Digitalisation in Chemical Engineering
Frankfurt, 1st March 2019

Deep knowledge in Process Industry digitalization

Costas Pantelides FIChemE FREng

gPROMS

Outline

- Digitalization – what is it ?
- Intelligent Digital Operations
- Online model-based Decision Support Systems
  - example: catalytic reactor monitoring, forecasting, optimization
- Conclusions

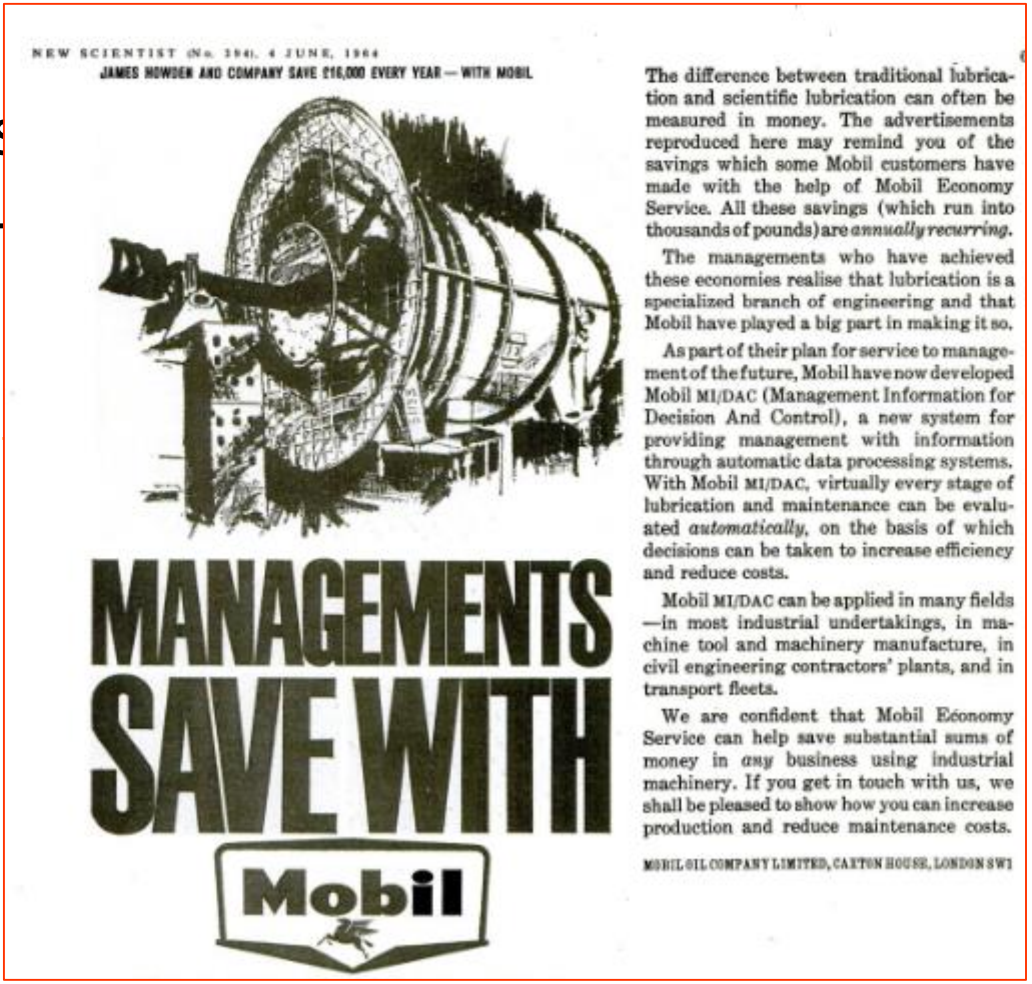
© 2019 Process Systems Enterprise Limited

Digitalization – what is it?

© 2019 Process Systems Enterprise Limited

Digitalization

is the use of digital te
to change a busines
and provide new revenue and value-
it is the process of moving to



© 2019 Process Systems Enterprise Limited

The use of computers & IT

The use of computers & IT

~~Digital~~ will have a significant impact on many areas of the chemical industry, with the potential to change value chains, lead to higher productivity and more innovation, and create new channels to market.

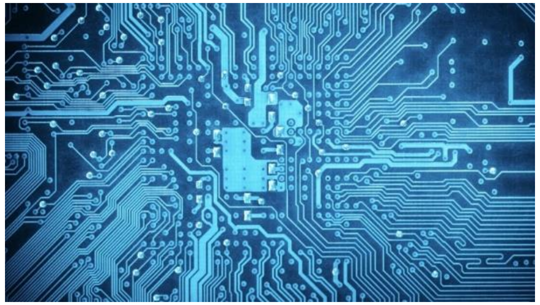
Given all the excitement about ~~digital~~, it is essential to **separate the substance from the hype and carefully evaluate what this will mean for the industry**.

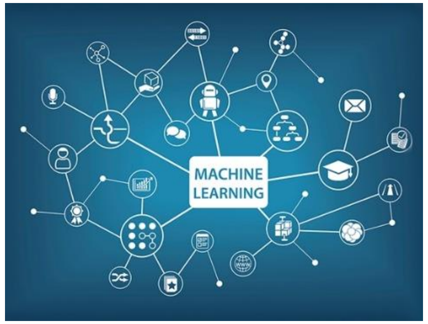
the use of computers & IT

The use of computers & IT in Chemicals: From Technology to Impact
A. Klei, M. Moder, O. Stockdale, U. Weihe, and G. Winkler
https://www.mckinsey.com/industries/chemicals/our-insights/digital-in-chemicals-from-technology-to-impact

