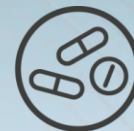
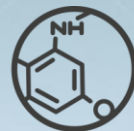


*Digitalisation in Chemical Engineering*  
Frankfurt, 1<sup>st</sup> March 2019

# Deep knowledge in Process Industry digitalization

Costas Pantelides FIChemE FREng



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

# Digitalization – what is it?



## Digitalization

is the use of digital technologies to change a business and provide new revenue and value. it is the process of moving to



NEW SCIENTIST (No. 194), 4 JUNE, 1964  
JAMES HOWDEN AND COMPANY SAVE £16,000 EVERY YEAR — WITH MOBIL

The difference between traditional lubrication and scientific lubrication can often be measured in money. The advertisements reproduced here may remind you of the savings which some Mobil customers have made with the help of Mobil Economy Service. All these savings (which run into thousands of pounds) are *annually recurring*.

The managements who have achieved these economies realise that lubrication is a specialized branch of engineering and that Mobil have played a big part in making it so.

As part of their plan for service to management of the future, Mobil have now developed Mobil MI/DAC (Management Information for Decision And Control), a new system for providing management with information through automatic data processing systems. With Mobil MI/DAC, virtually every stage of lubrication and maintenance can be evaluated *automatically*, on the basis of which decisions can be taken to increase efficiency and reduce costs.

Mobil MI/DAC can be applied in many fields—in most industrial undertakings, in machine tool and machinery manufacture, in civil engineering contractors' plants, and in transport fleets.

We are confident that Mobil Economy Service can help save substantial sums of money in *any* business using industrial machinery. If you get in touch with us, we shall be pleased to show how you can increase production and reduce maintenance costs.

MOBIL OIL COMPANY LIMITED, CARTON HOUSE, LONDON SW1

# MANAGEMENTS SAVE WITH

# Digitalization – what is it?

*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

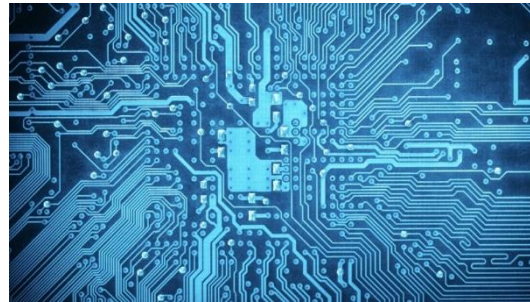
<https://www.mckinsey.com/industries/chemicals/our-insights/digital-in-chemicals-from-technology-to-impact>

