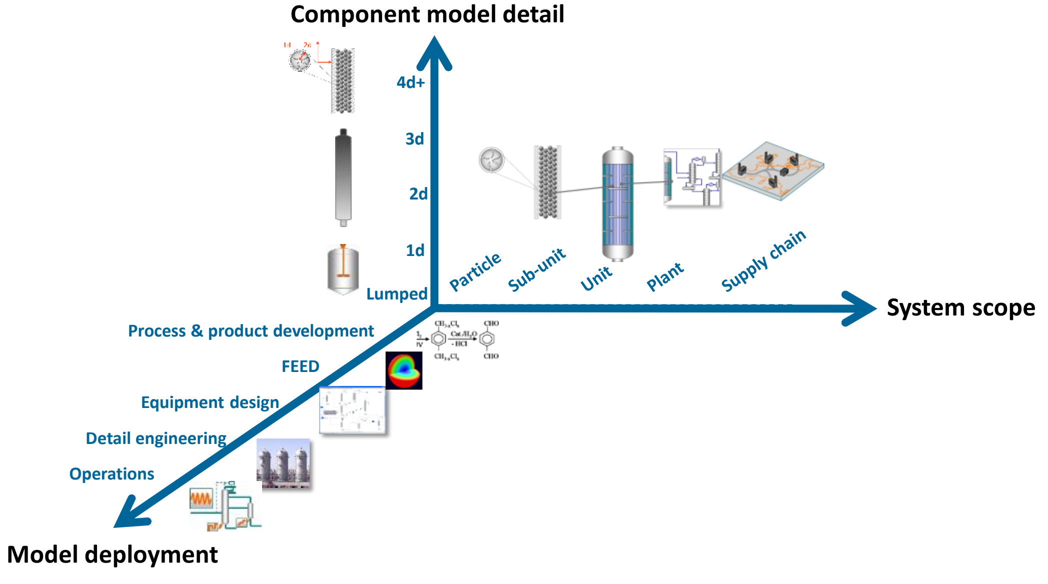


Outline

- Process modelling technology: where are we now?
  - Component model detail
  - System scope
  - Model deployment
- Process modelling technology: the next decade
  - Advances in underpinning IT technologies
  - Understanding global system behaviour
  - Impact of advances in Data Sciences
- Concluding remarks

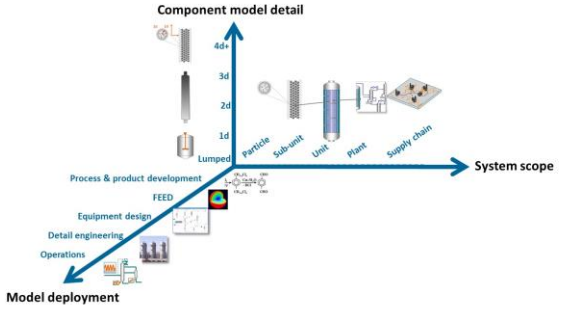
Process Modelling Technology: Where are we now?

Understanding process modelling



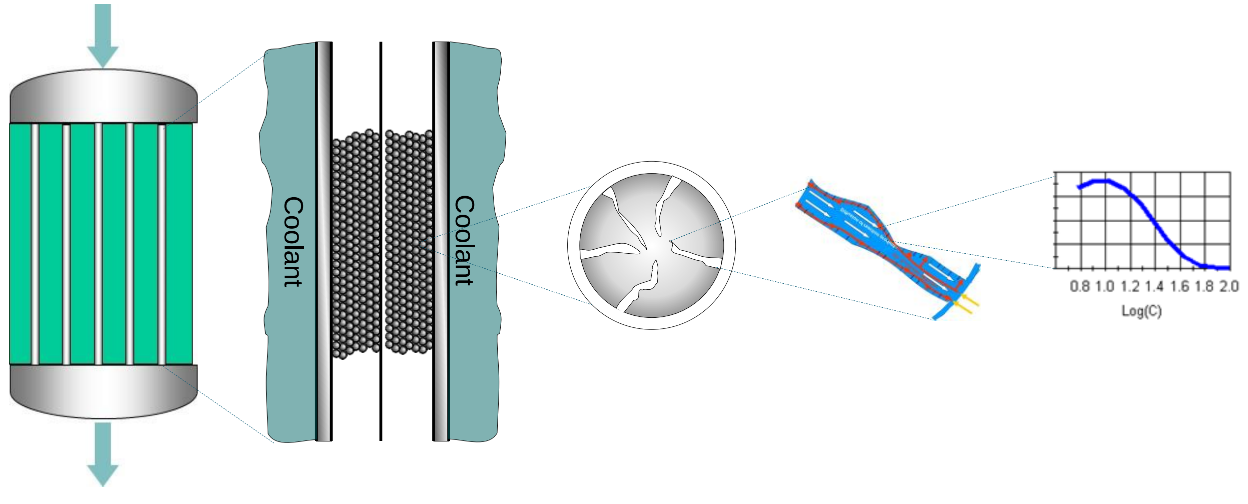
Process Modelling
Key drivers

1. Use *validated* models that are *predictive* over sufficiently wide ranges of design & operating parameters
➔ **increase reliability/reduce risk in model-based decisions**



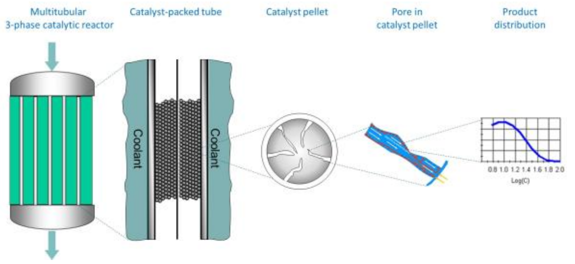
Complexity in component-level modelling
Example: multitubular 3-phase reactors

Multitubular 3-phase catalytic reactor | Catalyst-packed tube | Catalyst pellet | Pore in catalyst pellet | Product distribution



Complexity in component-level modelling

Example: multitubular 3-phase reactors



Shell GTL plant
Ras Lafaan, Qatar

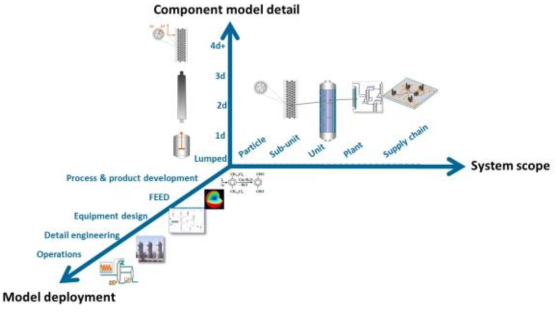
Diameter 8m
Height 22m
Weight 1,200 te

© Man DWE

Process Modelling

Key drivers

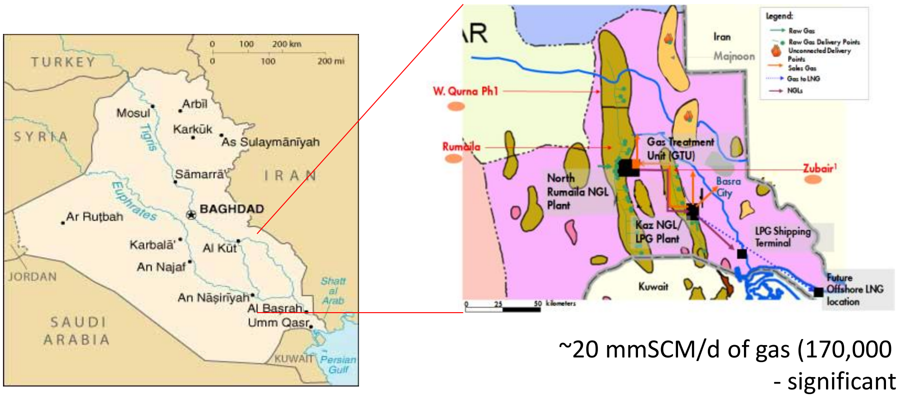
1. Use *validated* models that are *predictive* over sufficiently wide ranges of design & operating parameters
➔ **increase reliability/reduce risk in model-based decisions**



2. Ensure system boundary encompasses *all* important interactions
➔ **formulate meaningful engineering objectives**

Complexity in system-level modelling

Example: integrated gas production & processing networks



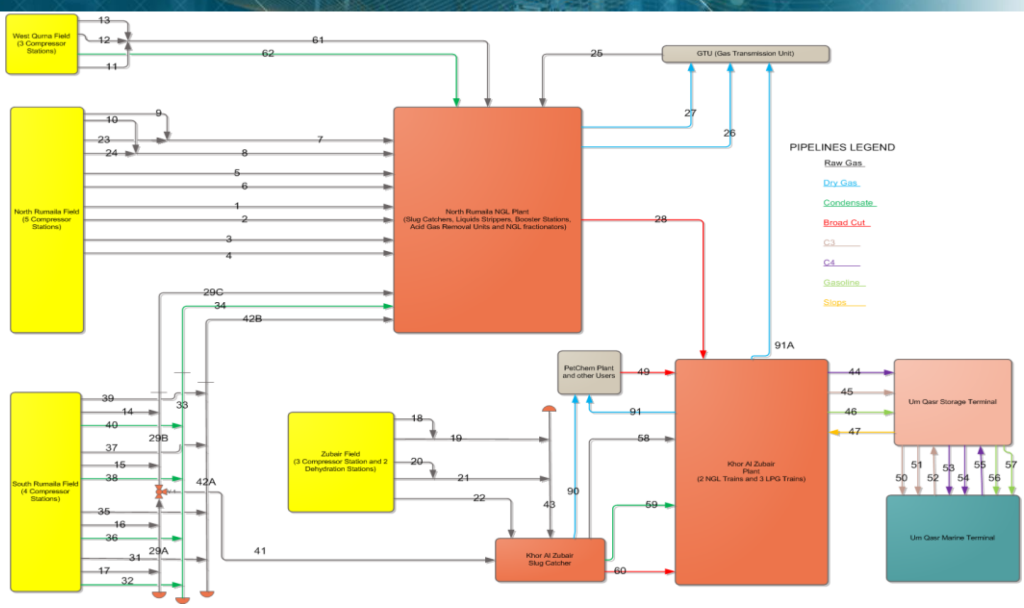
~20 mmSCM/d of gas (170,000 boe/d)
- significant flaring

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.