© 2019 Process Systems Enterprise Limited

Exploitation of a set of IT technologies





Data

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

Computation

- More power
- Lower cost
- More flexibility

Algorithms

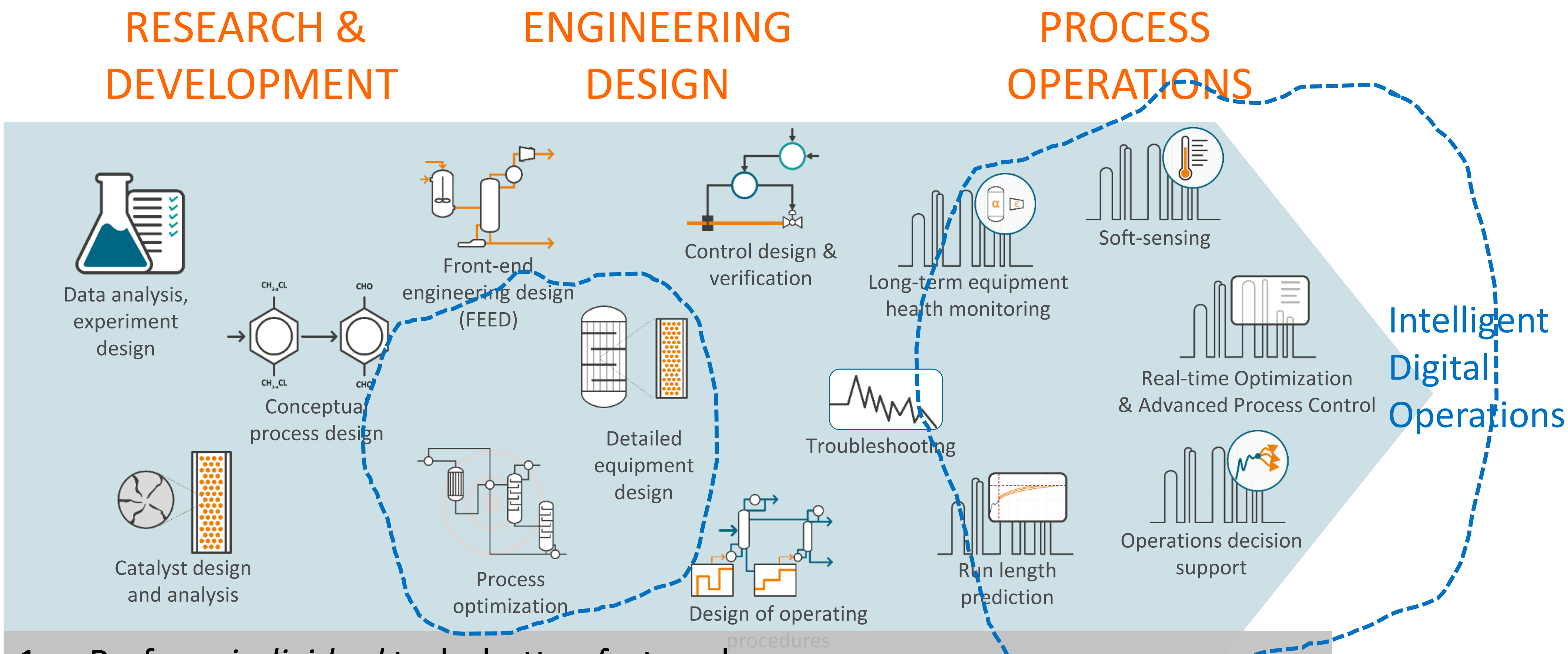
- Machine Learning
- Artificial Intelligence
- Meta-modelling
- Data Mining
- . . . .

…that have matured over the last couple of decades
…to the point where they can now usefully be applied to practical problems
…across the process lifecycle

© 2019 Process Systems Enterprise Limited

Model-based engineering along the process lifecycle

Impact of digitalization



1. Perform *individual* tasks better, faster, cheaper
2. Perform tasks that are not directly amenable to first-principles modelling
3. *Combine* tasks ➔ better solutions, fewer iterations
4. Integrate workflows, automate data transfer
5. Perform tasks that were previously computationally infeasible

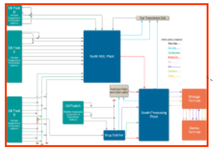
© 2019 Process Systems Enterprise Limited

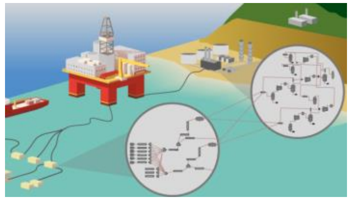
Towards intelligent Digital Operations

© 2019 Process Systems Enterprise Limited

Intelligent Digital Operations

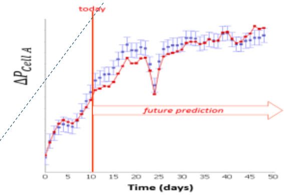
Model-Based Decision Support & Control Systems



Level 4: Supply Chain Planning

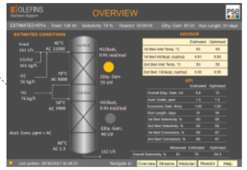
Production & inventory management
Multi-plant coordination

Level 3: Plant Operations Management

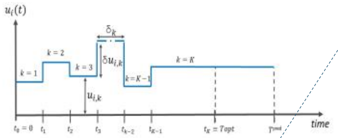
Data Reconciliation
Real-time Optimization
What-if analysis

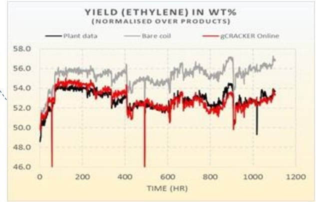
Opportunity: exploit
Deep Process Knowledge
↓
Improved quality of results
Reduced cost of deployment

Level 2: Supervisory Control

(linear, nonlinear, economic)
Real-time Soft Sensing



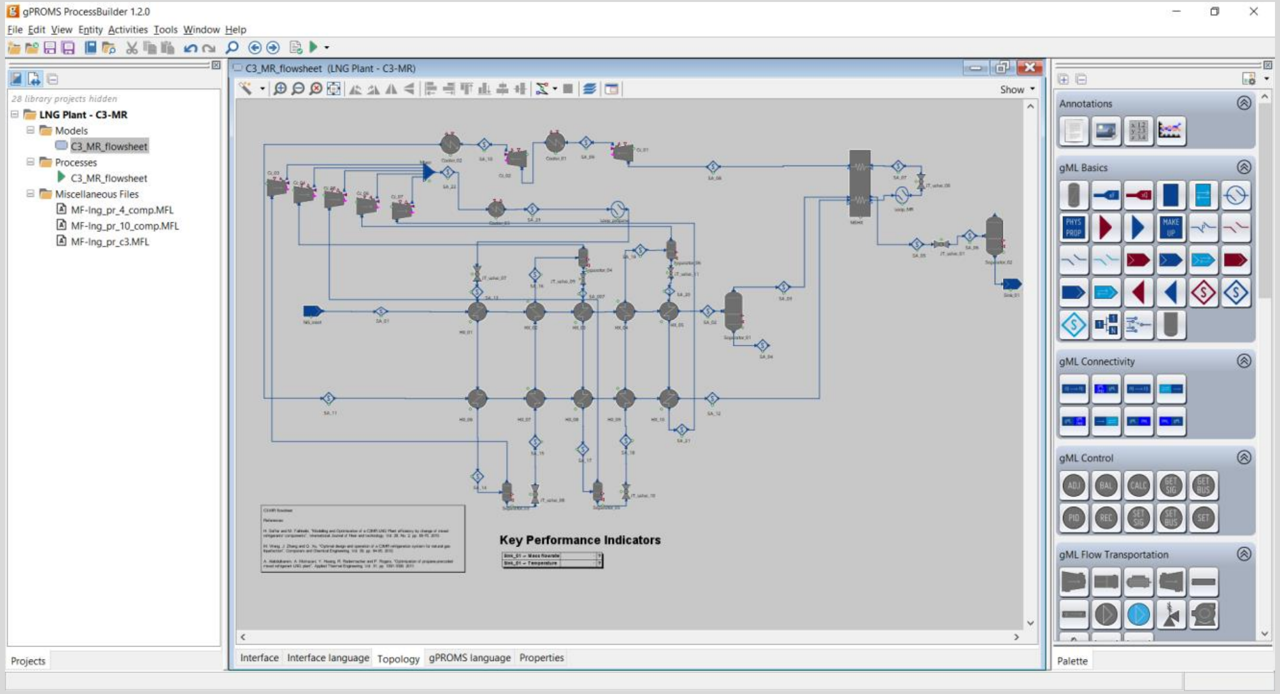
Level 1: Regulatory Control

Distributed Control Systems

© 2019 Process Systems Enterprise Limited

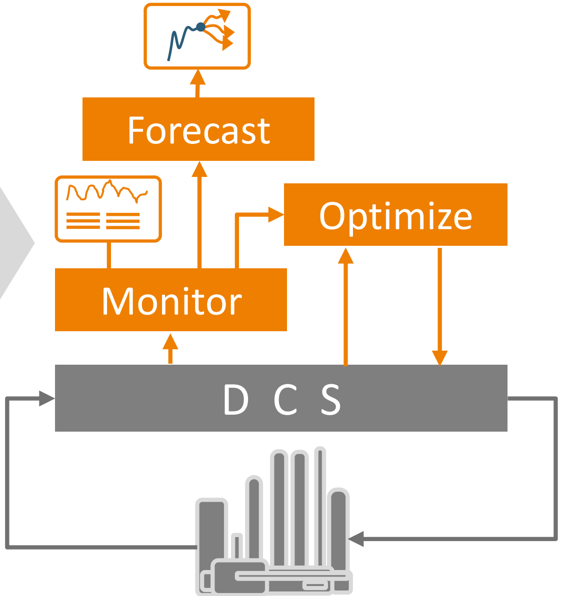
Deep process knowledge in online model-based applications