## 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

# Model-based engineering along the process lifecycle

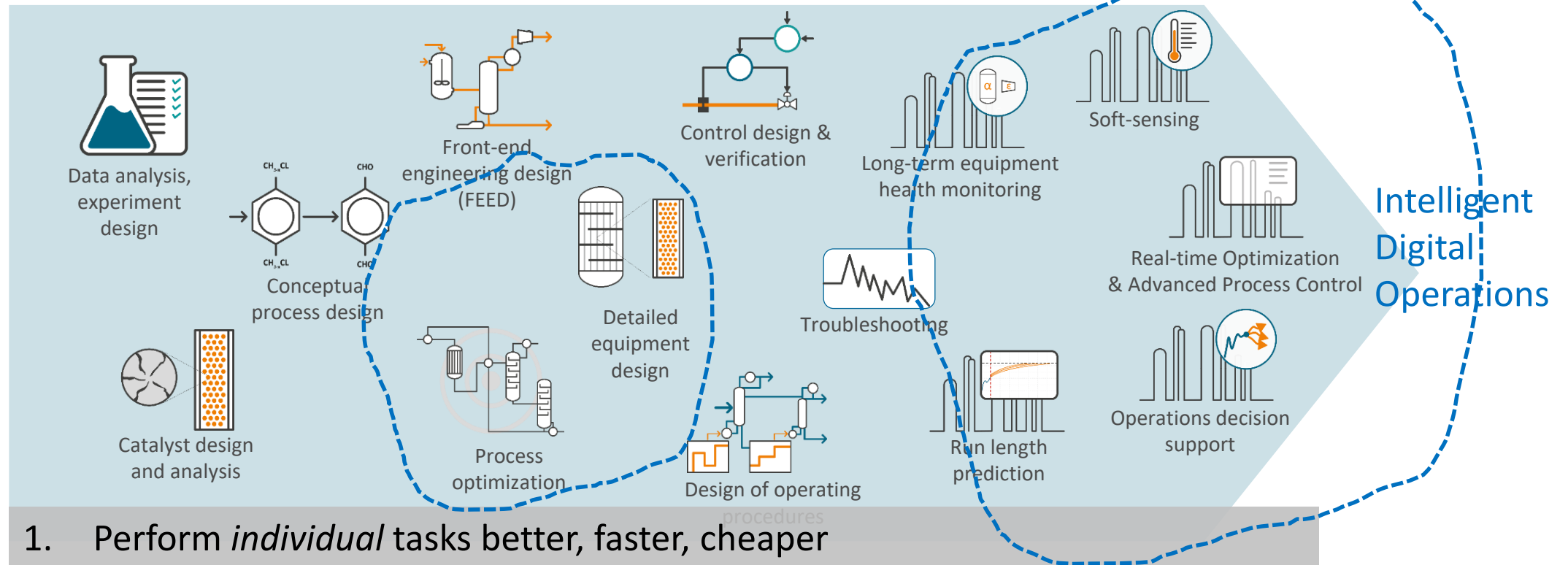
## Impact of digitalization



### RESEARCH & DEVELOPMENT

### ENGINEERING DESIGN

### PROCESS OPERATIONS



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