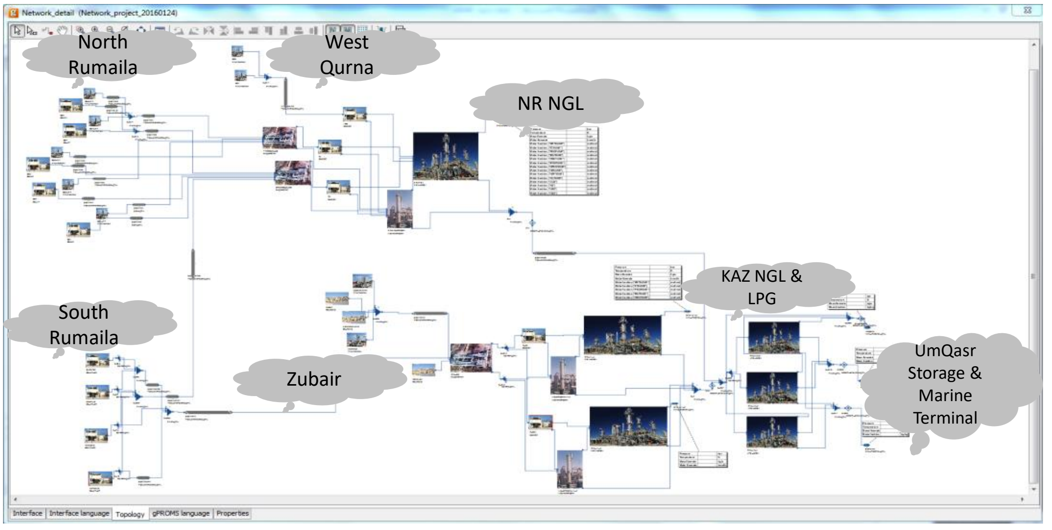
Acknowledgements: Shell, Basrah Gas Company

Integrated gas production & processing network

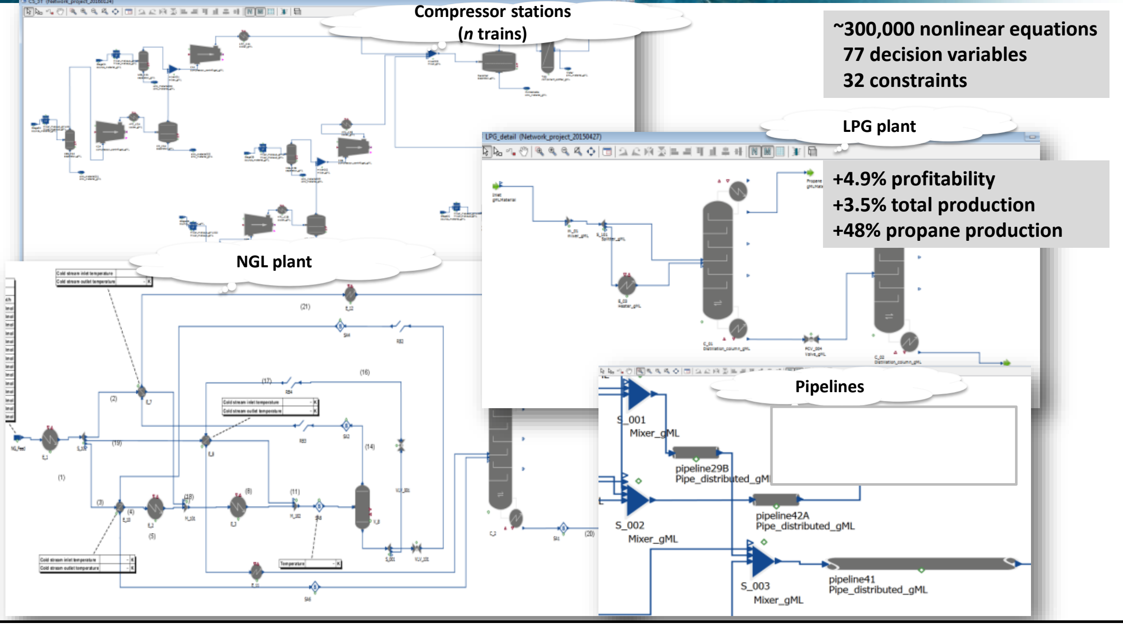
4 fields + 2 processing facilities + connecting pipelines



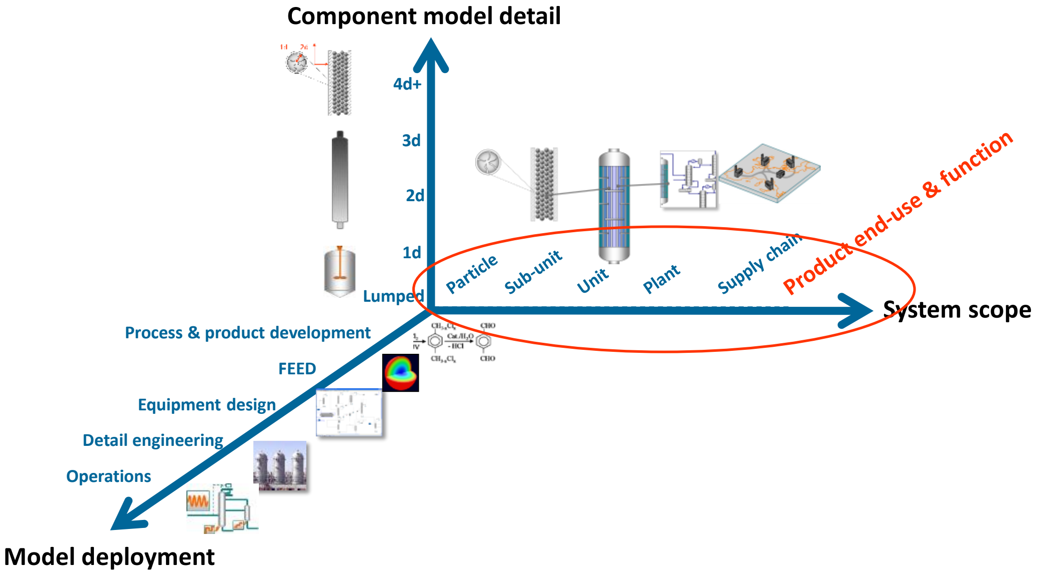
Integrated gas production & processing network
High-level model



Integrated gas production & processing network
Detailed plant models

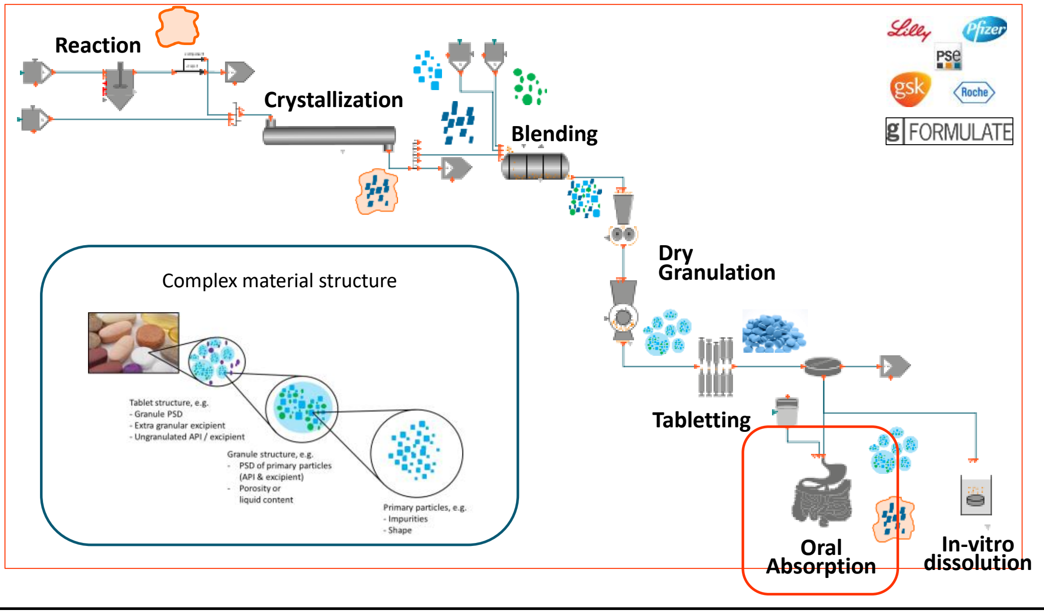


Dimensions of process modelling



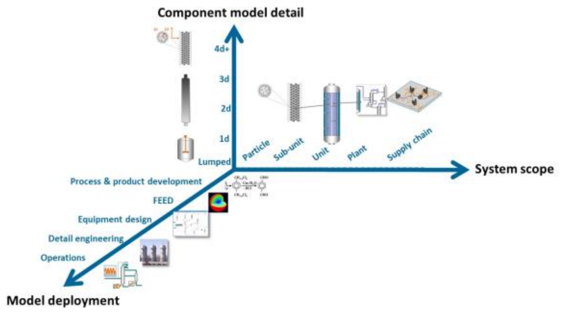
Systems-based Pharmaceutics

Process Systems Engineering tools & workflows



Process Modelling
Key drivers

1. Use *validated* models that are *predictive* over sufficiently wide ranges of design & operating parameters
➔ increase reliability/reduce risk in model-based decisions