Leveraging the offline modelling investment



DESKTOP
EMBEDDED

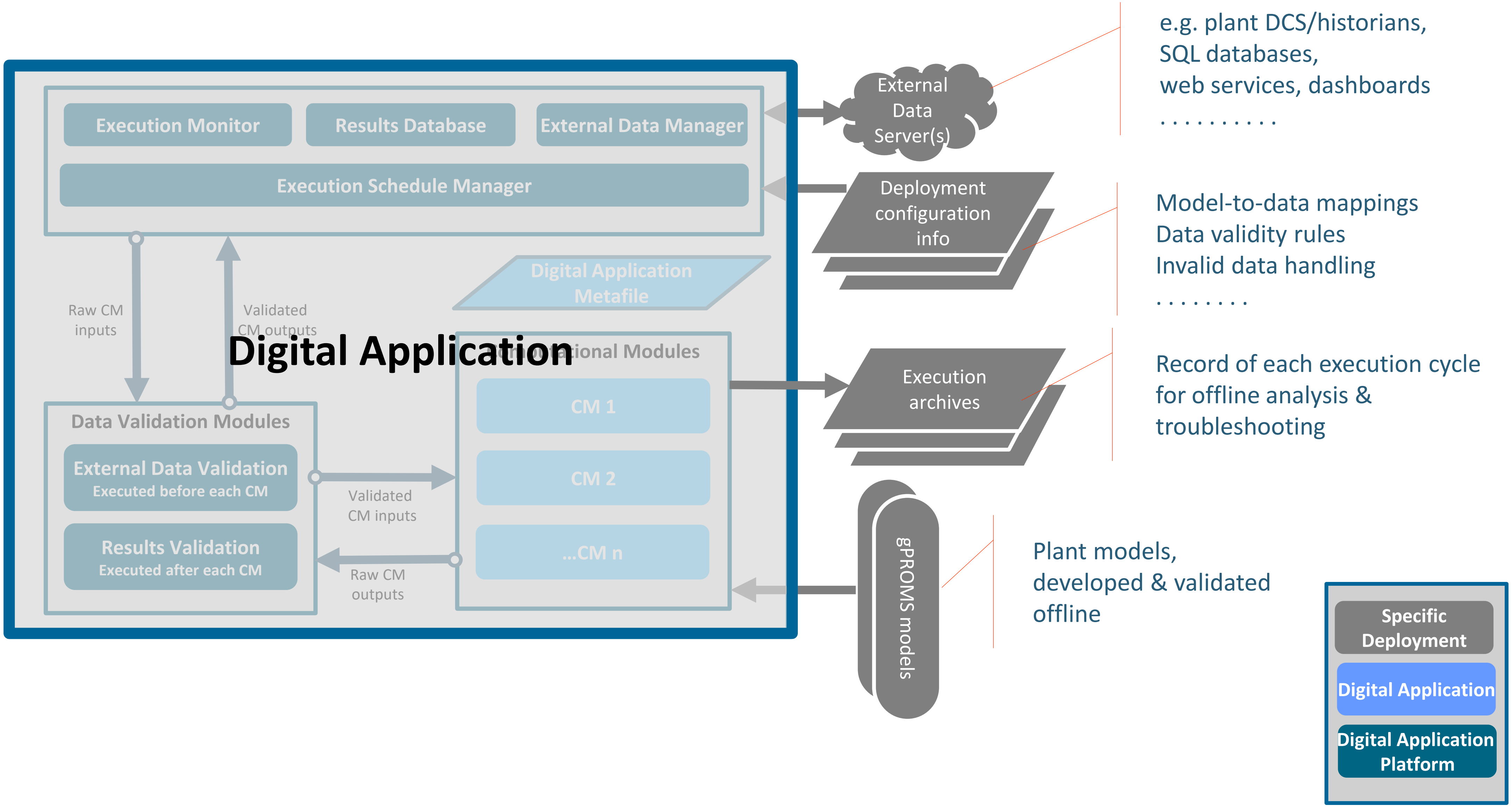
Digital Applications
for
Process Operations