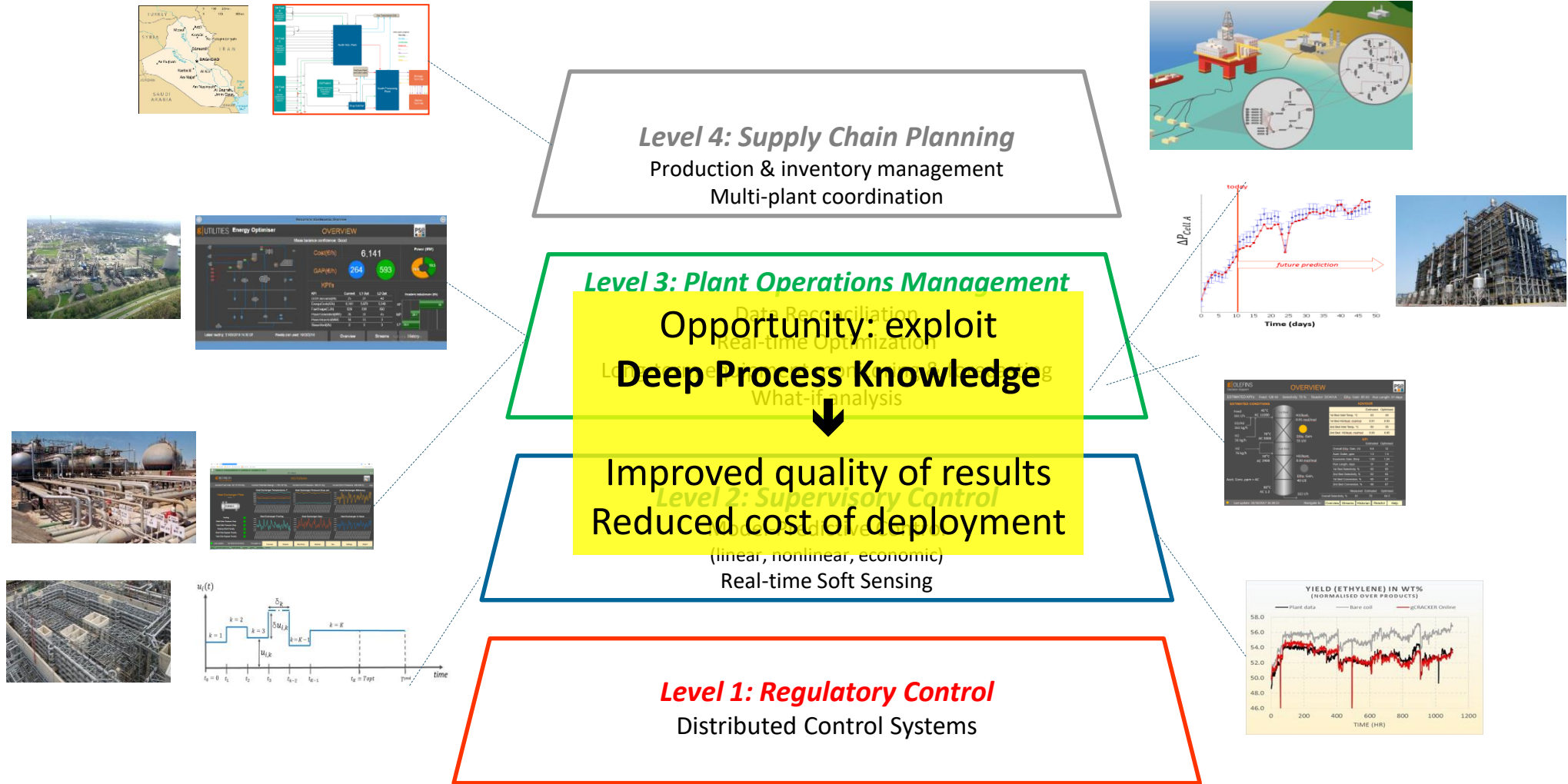
# Towards intelligent Digital Operations





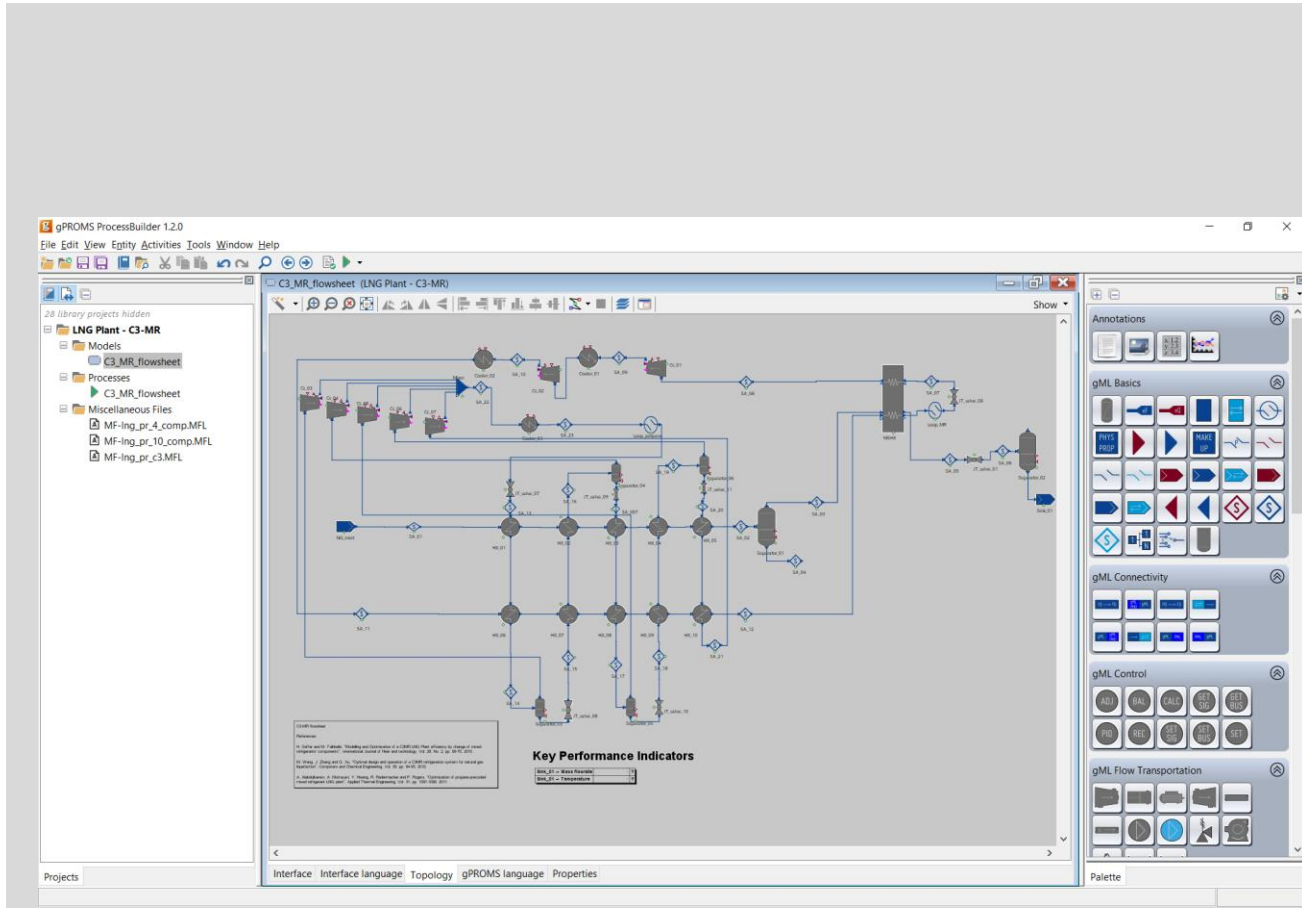
# Intelligent Digital Operations

## Model-Based Decision Support & Control Systems



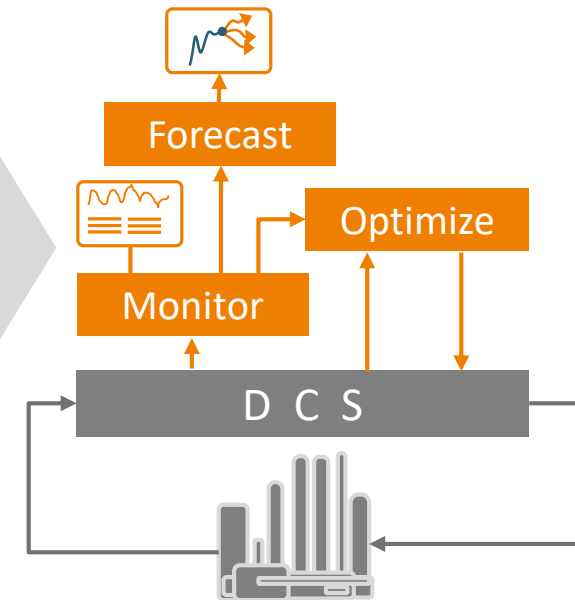
# Deep process knowledge in online model-based applications