2. Ensure system boundary encompasses *all* important interactions
➔ formulate meaningful engineering objectives

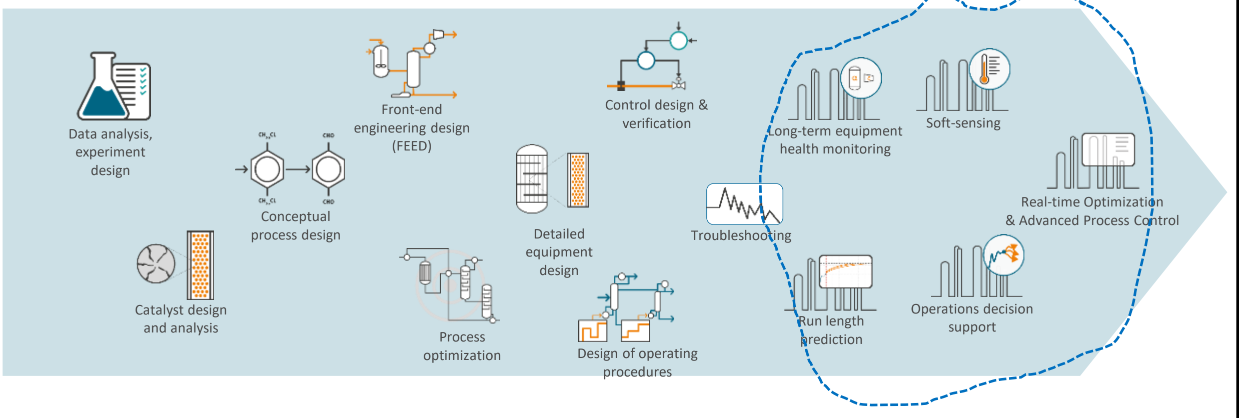
3. *Re-use* models across process lifecycle
➔ ensure consistency, reduce cost of model development & maintenance

Model-based engineering along the process lifecycle

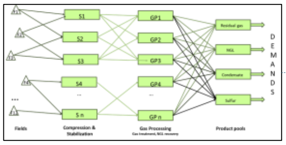
RESEARCH & DEVELOPMENT

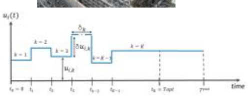
ENGINEERING DESIGN

PROCESS OPERATIONS



Model-based process operations





Opportunity

Exploit

Deep Process Knowledge

🡻

Improved quality of results

Reduced cost of deployment

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*, **51**, 136-148, 2012.

Level 2: Supervisory Control

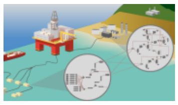
Model-Predictive Control

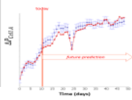
(linear, nonlinear, economic)

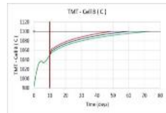
Real-time Soft Sensing

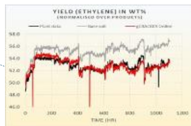
Level 1: Regulatory Control

Distributed Control Systems









Process Modelling Technology: the next decade

Process modelling technology: the next decade

Advances in underpinning IT technologies

Data

- Bigger volume
- Wider range
- Higher quality
- More accessible

Computation

- More power
- Lower cost
- More flexibility

Algorithms

- Data-driven modelling
- Hybrid modelling
- Surrogate modelling
- Data Mining
- . . . .

A set of technologies that have matured over the last couple of decades
…to be usefully applicable to practical problems
…across the process & product lifecycle

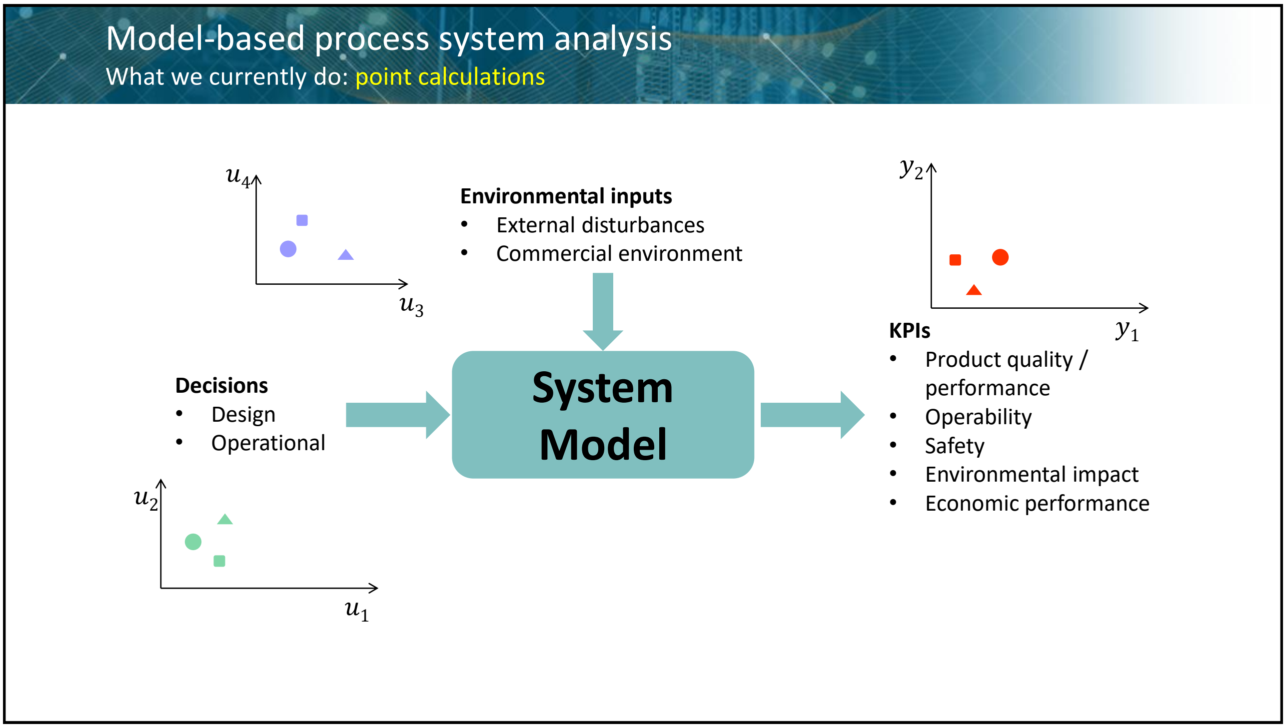

Perspective

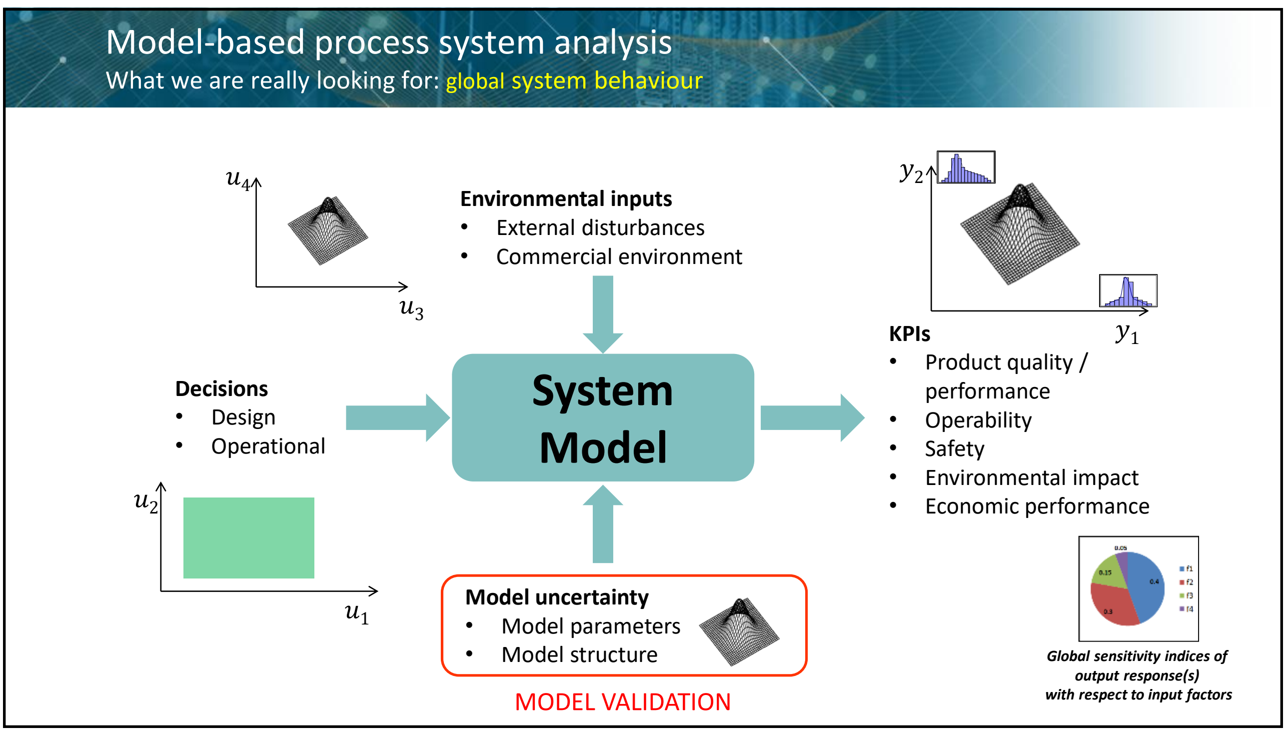
The Promise of Artificial Intelligence in Chemical Engineering: Is It Here, Finally?