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.**

© 2019 Process Systems Enterprise Limited

A general software platform for model-based Digital Applications

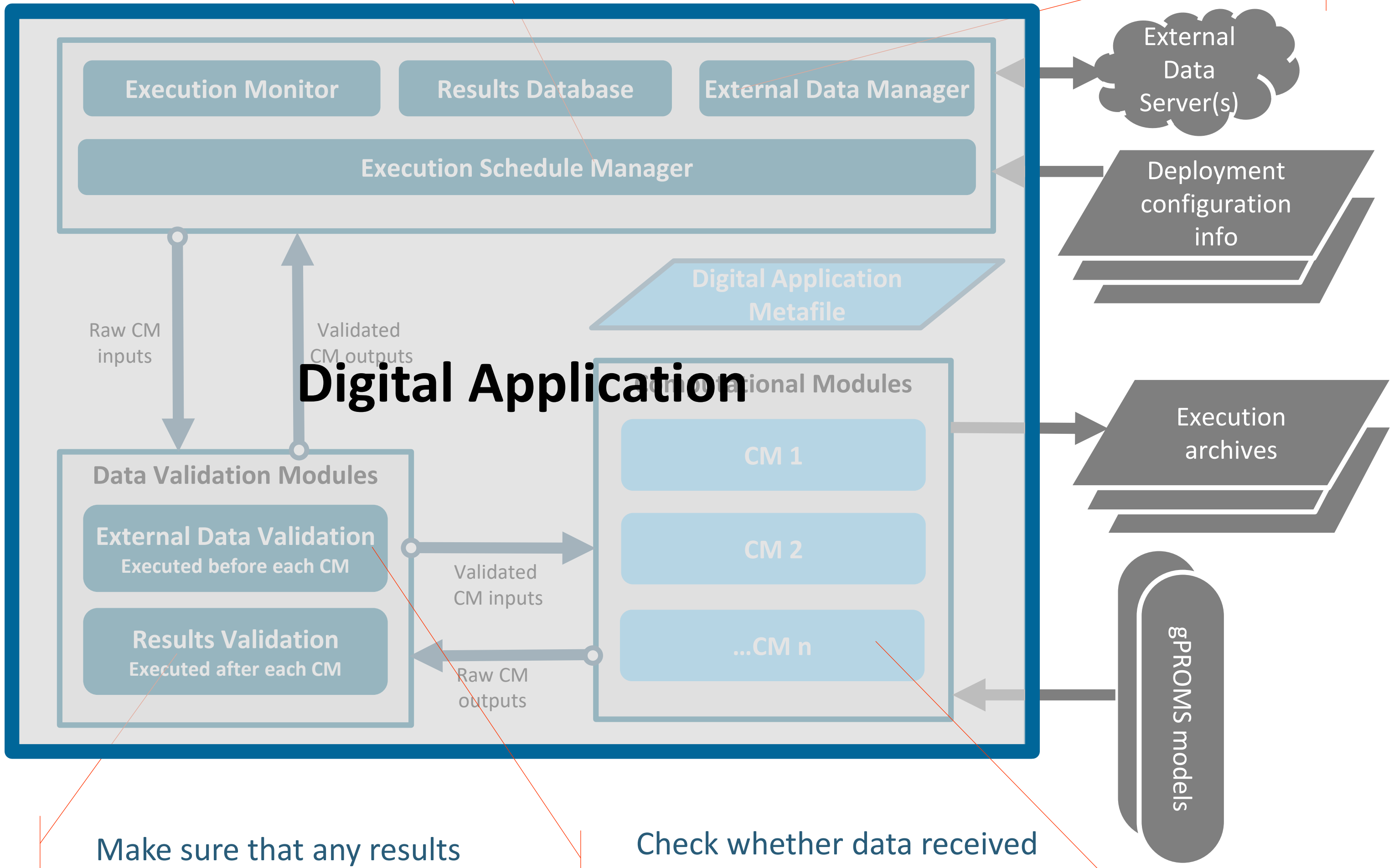


© 2019 Process Systems Enterprise Limited

A general software platform for model-based Digital Applications

Schedule & manage the execution of the various computations

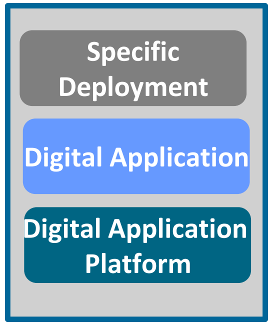
Manage communication with External Data Servers



Make sure that any results being sent to the outside world are valid

Check whether data received from outside world are valid – and take appropriate action if they aren't

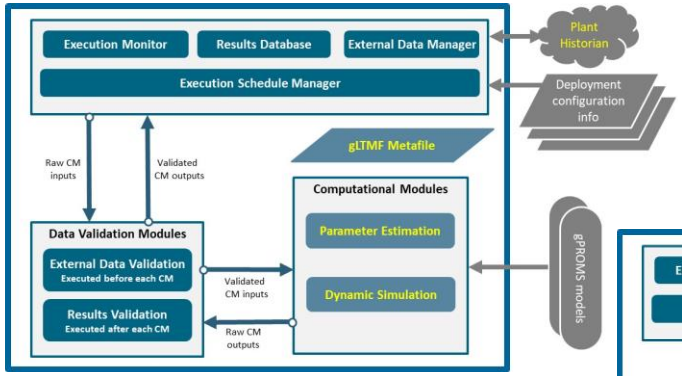
Perform model-based computations



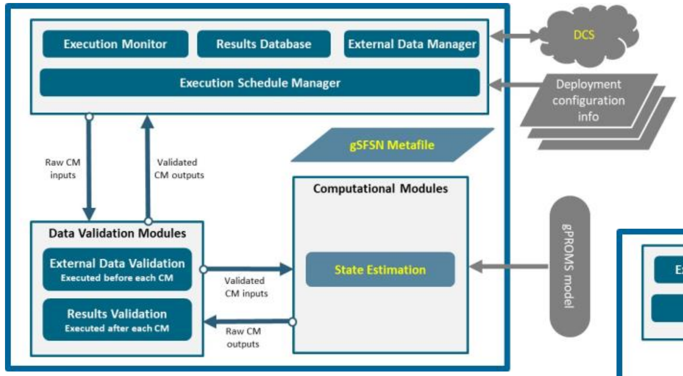
© 2019 Process Systems Enterprise Limited

Model-based Digital Applications

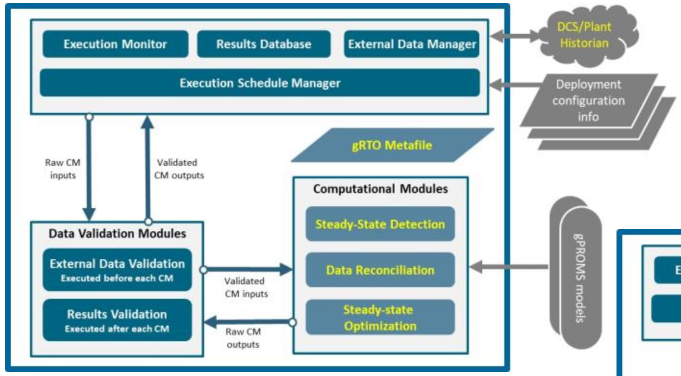
based on the gPROMS Digital Applications Platform



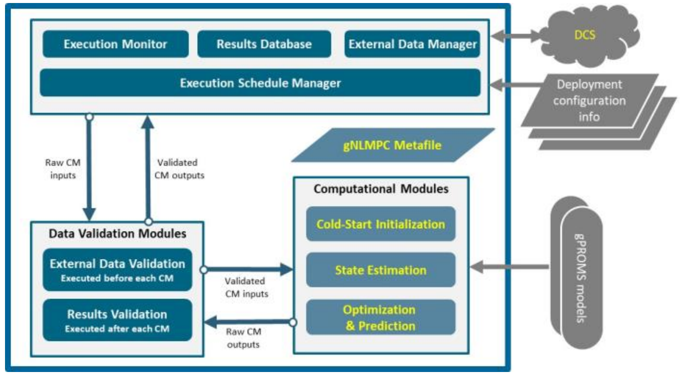
Long-Term
Equipment Monitoring
& Forecasting