## Leveraging the offline modelling investment



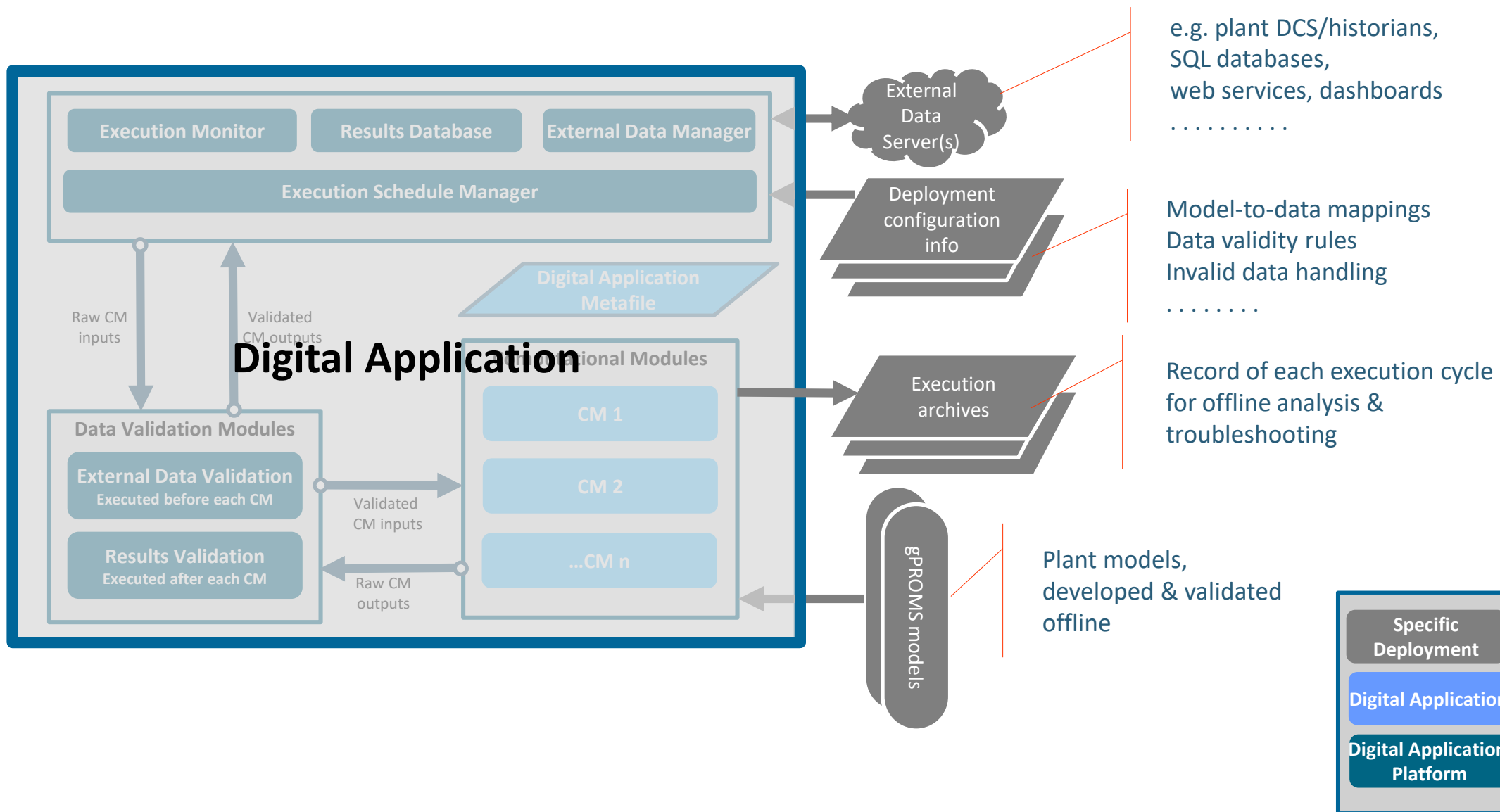
DESKTOP  
EMBEDDED

## 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.

# A general software platform for model-based Digital Applications

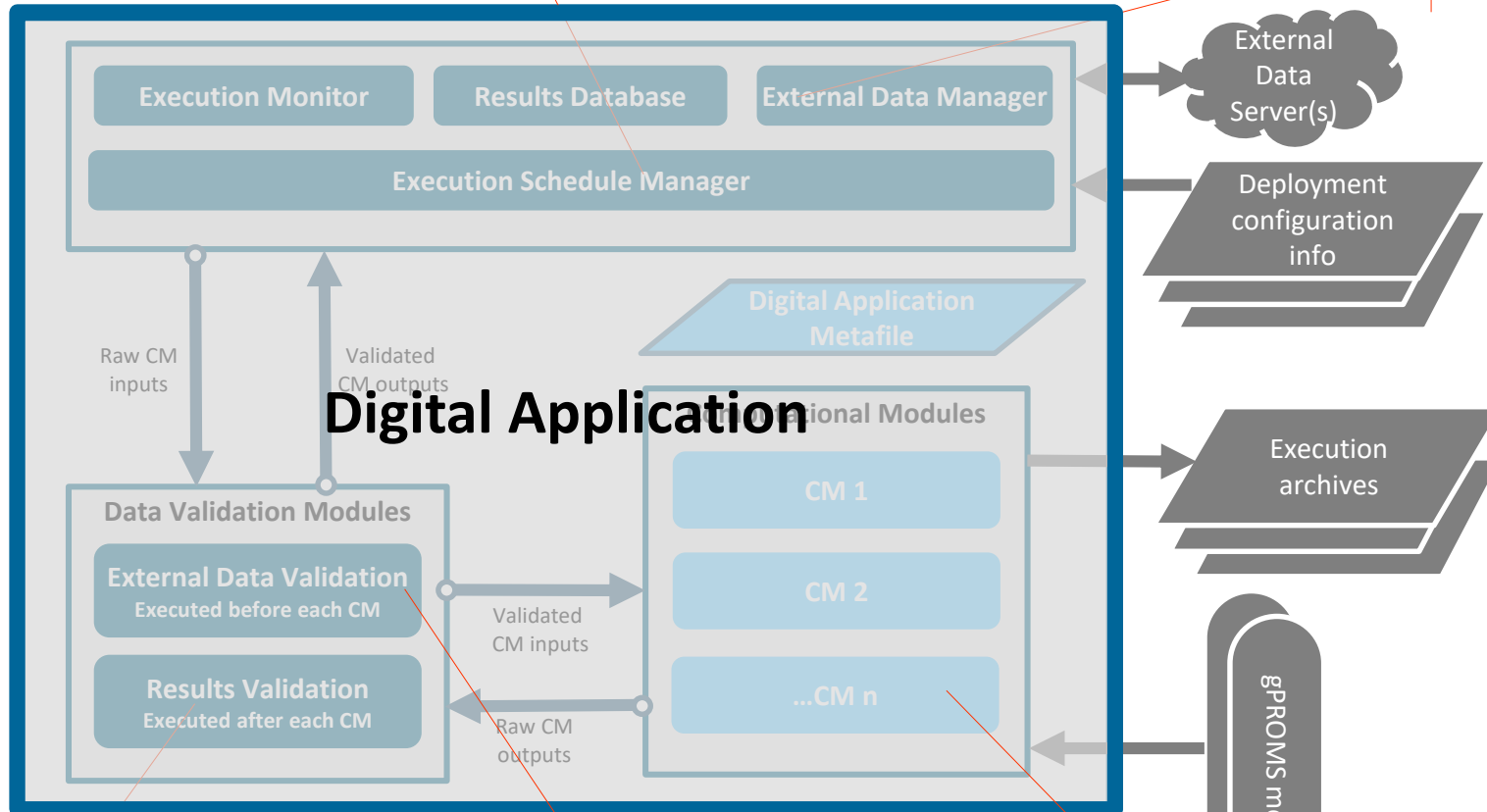


# A general software platform for model-based Digital Applications



Schedule & manage the execution of the various computations

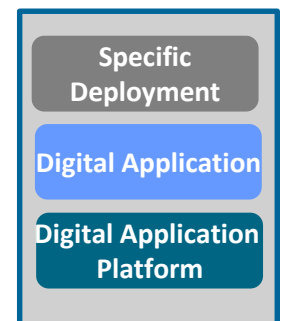
Manage communication with External Data Servers



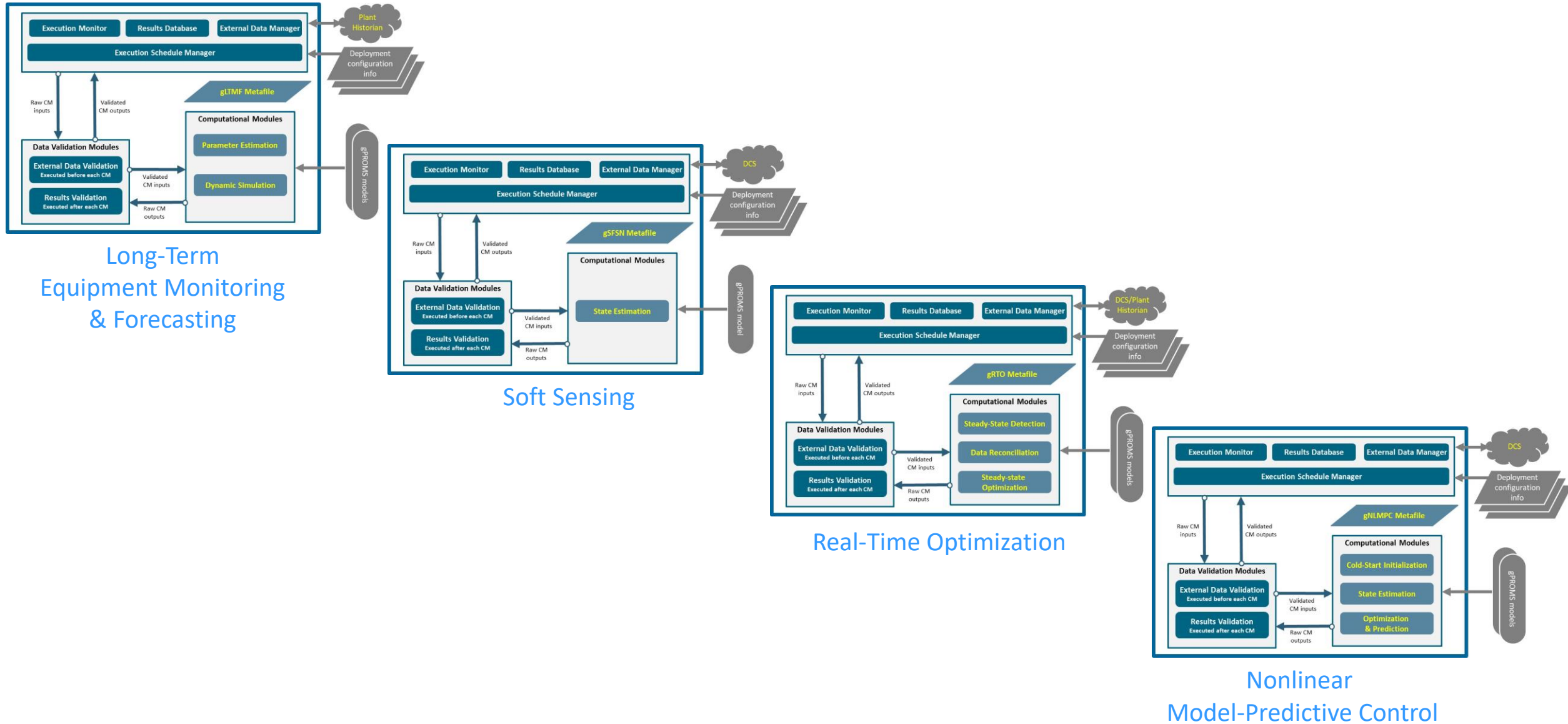
Make sure that any results being sent to the outside world are valid