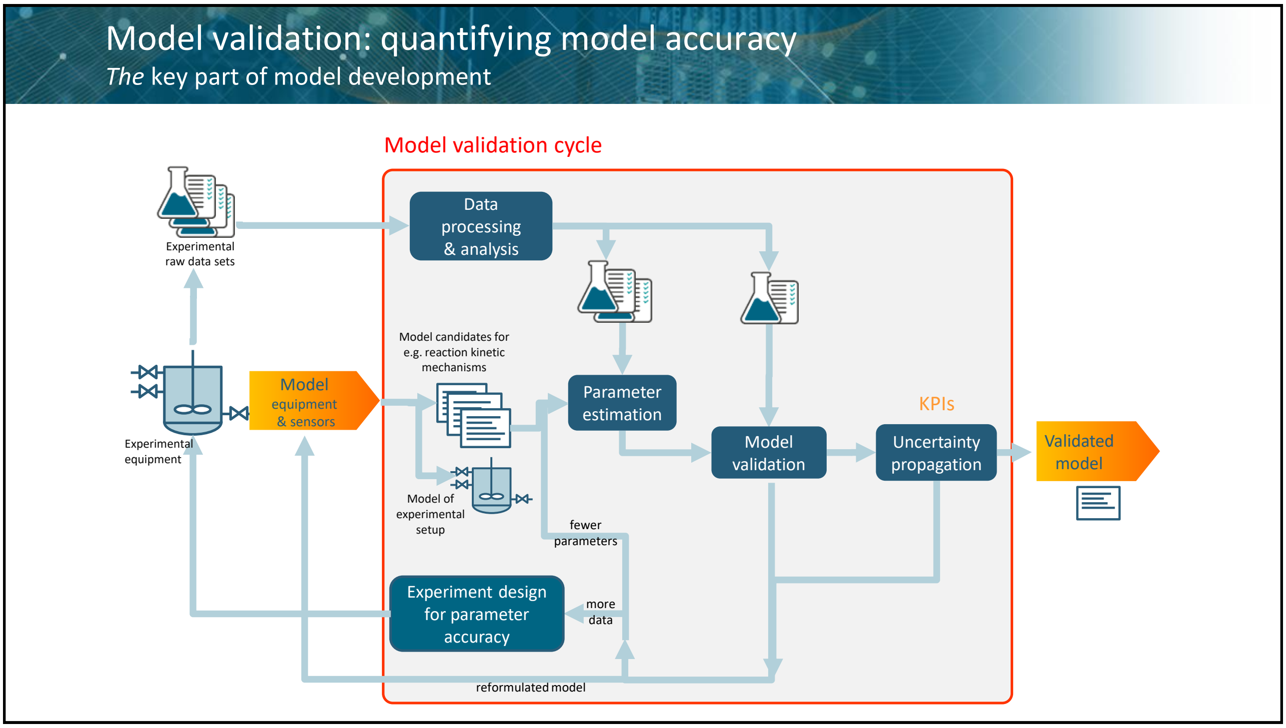
Venkat Venkatasubramanian

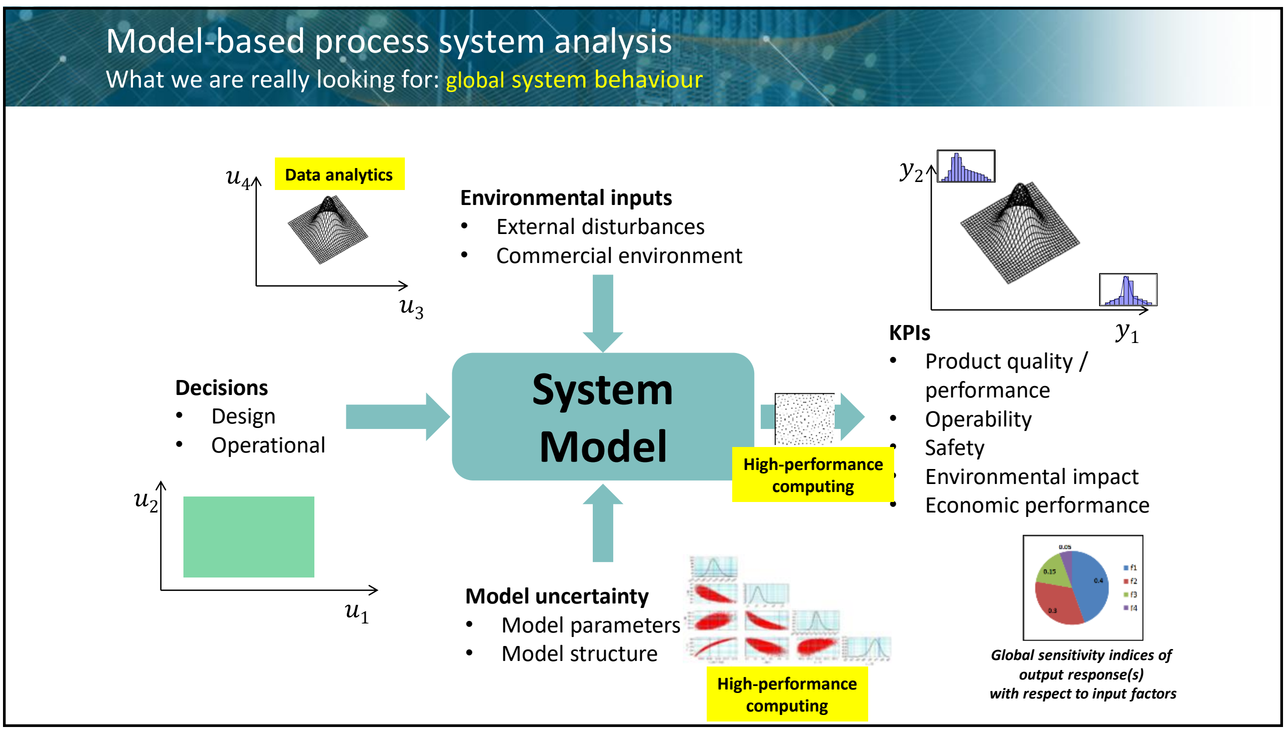
Process modelling technology: the next decade

Understanding global system behaviour

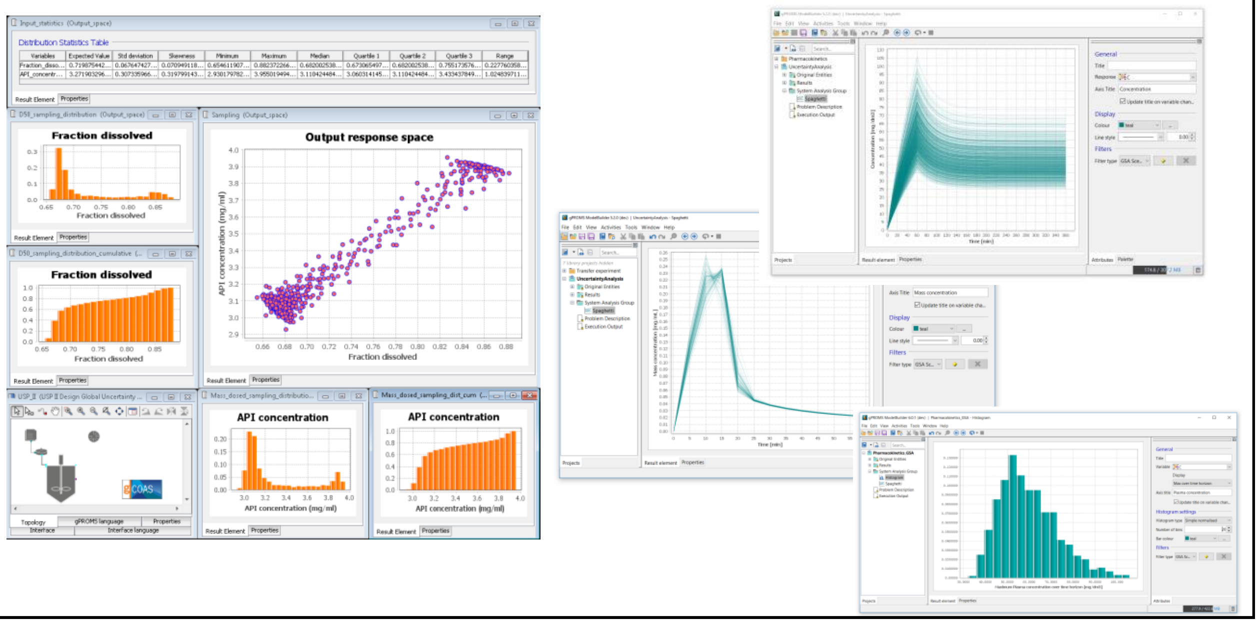

Model-based process system analysis
What we currently do: point calculations
u_4
u_3
Environmental inputs
• External disturbances
• Commercial environment
y_2
y_1
KPIs
• Product quality / performance
• Operability
• Safety
• Environmental impact
• Economic performance
Decisions
• Design
• Operational
System Model
u_2
u_1


Model-based process system analysis
What we are really looking for: global system behaviour
u_4
u_3
Environmental inputs
• External disturbances
• Commercial environment
y_2
y_1
KPIs
• Product quality / performance
• Operability
• Safety
• Environmental impact
• Economic performance
Decisions
• Design
• Operational
System Model
u_2
u_1
Model uncertainty
• Model parameters
• Model structure
MODEL VALIDATION
Global sensitivity indices of output response(s) with respect to input factors


Model validation: quantifying model accuracy
The key part of model development
Model validation cycle
Experimental raw data sets
Data processing & analysis
Experimental equipment
Model equipment & sensors
Model candidates for e.g. reaction kinetic mechanisms
Parameter estimation
Model of experimental setup
Model validation
KPIs
Uncertainty propagation
Validated model
fewer parameters
Experiment design for parameter accuracy
more data
reformulated model