Soft Sensing



Real-Time Optimization



Nonlinear
Model-Predictive Control

© 2019 Process Systems Enterprise Limited

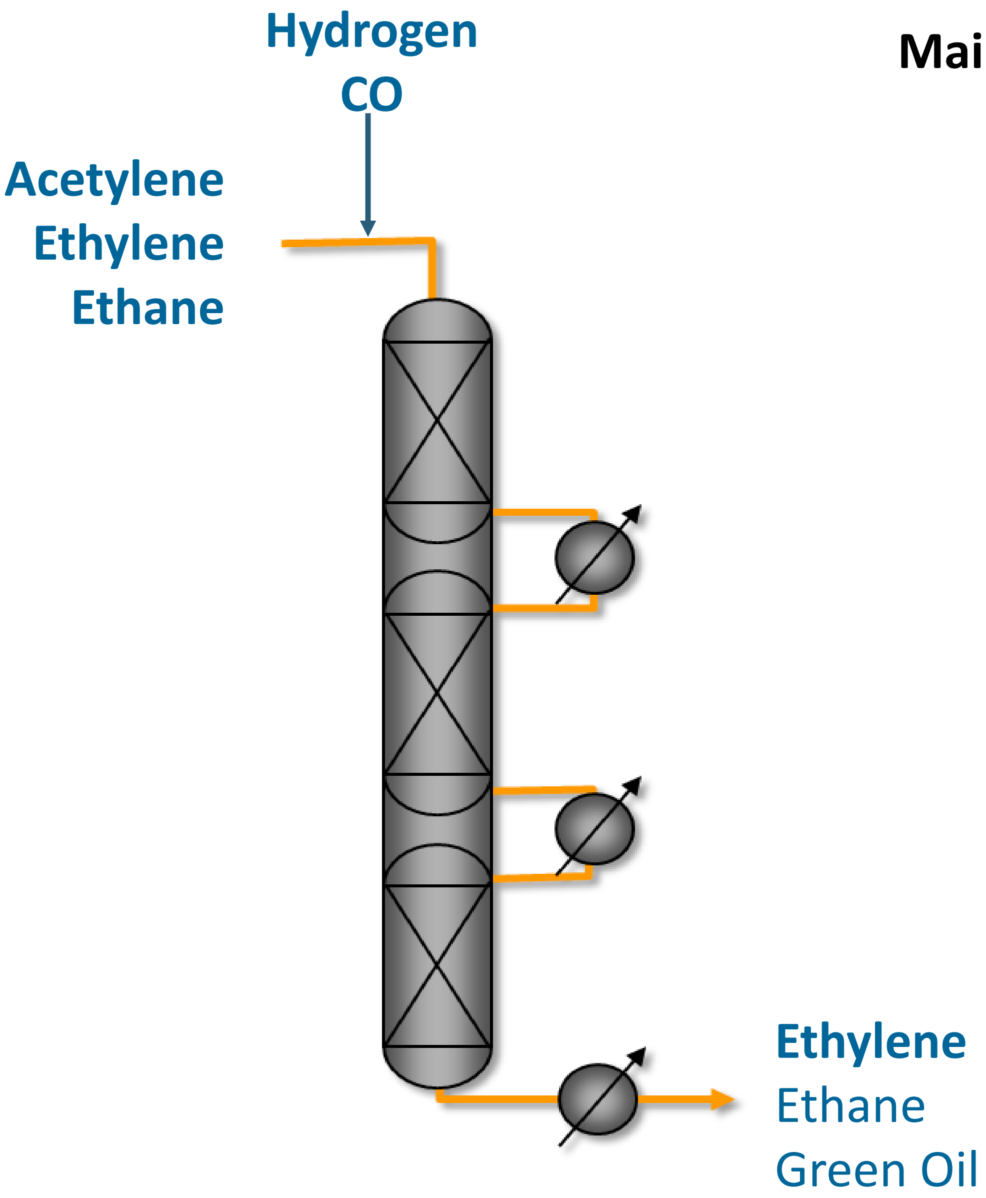
Online model-based Decision Support Systems

Example: catalytic reactor monitoring, forecasting, optimization

© 2019 Process Systems Enterprise Limited

Example

Acetylene converters in olefin plants



Main Reaction:

Desired reaction

- $C_2H_2 + H_2 \rightarrow C_2H_4$ Acetylene hydrogenation

Undesired reactions

- $C_2H_4 + H_2 \rightarrow C_2H_6$ Ethylene hydrogenation
- $2C_2H_2 + xH_2 \rightarrow C_4H_{4+2x}$ Green Oil formation (➔ catalyst deactivation)