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

Perform model-based computations

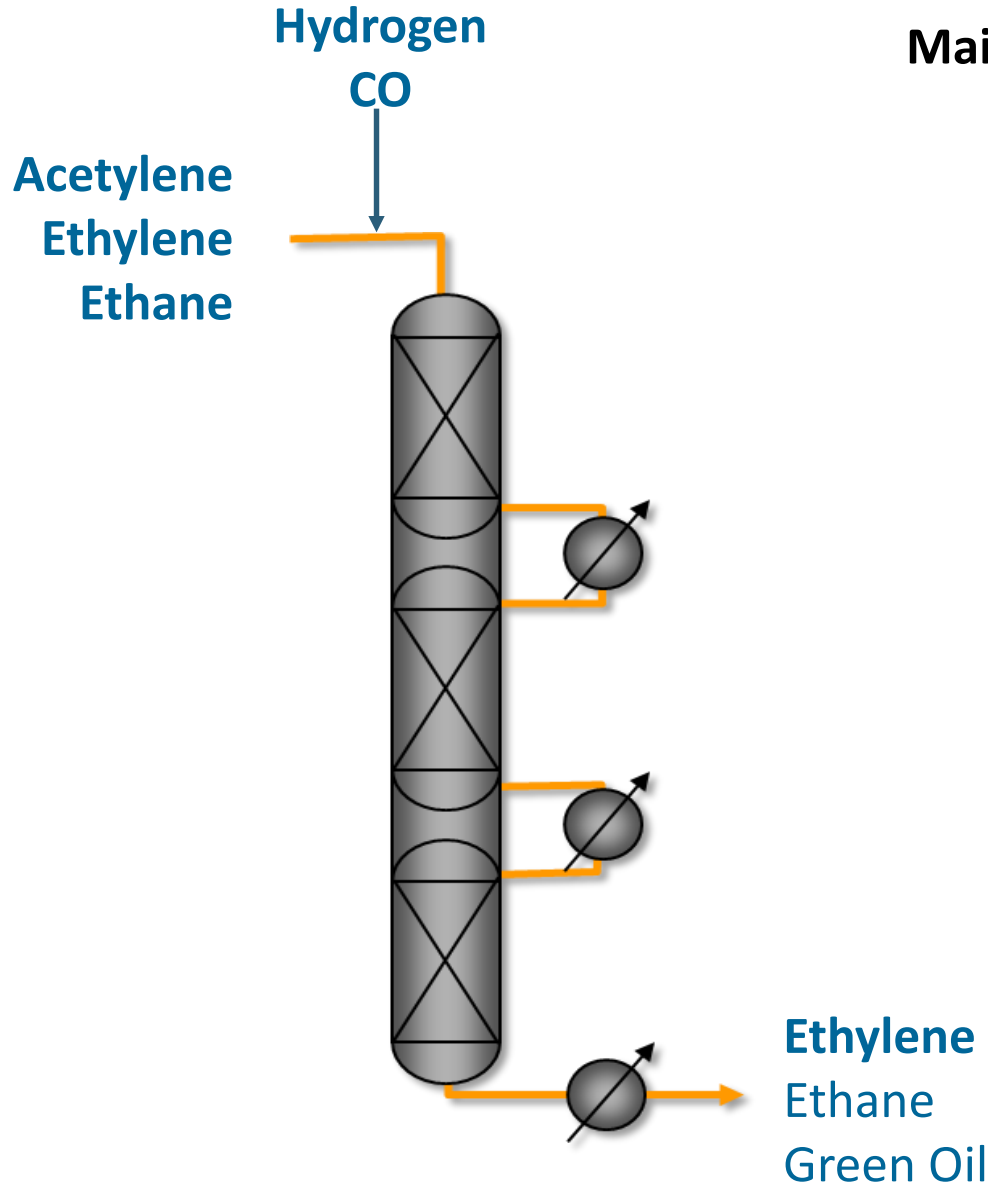


# Model-based Digital Applications based on the gPROMS Digital Applications Platform



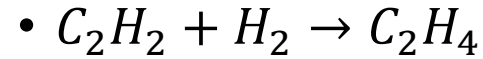
- Online model-based Decision Support Systems
- Example: catalytic reactor monitoring, forecasting, optimization





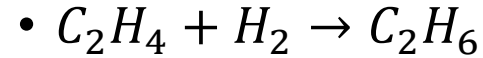
### Main Reaction:

#### Desired reaction

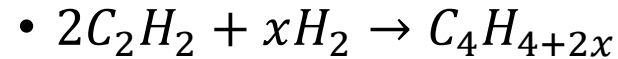


Acetylene hydrogenation

#### Undesired reactions



Ethylene hydrogenation



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

# Configuring the catalytic reactor model via off-line process modelling tool



gPROMS ProcessBuilder 1.3.0 (dev)

File Edit View Entity Activities Tools Window Help

36 library projects hidden

- AML-FBCR Kinetics
- AML-FBCR Properties
- Variable Types
- Models
  - fs\_reactor\_2\_beds
  - fs\_reactor\_2\_beds\_RLP
  - kinetics\_in\_1D\_bed
  - MassBalance
  - MassBalance\_Test
  - Measurements
- Processes
  - fs\_reactor\_2\_beds\_A
  - fs\_reactor\_2\_beds\_A\_initial
  - fs\_reactor\_2\_beds\_A\_OPT
  - fs\_reactor\_2\_beds\_A\_RLP
  - fs\_reactor\_2\_beds\_B
  - fs\_reactor\_2\_beds\_B\_initial
  - fs\_reactor\_2\_beds\_B\_OPT
  - fs\_reactor\_2\_beds\_B\_RLP
- Optimisations
  - fs\_reactor\_2\_beds\_OPT\_A
  - fs\_reactor\_2\_beds\_OPT\_B
- Saved Variable Sets
- Miscellaneous Files

Projects

Interface Interface language Topology gPROMS language Pre

**Bed\_1 (Catalyst\_pellets\_section\_1D)**

General settings

Bed porosity calculation: Mass of catalyst

Reactor geometry

- Catalyst section length: 3000 mm
- Bed radius: 1500 mm
- Thermo-well radius: 0 m
- Number of tubes: 1

Bed properties

- Catalyst volumetric fraction: 1
- Catalyst mass per tube: ...18...35 t

OK Cancel Reset all Help

**Bed\_2 (Catalyst\_pellets\_section\_1D)**

General settings

Catalyst pellet type: Whole pellet

Catalyst pellet shape: Sphere

Catalyst model: Lumped

Pellet geometry

- Pellet radius: 3(avg) mm

Pellet properties

- Pellet bulk density: 1250 kg/m<sup>3</sup>
- Pellet specific heat capacity: 880 J kg<sup>-1</sup> K<sup>-1</sup>
- Pellet conductivity: 18 W m<sup>-1</sup> K<sup>-1</sup>
- Pellet porosity: 0.2 m<sup>3</sup>/m<sup>3</sup>
- Pellet emissivity: 0.8

Inert pellet (for catalyst fraction less than 1)

- Inert pellet bulk density: 2000 kg/m<sup>3</sup>
- Inert pellet specific heat capacity: 2000 J kg<sup>-1</sup> K<sup>-1</sup>