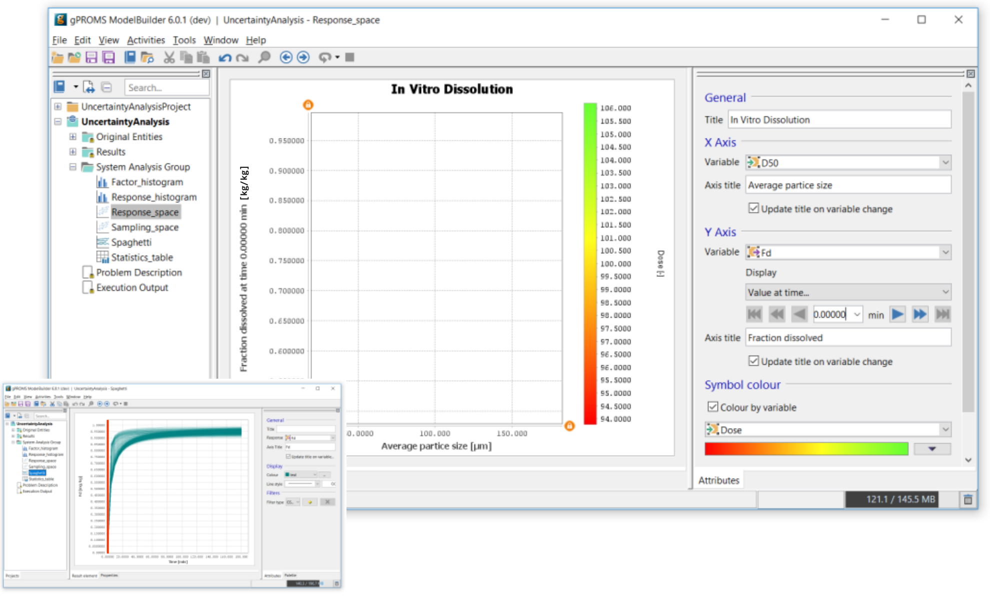

Model-based process system analysis
What we are really looking for: global system behaviour
Data analytics
u_4
u_3
Environmental inputs
• External disturbances
• Commercial environment
y_2
y_1
KPIs
• Product quality / performance
• Operability
• Safety
• Environmental impact
• Economic performance
Decisions
• Design
• Operational
System Model
High-performance computing
u_2
u_1
Model uncertainty
• Model parameters
• Model structure
High-performance computing
Global sensitivity indices of output response(s) with respect to input factors

Global System Analysis in practice



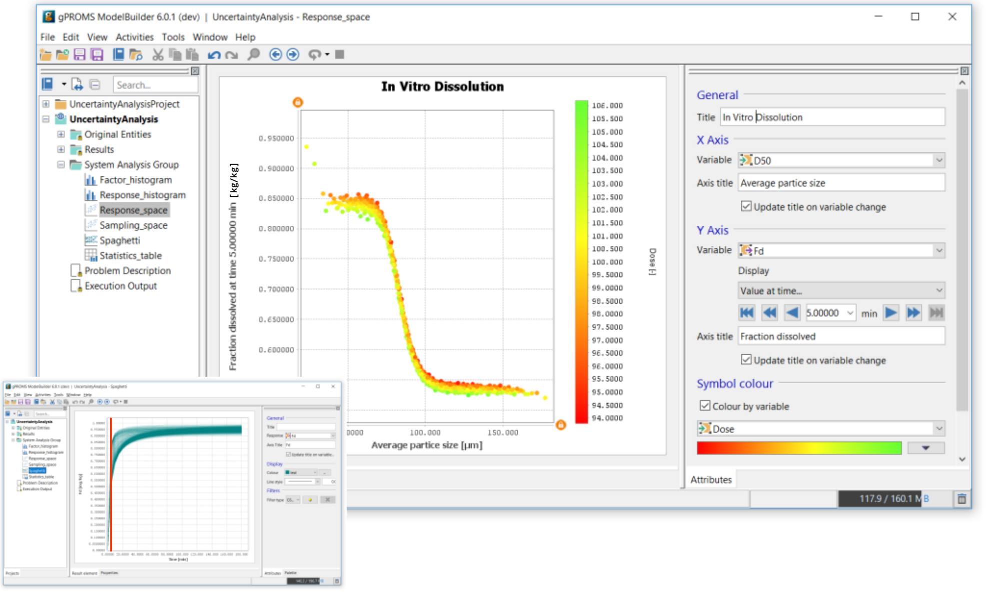
Global System Analysis of dynamic systems

KPI at start of process



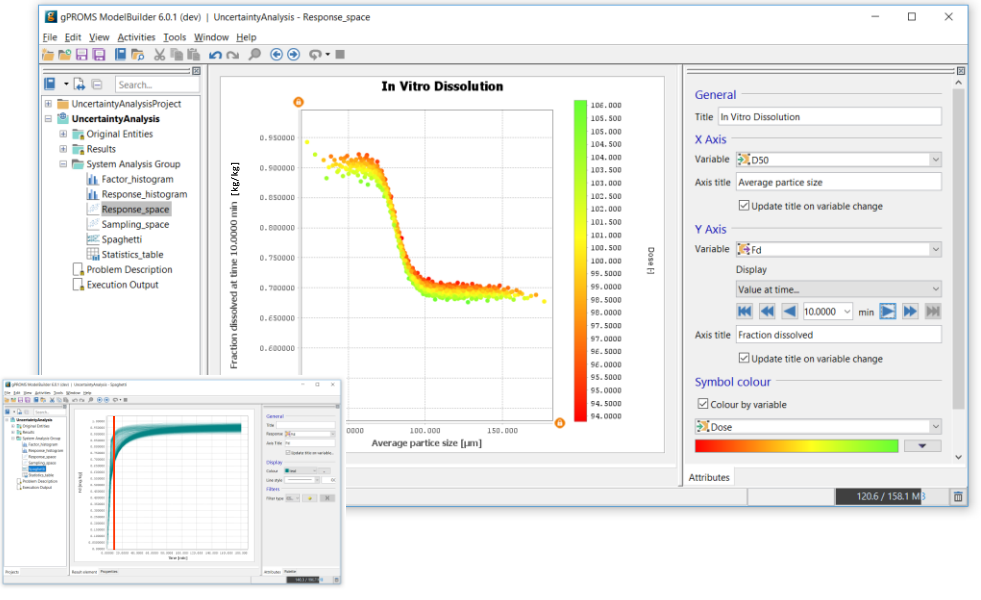
Global System Analysis of dynamic systems

KPI at 5 minutes



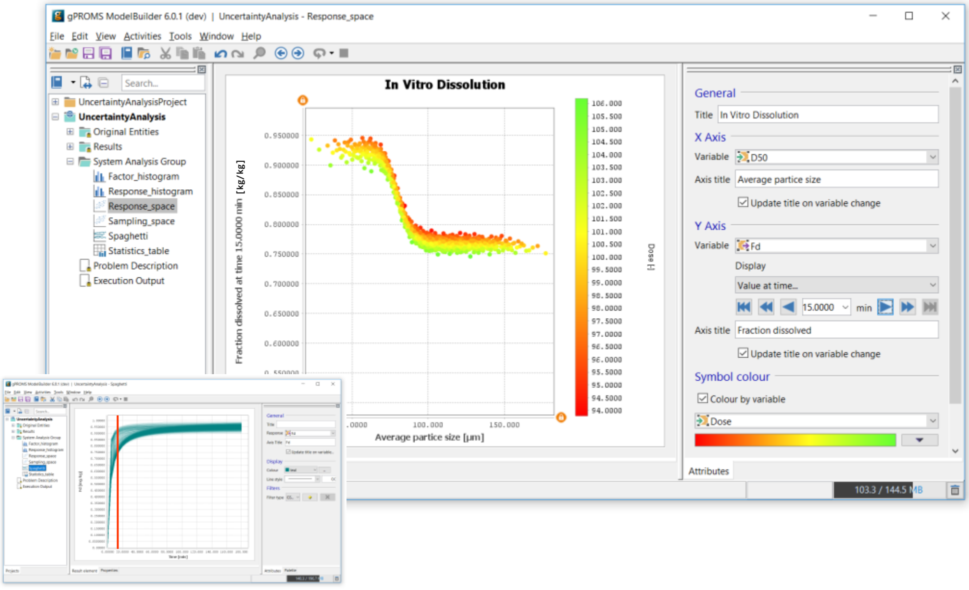
Global System Analysis of dynamic systems

KPI at 10 minutes



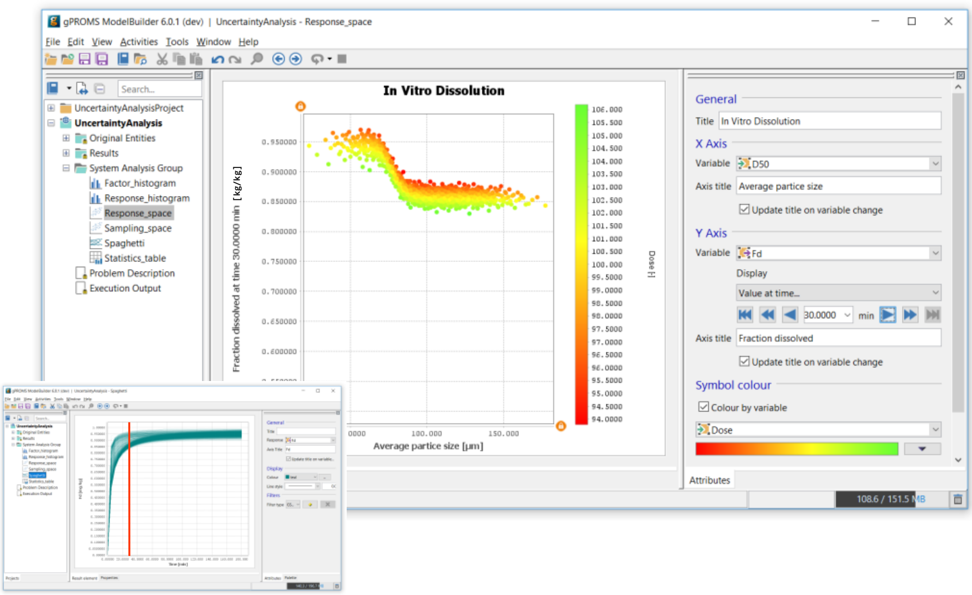
Global System Analysis of dynamic systems