Key business objectives

- maximize *net* ethylene gain
- increase run-length

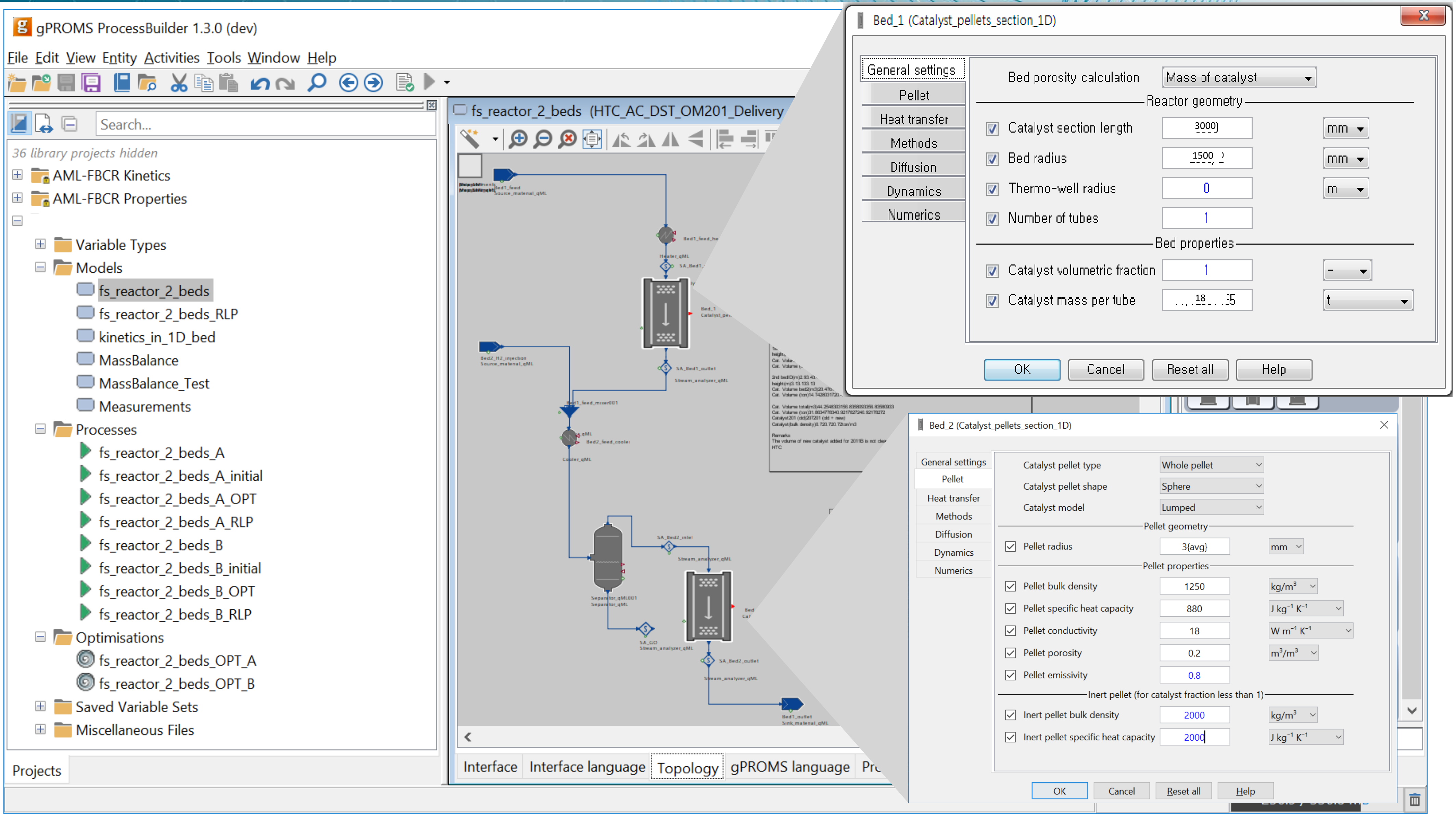
Decision variables

- bed inlet temperatures
- hydrogen addition rate
- CO addition rate

© 2019 Process Systems Enterprise Limited

Configuring the catalytic reactor model

via off-line process modelling tool



© 2019 Process Systems Enterprise Limited

Catalytic reactor

Online model-based Decision Support System

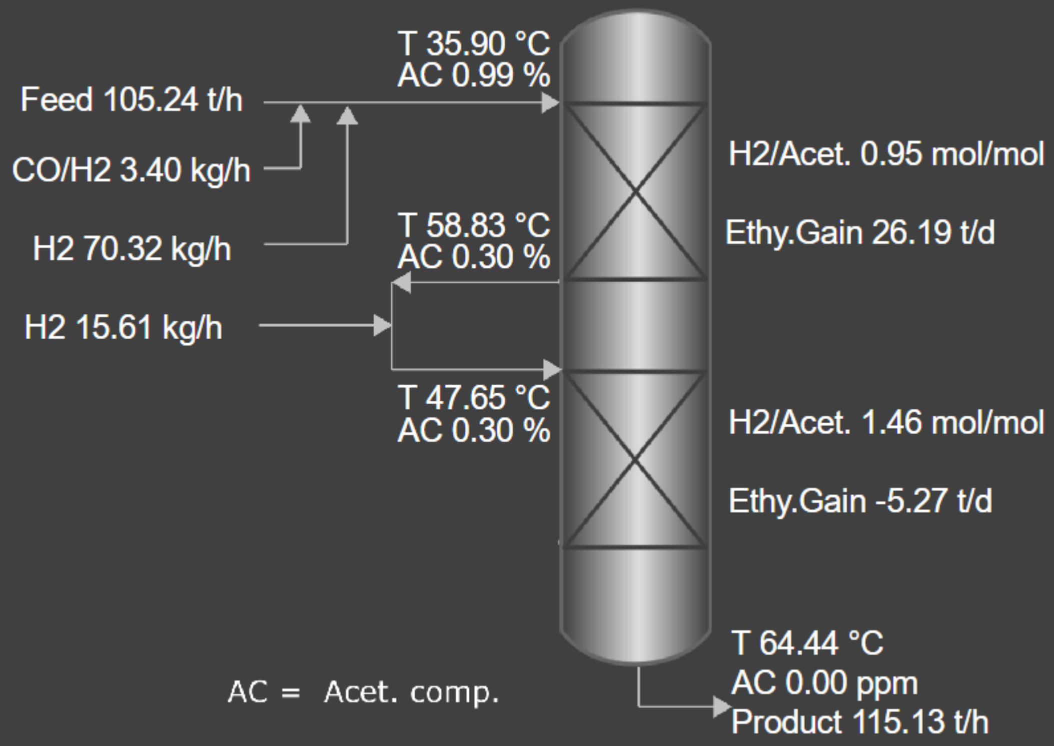
g | OLEFINS DECISION SUPPORT

OVERVIEW

ABC Petrochemicals

Feed: 105.2 t/h | Selectivity: 55.2 % | Reactor: RC201 | Overall Ethy. Gain: 20.9 t/d | Opt. Economic Gain: 16.9 % | Run Length: 146.3 days

ESTIMATED CONDITIONS



1st Bed

2nd Bed

ADVISOR

	Units	Estimated	Optimised
1st Bed H2/Acet.	mol/mol	0.95	0.95
2nd Bed H2/Acet.	mol/mol	1.46	1.42
1st Bed Inlet Temp	°C	35.90	37.90
2nd Bed Inlet Temp	°C	47.65	45.65

KPIs

KPI	Units	Estimated	Optimised
Overall Ethy. Gain	t/d	20.9	22.0
1st Bed Selectivity	%	99.9	99.9
2nd Bed Selectivity	%	-45.2	-40.2
1st Bed Conversion	%	69.2	70.1
2nd Bed Conversion	%	100.0	100.0
2nd Bed Acet. Outlet	ppm	0.0	0.0
Selectivity	%	55.2	58.1

Last update: 07/26/2018 23:07:47

Navigate to: Overview | Streams | Historian | Reactor | Help

© 2019 Process Systems Enterprise Limited

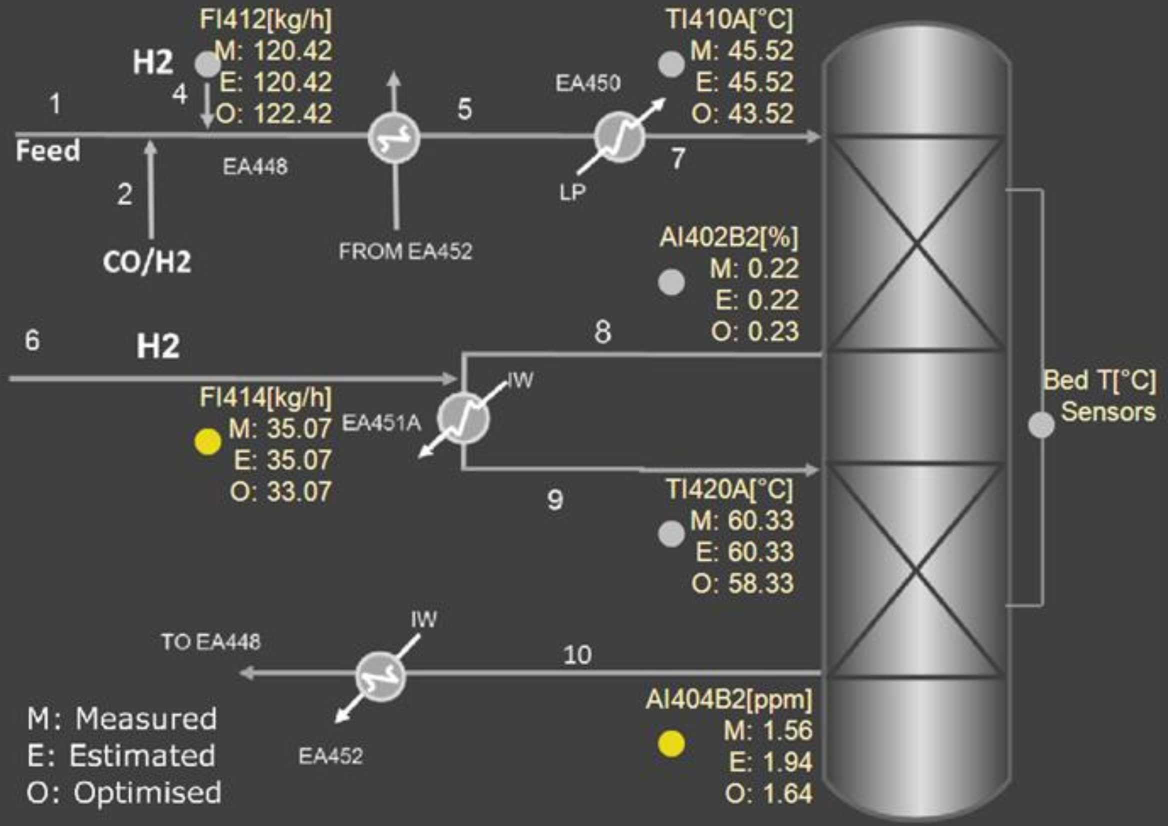
Catalytic reactor

Online model-based Decision Support System

g | OLEFINS DECISION SUPPORT

STREAMS

Reactor: DXXXXX | Feed: 157.9 t/h | Selectivity: 25.4 % | Ethy. Gain (Est./Opt.): 9.2 / 10.8 t/d | SOR: 15 Jun 2018 | Est. EOR: 21 Sep 2018