OK Cancel Reset all Help



# Catalytic reactor

## Online model-based Decision Support System



### OVERVIEW



ABC  
Petrochemicals



Feed: 105.2 t/h

Selectivity: 55.2 %

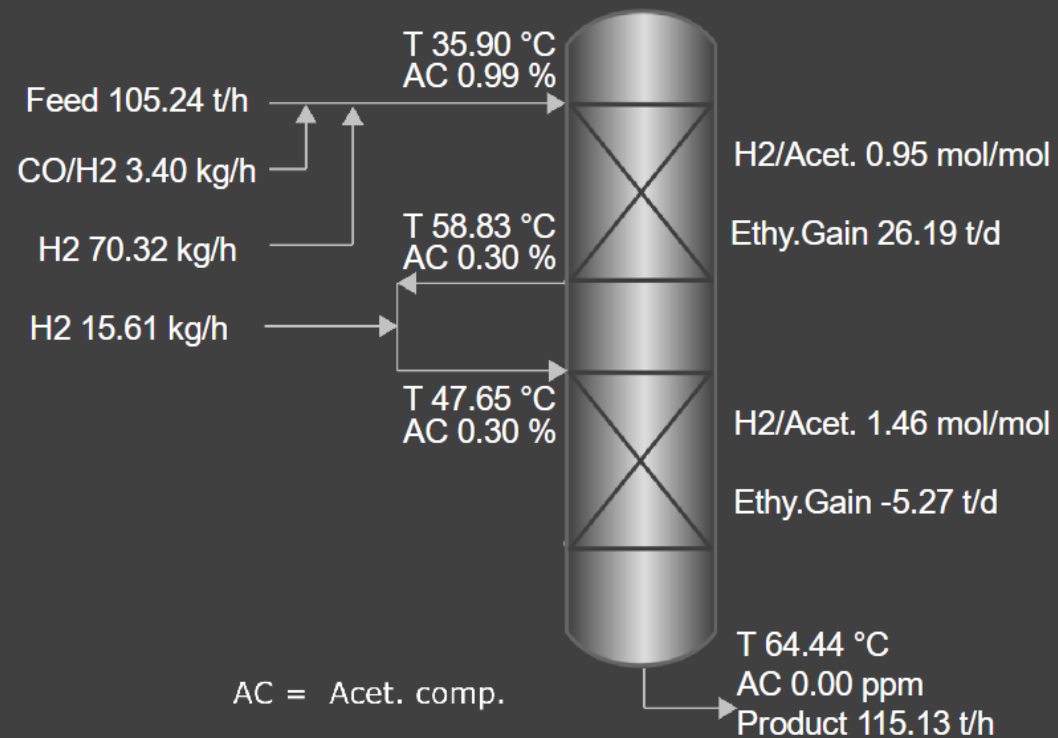
Reactor: RC201

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 H <sub>2</sub> /Acet.	mol/mol	0.95	0.95
2nd Bed H <sub>2</sub> /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

# Catalytic reactor

## Online model-based Decision Support System



**g|OLEFINS**  
DECISION SUPPORT

### STREAMS



Reactor: DXXXXX

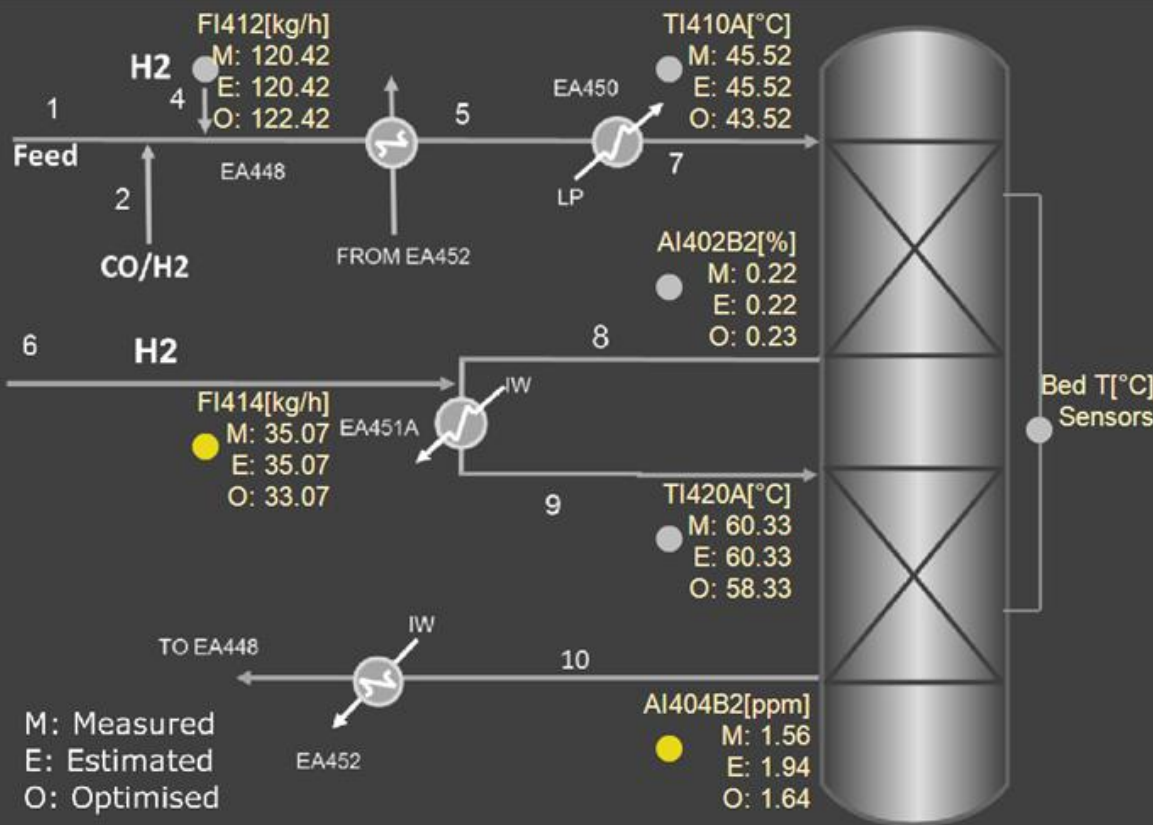
Feed: 157.9 t/h

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](#)