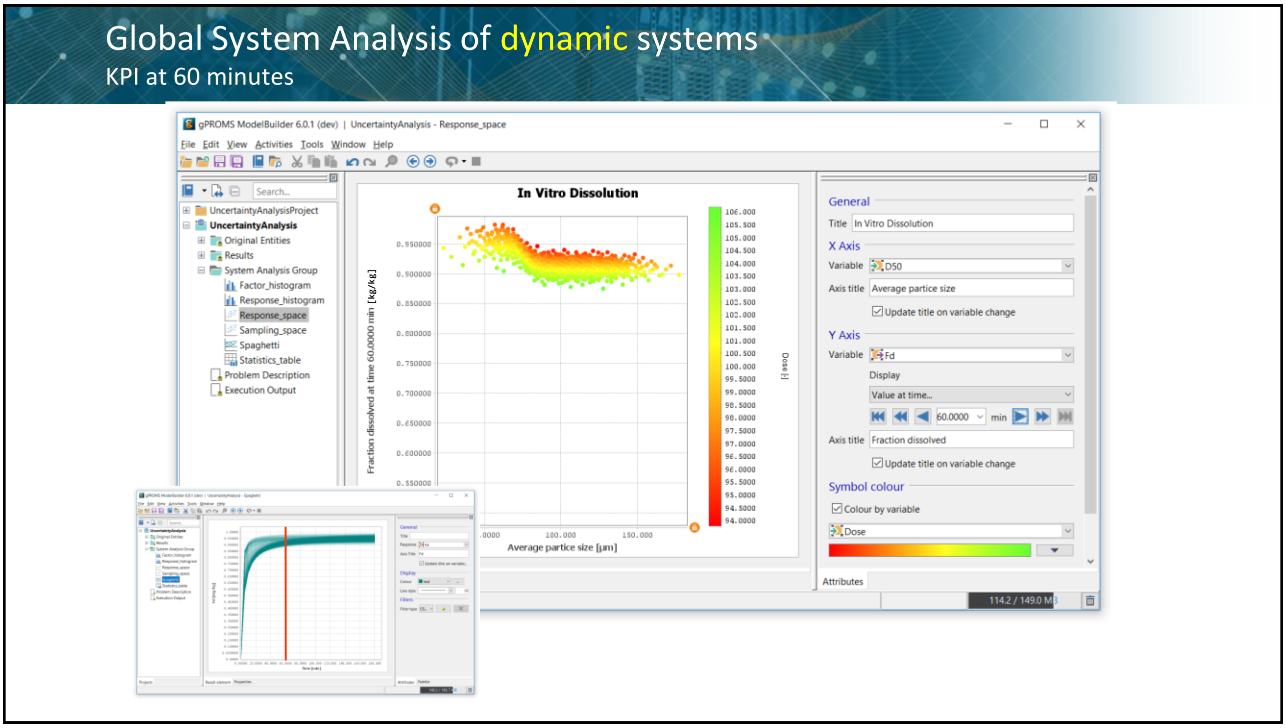
KPI at 15 minutes

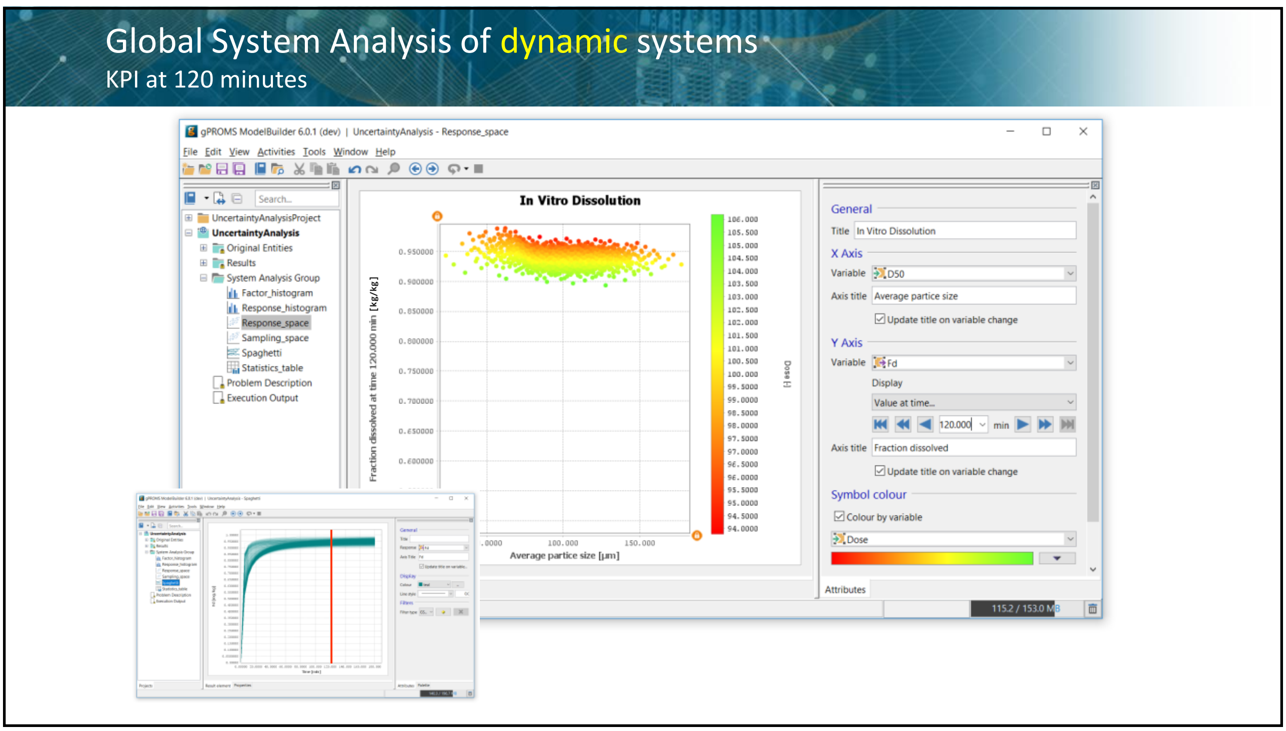


Global System Analysis of dynamic systems

KPI at 30 minutes




Global System Analysis of dynamic systems
KPI at 60 minutes
gPROMS ModelBuilder 6.0.1 (dev) | UncertaintyAnalysis - Response_space
File Edit View Activities Tools Window Help
UncertaintyAnalysisProject
UncertaintyAnalysis
Original Entities
Results
System Analysis Group
Factor_histogram
Response_histogram
Response_space
Sampling_space
Spaghetti
Statistics_table
Problem Description
Execution Output
In Vitro Dissolution
Fraction dissolved at time 60.0000 min [kg/kg]
Average partice size [µm]
Dose [-]
General
Title In Vitro Dissolution
X Axis
Variable D50
Axis title Average partice size
Update title on variable change
Y Axis
Variable Fd
Display
Value at time...
60.0000 min
Axis title Fraction dissolved
Update title on variable change
Symbol colour
Colour by variable
Dose
Attributes
114.2 / 149.0 MB


Global System Analysis of dynamic systems
KPI at 120 minutes
gPROMS ModelBuilder 6.0.1 (dev) | UncertaintyAnalysis - Response_space
File Edit View Activities Tools Window Help
UncertaintyAnalysisProject
UncertaintyAnalysis
Original Entities
Results
System Analysis Group
Factor_histogram
Response_histogram
Response_space
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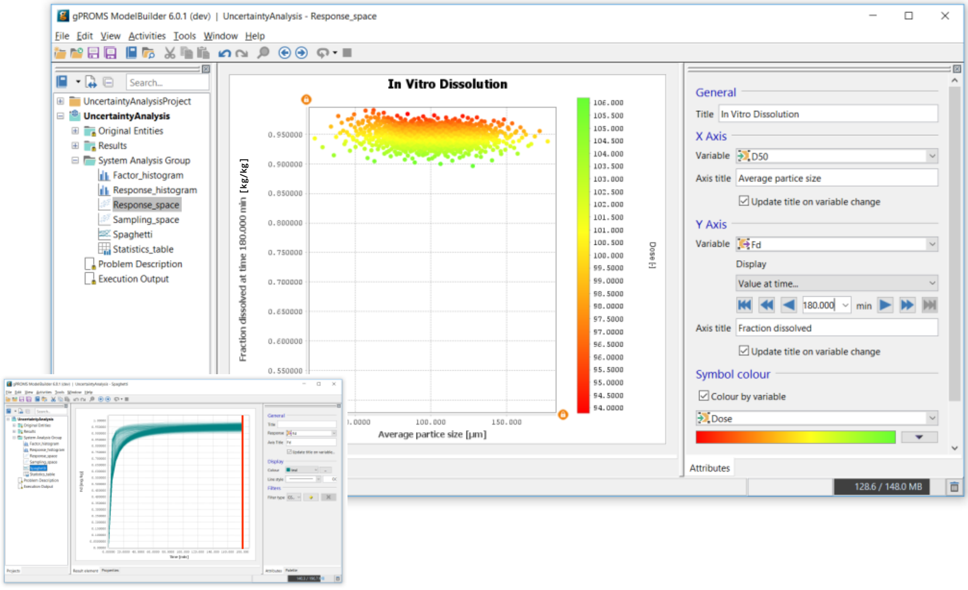
In Vitro Dissolution
Fraction dissolved at time 120.000 min [kg/kg]
Average partice size [µm]
Dose [-]
General
Title In Vitro Dissolution
X Axis
Variable D50
Axis title Average partice size
Update title on variable change
Y Axis
Variable Fd
Display
Value at time...
120.000 min
Axis title Fraction dissolved
Update title on variable change
Symbol colour
Colour by variable
Dose
Attributes
115.2 / 153.0 MB