Stream Conditions

Stream ID: 4 Hydrogen to 1st Bed

KPI	Units	Measured	Estimated	Optimised
Acetylene	%		0.00	0.00
Ethylene	%		0.00	0.00
Ethane	%		0.00	0.00
Hydrogen	%		100.00	100.00
C4+	%		0.00	0.00
Flowrate	kg/h	120.42	120.42	122.42
Temperature	°C		30.00	30.00

Overall KPIs

KPI	Units	Measured	Estimated	Optimised
1st Bed Conversion	%	76.96	77.00	76.63
2nd Bed Conversion	%	99.92	99.91	99.92
Overall Selectivity	%	53.90	25.45	29.87

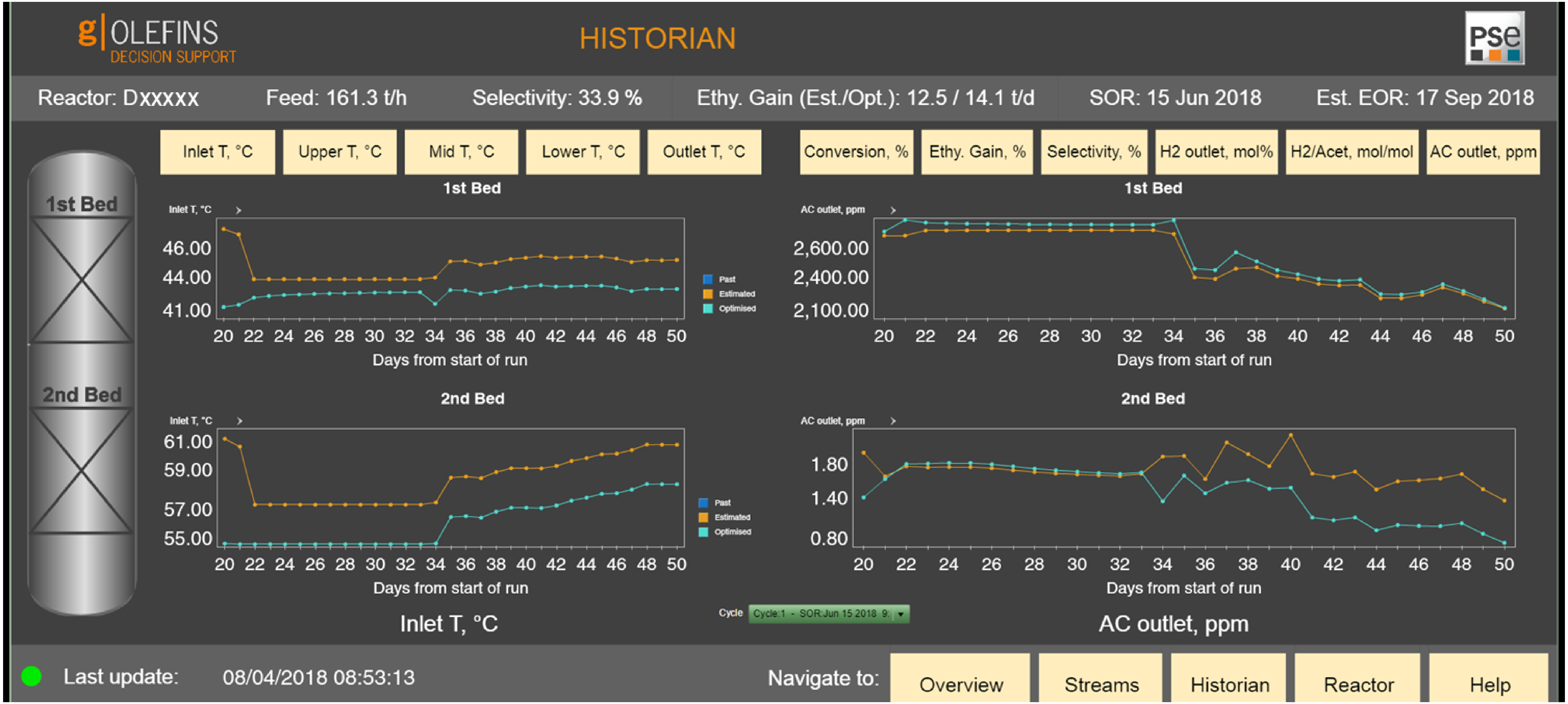
Last update: 08/04/2018 16:52:17

Navigate to: Overview | Streams | Historian | Reactor | Help

© 2019 Process Systems Enterprise Limited

Catalytic reactor

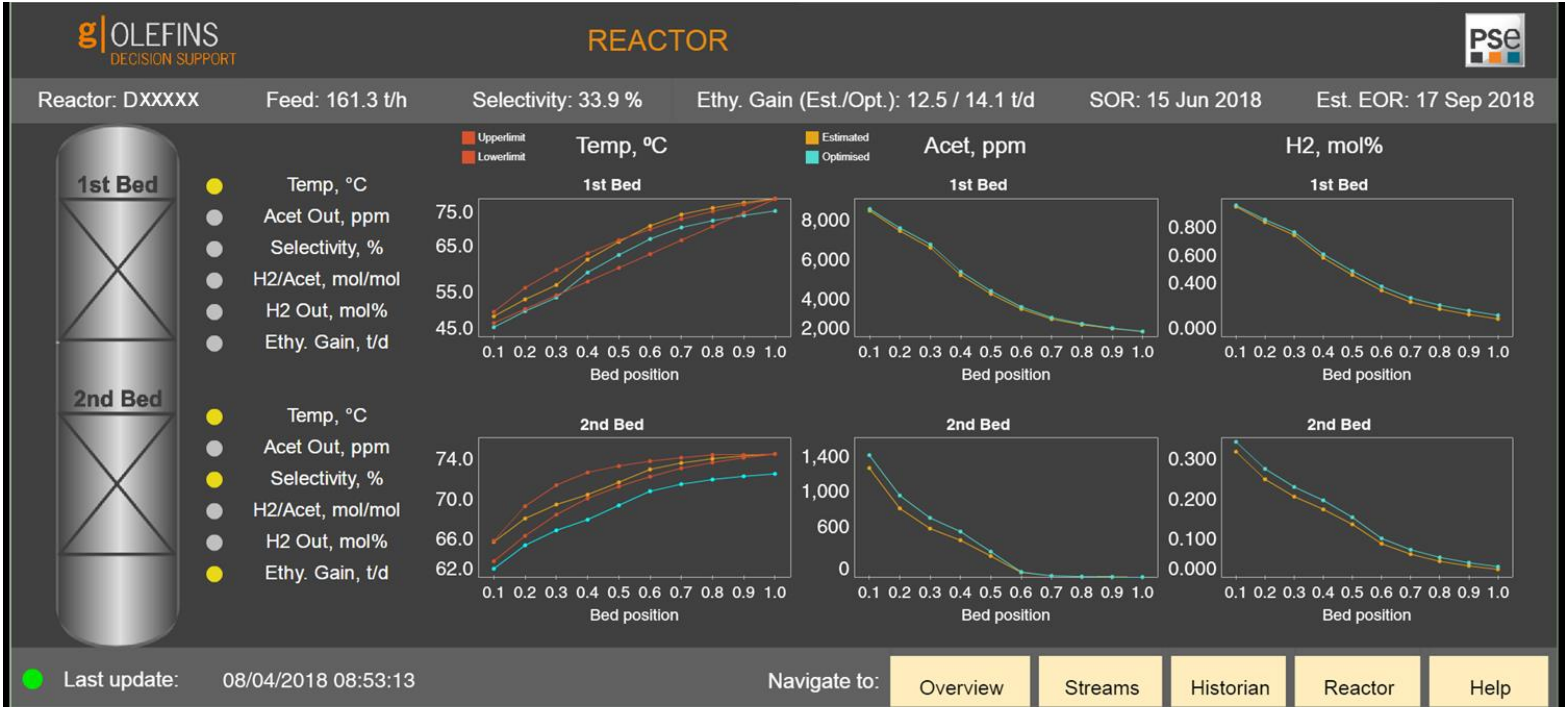
Online model-based Decision Support System