# Catalytic reactor

## Online model-based Decision Support System



### HISTORIAN



Reactor: DXXXXX

Feed: 161.3 t/h

Selectivity: 33.9 %

Ethy. Gain (Est./Opt.): 12.5 / 14.1 t/d

SOR: 15 Jun 2018

Est. EOR: 17 Sep 2018

Inlet T, °C

Upper T, °C

Mid T, °C

Lower T, °C

Outlet T, °C

Conversion, %

Ethy. Gain, %

Selectivity, %

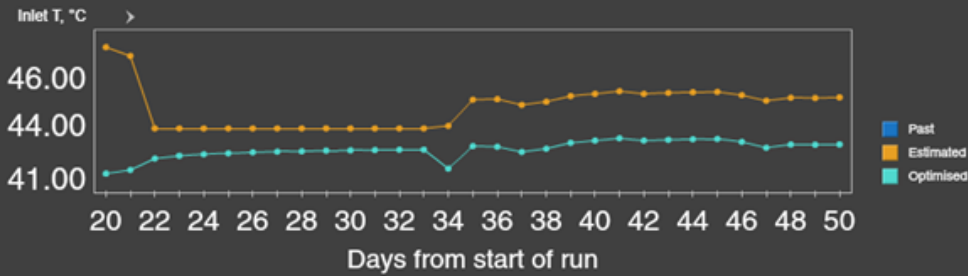
H2 outlet, mol%

H2/Acet, mol/mol

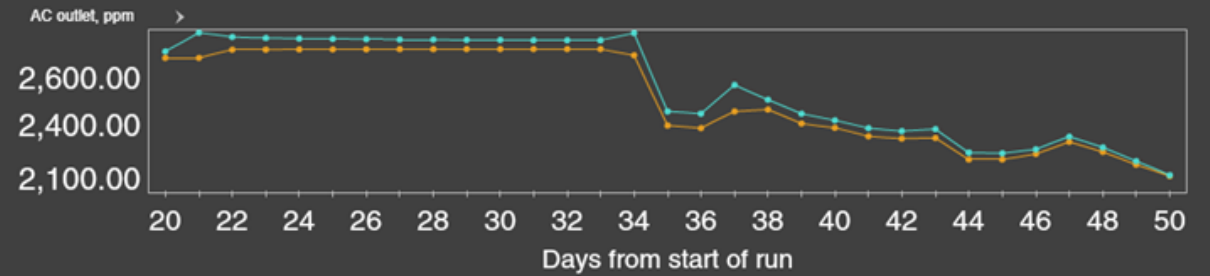
AC outlet, ppm



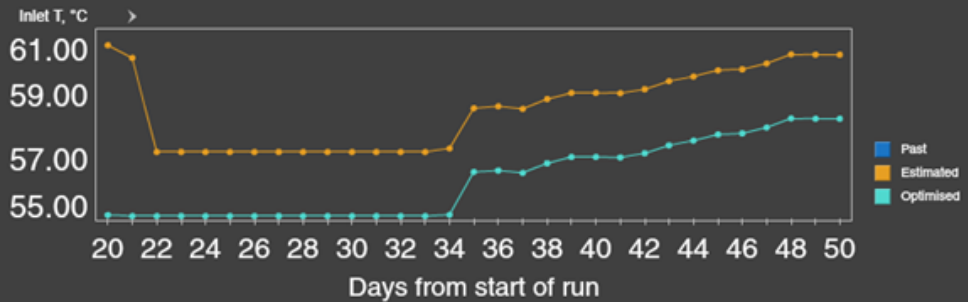
1st Bed



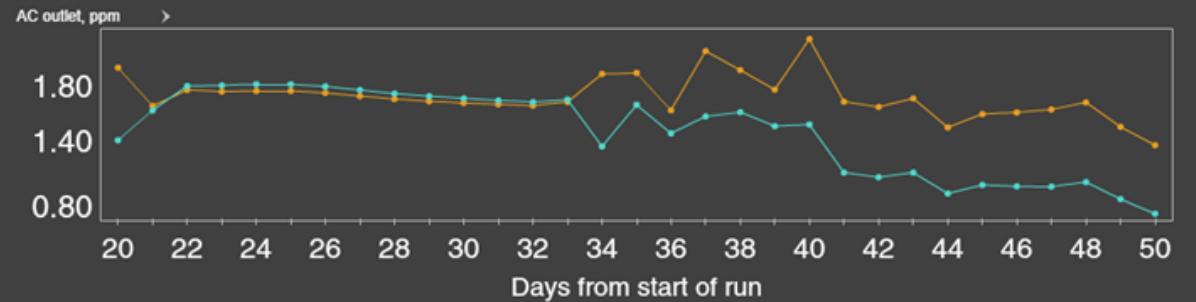
1st Bed



2nd Bed



2nd Bed



Cycle: Cycle 1 - SOR Jun 15 2018 9: [dropdown]

AC outlet, ppm

Last update: 08/04/2018 08:53:13

Navigate to:

[Overview](#)

[Streams](#)

[Historian](#)

[Reactor](#)

[Help](#)

# Catalytic reactor

## Online model-based Decision Support System



**g|OLEFINS**  
DECISION SUPPORT

### REACTOR



Reactor: DXXXXX

Feed: 161.3 t/h

Selectivity: 33.9 %

Ethy. Gain (Est./Opt.): 12.5 / 14.1 t/d

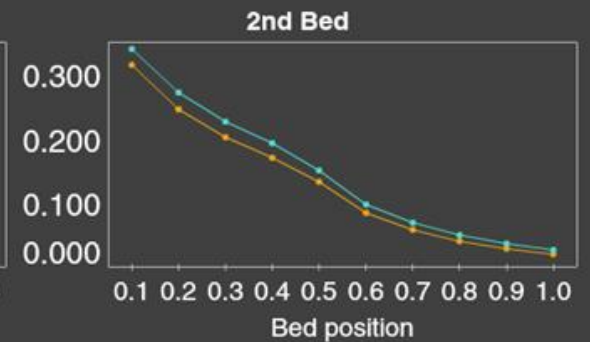
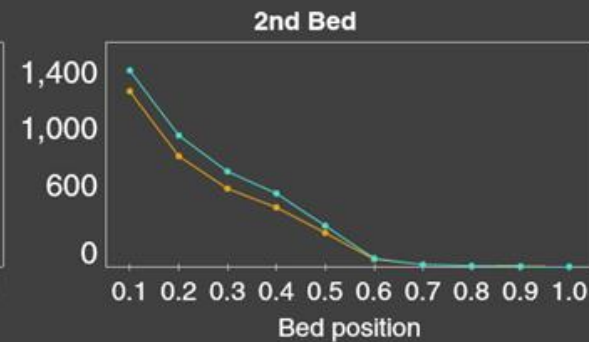
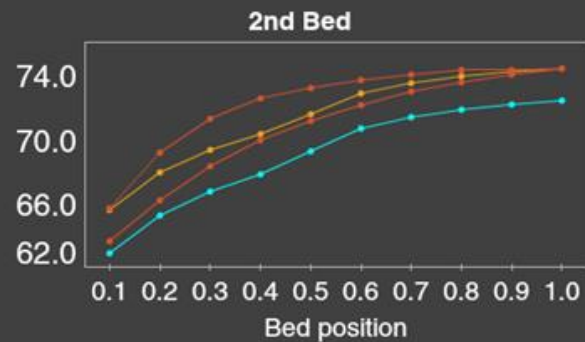
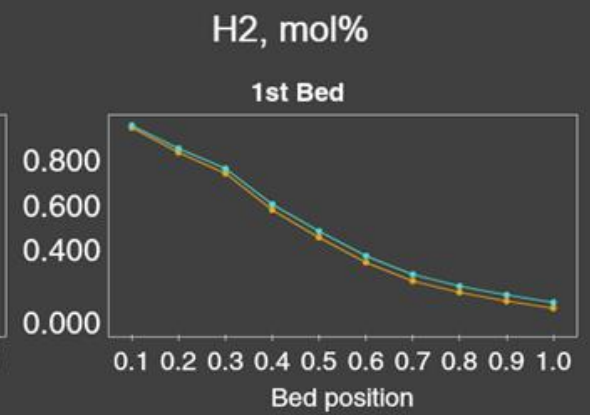
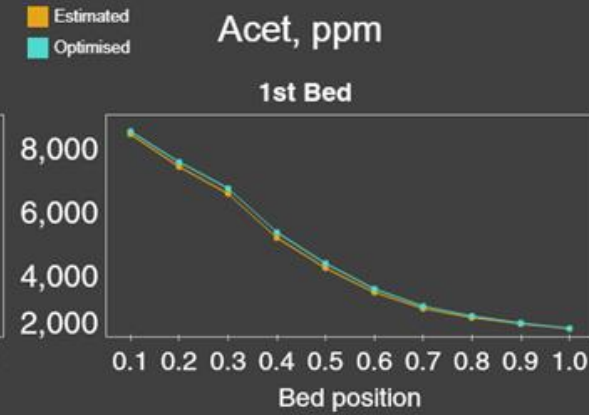
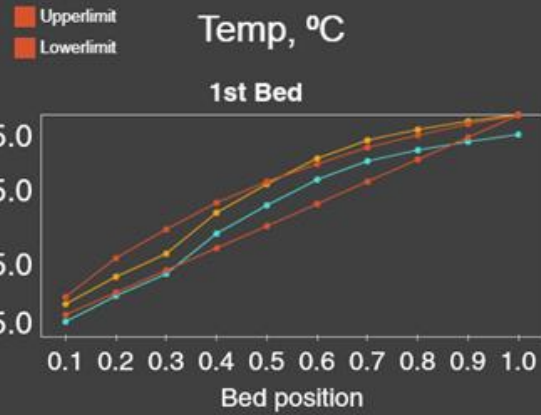
SOR: 15 Jun 2018