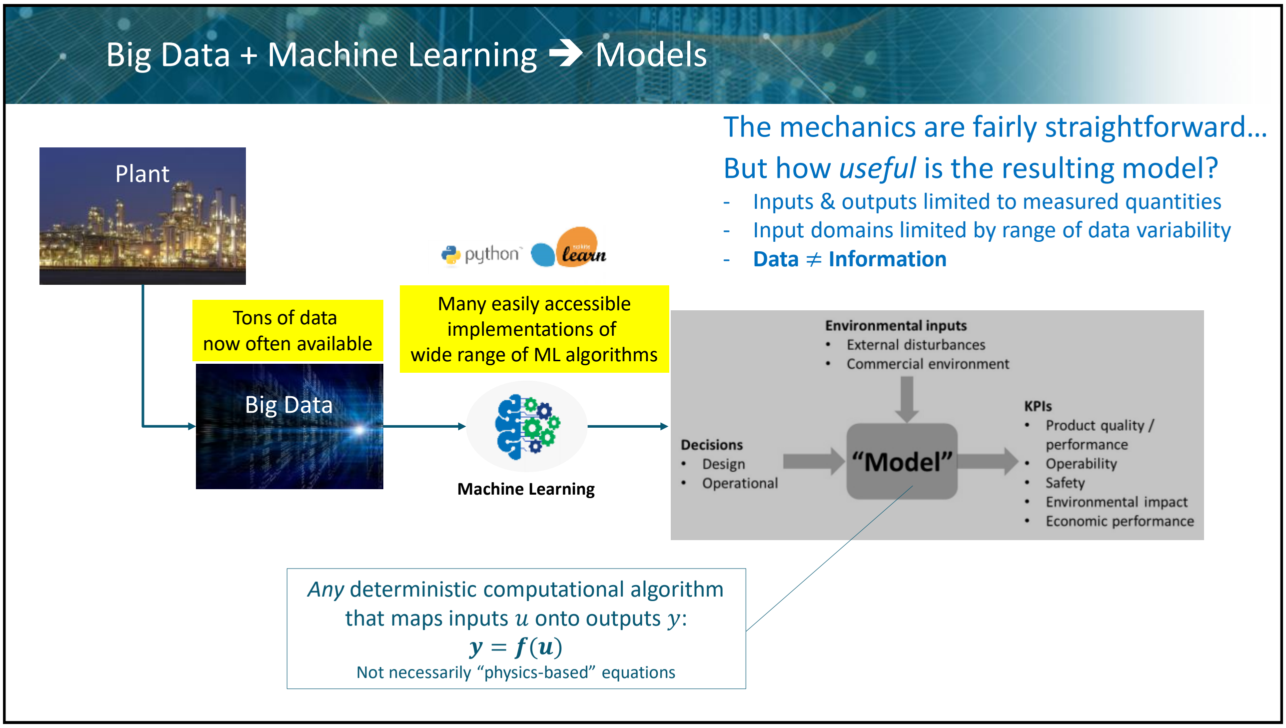
Global System Analysis of dynamic systems

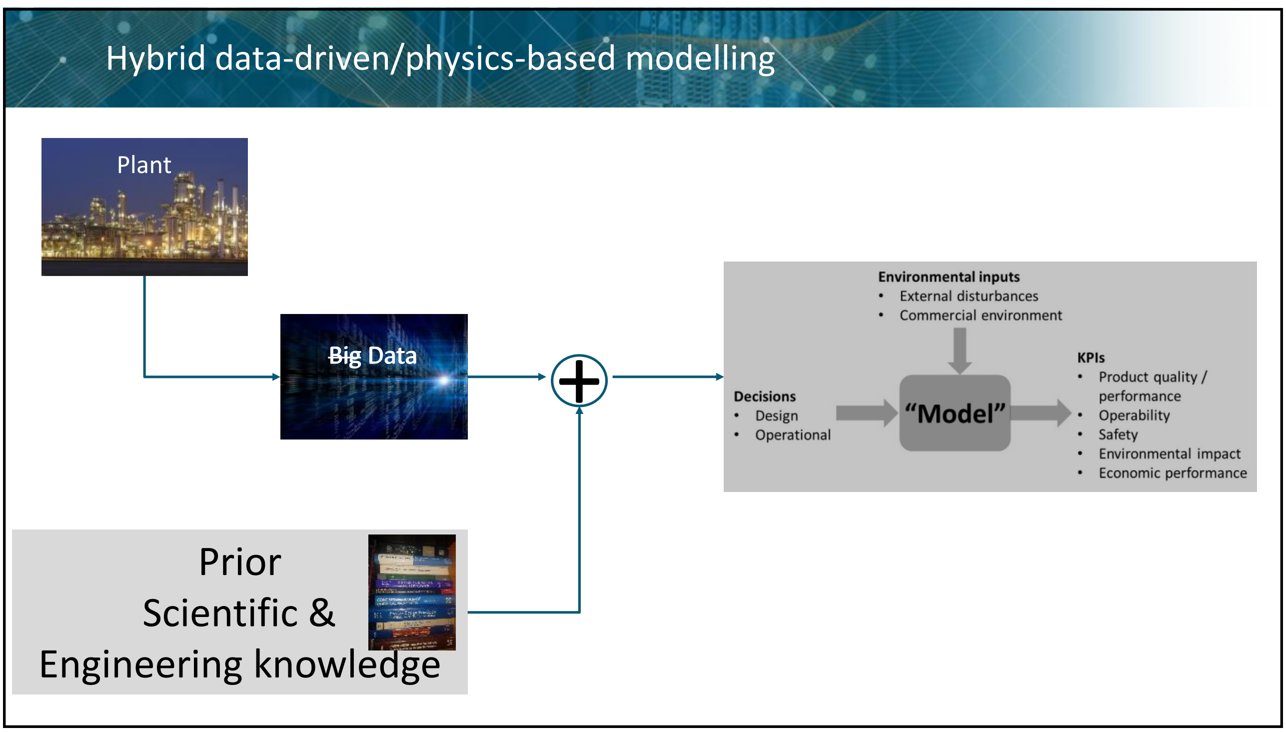
KPI at 180 minutes



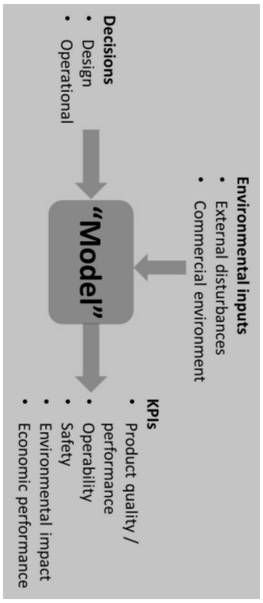
Process modelling technology: the next decade

The impact of advances in Data Science

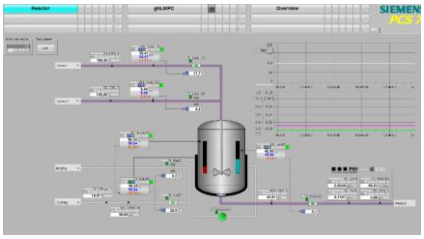

Big Data + Machine Learning ➔ Models
The mechanics are fairly straightforward…
But how *useful* is the resulting model?
- Inputs & outputs limited to measured quantities
- Input domains limited by range of data variability
- **Data ≠ Information**
Plant
Tons of data now often available
Big Data
python
learn
Many easily accessible implementations of wide range of ML algorithms
Machine Learning
Environmental inputs
• External disturbances
• Commercial environment
Decisions
• Design
• Operational
"Model"
KPIs
• Product quality / performance
• Operability
• Safety
• Environmental impact
• Economic performance
Any deterministic computational algorithm that maps inputs u onto outputs y:
$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{u})$
Not necessarily "physics-based" equations

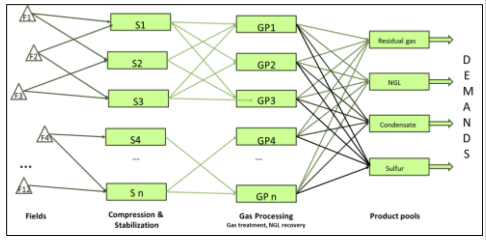

Hybrid data-driven/physics-based modelling
Plant
Big Data
Environmental inputs
• External disturbances
• Commercial environment
Decisions
• Design
• Operational
"Model"
KPIs
• Product quality / performance
• Operability
• Safety
• Environmental impact
• Economic performance
Prior Scientific & Engineering knowledge

Some models are just *too* computationally complex for *some* applications…



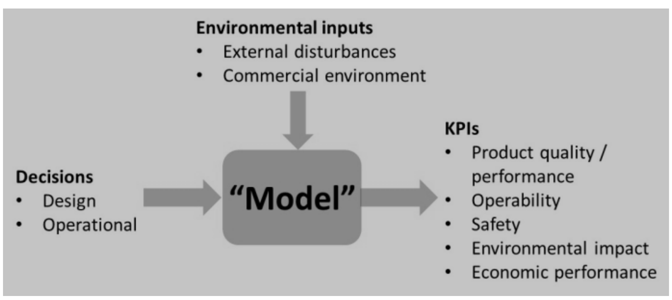
- Model may exhibit satisfactory predictive accuracy…
- …but is unsuitable for intended application
  - too large ➔ computationally intractable
  - not robust enough ➔ unreliable performance





➔ generate & use **surrogate** model

A surrogate model is…



- an *explicit* relation between inputs and outputs: $y = f(u)$
- …derived from the results of a (much) more *detailed* model
- …guaranteed to match the predictions of the detailed model
  - within a specified accuracy
  - for *all* input combinations within a given domain

NOT plant data ("big" or otherwise)