© 2019 Process Systems Enterprise Limited

Catalytic reactor

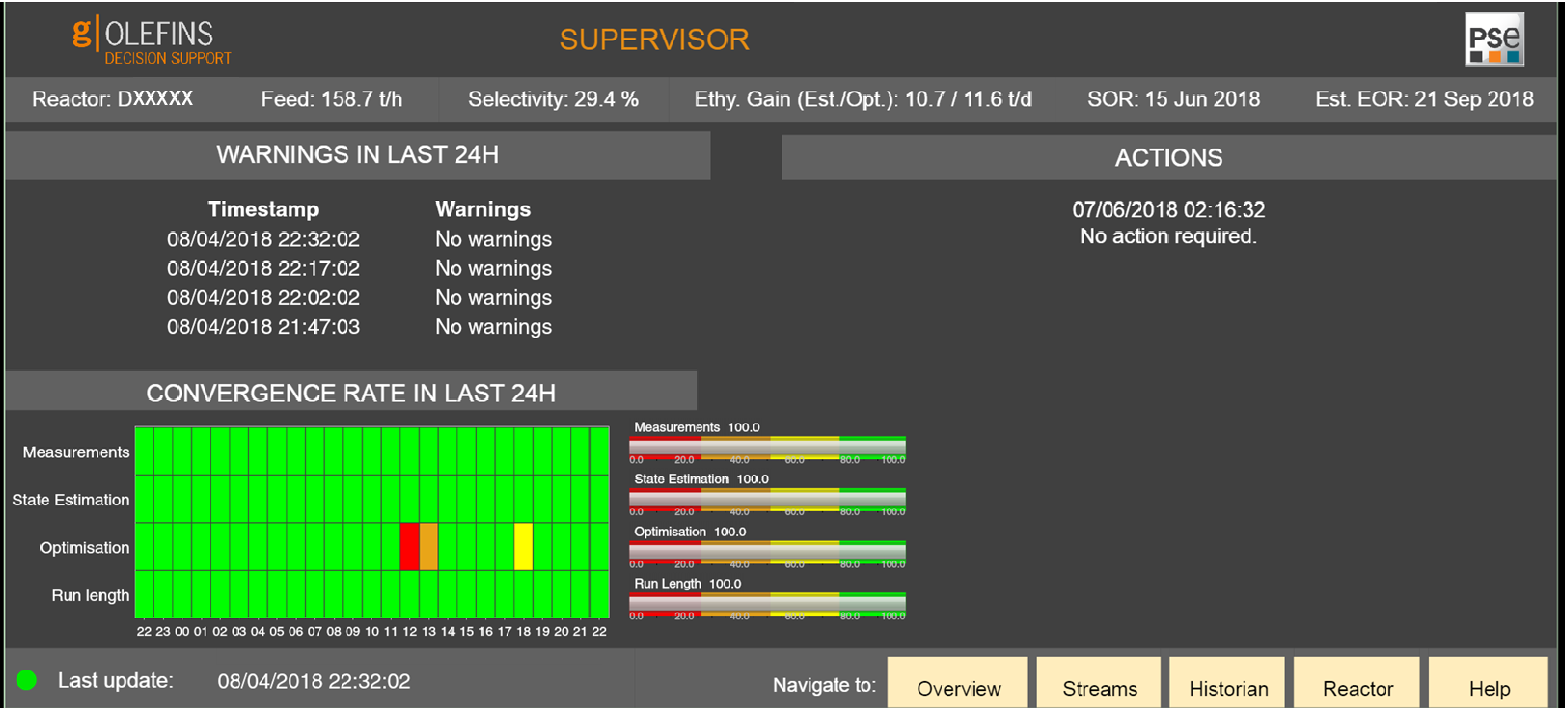
Online model-based Decision Support System



© 2019 Process Systems Enterprise Limited

Catalytic reactor

Online model-based Decision Support System



© 2019 Process Systems Enterprise Limited

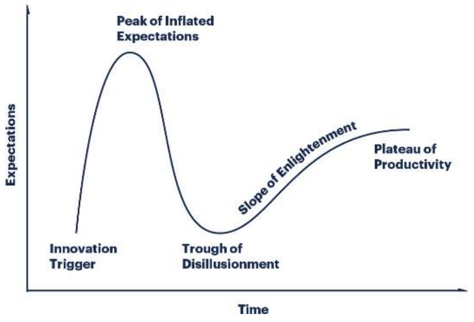
In conclusion…

© 2019 Process Systems Enterprise Limited

Digitalization in Process Engineering

3 key messages

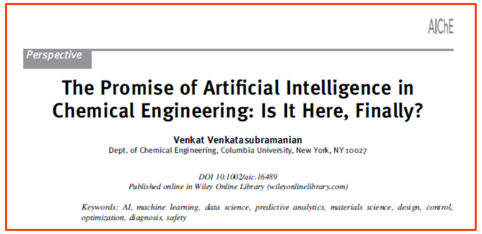
https://www.gartner.com/en/research/methodologies/gartner-hype-cycle



1. Digitalization: it's not *all* hype

- New power and capability based on significant recent advances in IT
- Opens new technical opportunities across process lifecycle

R&D → Engineering Design → Operations


AIChE

Perspective

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

Venkat Venkatasubramanian

Dept. of Chemical Engineering, Columbia University, New York, NY 10027

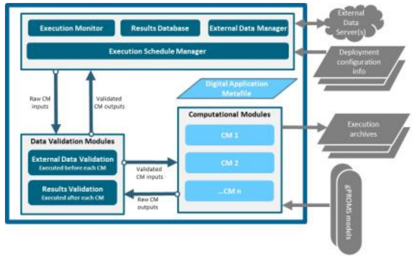
DOI 10.1002/aic.16489

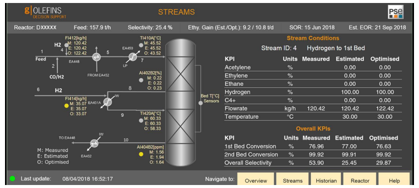
Published online in Wiley Online Library (wileyonlinelibrary.com)

Keywords: AI, machine learning, data science, predictive analytics, materials science, design, control, optimization, diagnosis, safety

2. Deep knowledge: don't re-invent the wheel (the hard way…)

- Plant data on their own do not always contain sufficient information
- Make full use of prior scientific & engineering knowledge
- …*combined* with plant data using sophisticated mathematical techniques





3. General Digital Applications Platforms: necessary *and* feasible

- Efficient & error-free development of complex applications
  - involving multiple communicating model-based computations
- Robust & efficient real-time deployment
- Visualization a key consideration

© 2019 Process Systems Enterprise Limited

Questions?