Est. EOR: 17 Sep 2018



- Temp, °C
- Acet Out, ppm
- Selectivity, %
- H2/Acet, mol/mol
- H2 Out, mol%
- Ethy. Gain, t/d

- Temp, °C
- Acet Out, ppm
- Selectivity, %
- H2/Acet, mol/mol
- H2 Out, mol%
- Ethy. Gain, t/d



Last update: 08/04/2018 08:53:13

Navigate to:

[Overview](#)

[Streams](#)

[Historian](#)

[Reactor](#)

[Help](#)

# Catalytic reactor

## Online model-based Decision Support System



### SUPERVISOR



Reactor: DXXXXX

Feed: 158.7 t/h

Selectivity: 29.4 %

Ethy. Gain (Est./Opt.): 10.7 / 11.6 t/d

SOR: 15 Jun 2018

Est. EOR: 21 Sep 2018

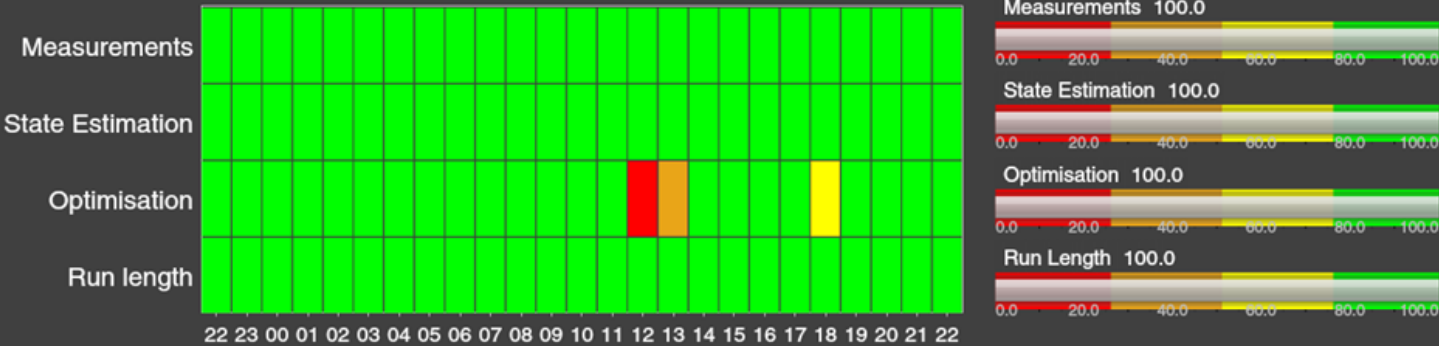
#### WARNINGS IN LAST 24H

Timestamp	Warnings
08/04/2018 22:32:02	No warnings
08/04/2018 22:17:02	No warnings
08/04/2018 22:02:02	No warnings
08/04/2018 21:47:03	No warnings

#### ACTIONS

07/06/2018 02:16:32  
No action required.

#### CONVERGENCE RATE IN LAST 24H



Last update: 08/04/2018 22:32:02

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[Overview](#)

[Streams](#)

[Historian](#)

[Reactor](#)

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In conclusion...



# Digitalization in Process Engineering

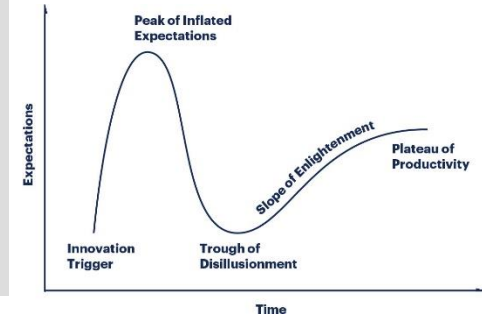
## 3 key messages



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

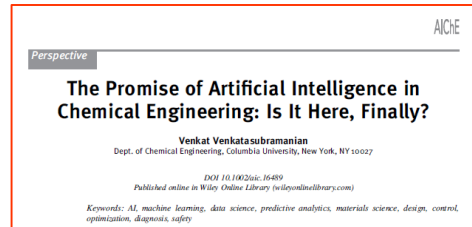
- New power and capability based on significant recent advances in IT
- Opens new technical opportunities across process lifecycle  
R&D → Engineering Design → Operations

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



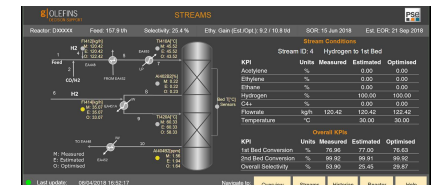
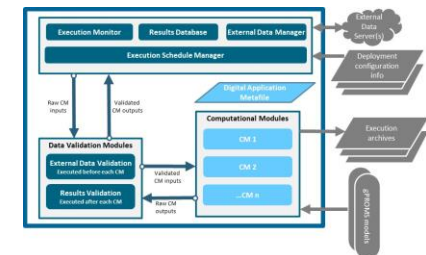
### 2. Deep knowledge: don't re-invent the wheel (the hard way...)

- 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



Questions?