Usually a *restricted* input domain

Surrogate modelling example: Gas-Oil Separator (GOSP) plant

Model structure

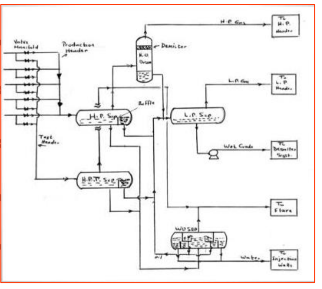
Water pumps in parallel u_1

HP Comp recycle rate u_2

LP Comp recycle rate u_3

Water pump recycle rate u_4

Inlet flowrate u_5



y_1 Power consumption

$y_2 \dots y_4$ HPPT compressor capacity & head margins

$y_5 \dots y_7$ LPPT compressor capacity & head margins

$y_8 \dots y_{10}$ Water pump capacity & pressure margins

$y_{11} \dots y_{13}$ GOSP oil and water capacity margins

y_{14} Oil production

Model Inputs
- 1 integer, u_1
- 4 continuous, $u_2 - u_5$

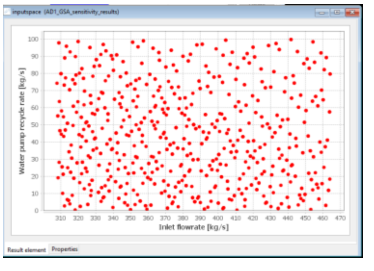
→

Model Outputs
- 14 continuous, $y_1 - y_{14}$

Surrogate modelling example: Gas-Oil Separator (GOSP) plant

Exploration of input space of interest via Global System Analysis

- 7,200 points
  - Sampled over input space using low-discrepancy sequences
  - Integer input handled automatically
- Generated in ~27.5’
  - 4-core desktop machine



WP_pressure_DST (AD1_GSA_sensitivity_results)

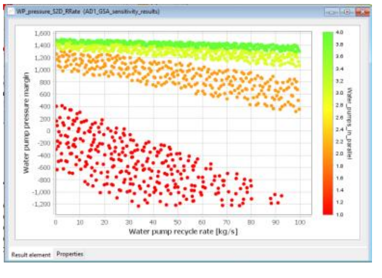
Distribution Statistics Table

Variable	Units	Expected Value	Std deviation	Minimum	Maximum
Water_pump_pressure_margin		765.9	810.3	-1230	1498

WP_pressure_FST (AD1_GSA_sensitivity_results)

Factor Sensitivity Table

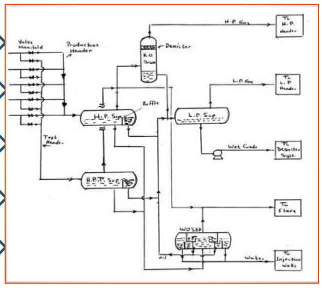
Factor	Water_pump_pressure_margin Total effect
HP_Compressor_recycle_rate	1.144E-12
Inlet_flowrate	0.5098
LP_Compressor_recycle_rate	1.658E-17
Pump_recycle_rate	0.6441



Surrogate modelling example: Gas-Oil Separator (GOSP) plant

Automatically generated surrogate model

Inputs:
- Water pumps in parallel (u_1)
- HP Comp recycle rate (u_2)
- LP Comp recycle rate (u_3)
- Water pump recycle rate (u_4)
- Inlet flowrate (u_5)



Outputs:
- y_1: Power consumption
- $y_2 \dots y_4$: HPPT compressor capacity & head margins
- $y_5 \dots y_7$: LPPT compressor capacity & head margins
- $y_8 \dots y_{10}$: Water pump capacity & pressure margins
- $y_{11} \dots y_{13}$: GOSP oil and water capacity margins
- y_{14}: Oil production

Algorithm automatically determines form of nonlinear functions

- Explicit nonlinear model for water pump pressure margin

$$y_{10} = 1014.12 - 14.5807 \times u_4 - 5.324 \times u_5 - 0.0128 \times u_4^2 - 0.00753 \times u_5^2 - 0.004918 \times u_4 \times u_5 - 0.000000334076 \times u_4^2 \times u_5^2 \quad \text{for } u_1 = 1$$

$$y_{10} = 1342.54 - 1.477 \times u_4 - 1.477 \times u_5 - 0.614122 \times u_4^2 - 0.00099132 \times u_5^2 - 0.00384918 \times u_4 \times u_5 - 0.00000099076 \times u_4^2 \times u_5^2 \quad \text{for } u_1 = 2$$

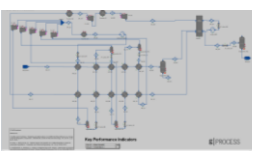
$$y_{10} = 1265.76 - 0.625 \times u_4 - 4.922 \times u_5 - 0.57122 \times u_4^2 - 0.00099132 \times u_5^2 - 0.00384918 \times u_4 \times u_5 - 0.00000099076 \times u_4^3 \times u_5^3 \quad \text{for } u_1 = 3$$

$$y_{10} = 2343.67 - 2.5107 \times u_4 - 2.922 \times u_5 - 0.6722 \times u_4^2 - 0.023289 \times u_5^2 - 0.012364 \times u_4 \times u_5 \quad \text{for } u_1 = 4$$

A. Cozad, N.V. Sahinidis, D.C. Miller, *AIChE J.*, **60**, 2211-2227 (2014); Z.T. Wilson, N.V. Sahinidis, *Comput. chem. Engng.*, **106**, 785-795 (2017)

Surrogate modelling: key enabling technology for Process Modelling in the next decade

Model detail/ predictive accuracy



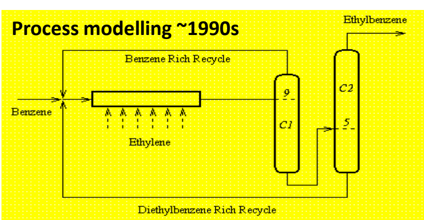
Computational complexity

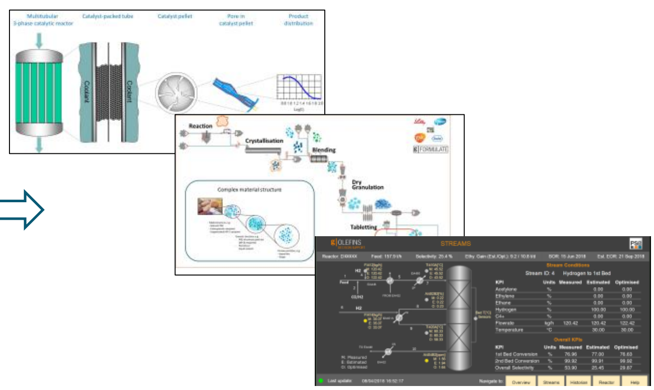
Process modelling: current perspectives, future visions

In conclusion…

Process modeling technology: current perspectives

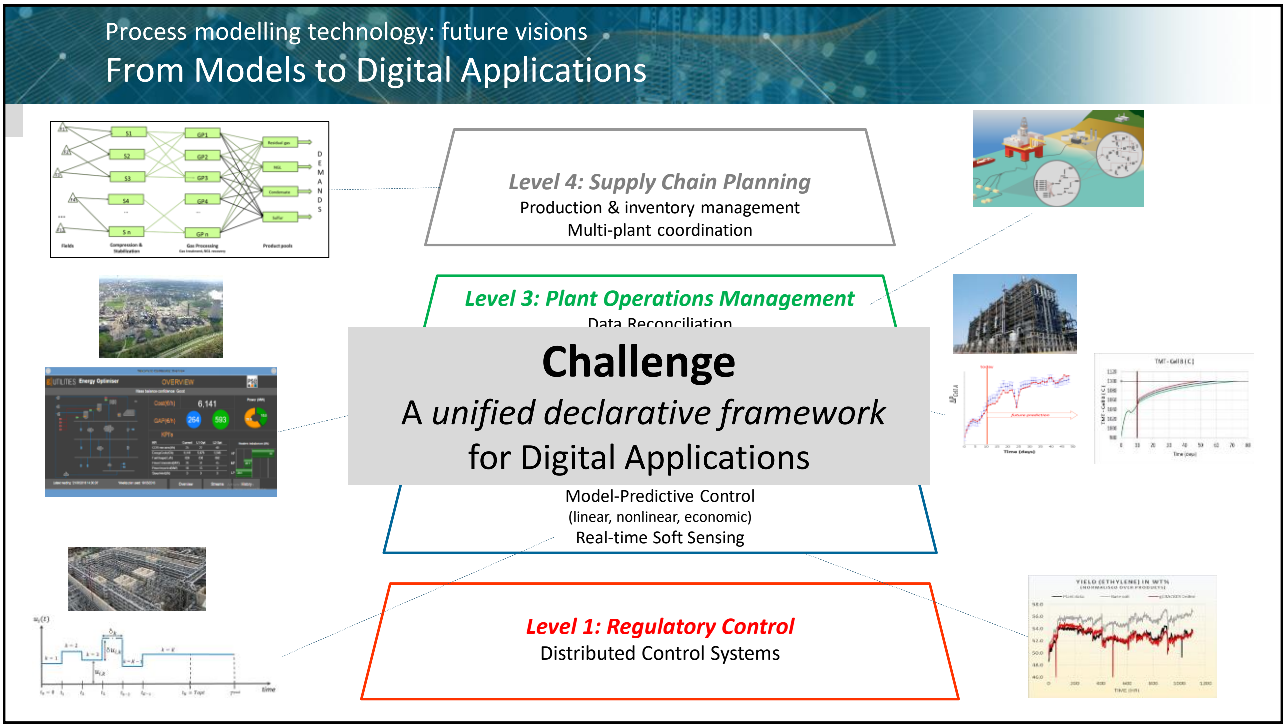
We've come a *long* way!





Key contributing factors

- Declarative modelling languages
- Multipurpose modelling environments – not just "simulators"
- Advances in computation
  - Algorithms
  - Hardware


Process modelling technology: future visions
From Models to Digital Applications
Level 4: Supply Chain Planning
Production & inventory management
Multi-plant coordination
Level 3: Plant Operations Management
Data Reconciliation
Challenge
A unified declarative framework
for Digital Applications
Model-Predictive Control
(linear, nonlinear, economic)
Real-time Soft Sensing
Level 1: Regulatory Control
Distributed Control Systems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Thank you for your attention!
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