Digital Process Technology

Sustainability and responsiveness in the Process Industries

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Decarbonization of Process Industry and Next-Generation Materials for Sustainability: DTSI session

23 June 2023

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Humanity’s #1 challenge

is climate change

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The process industries are a major contributor to GHG emissions

Global direct CO_2 emissions from primary chemical production alone was nearly 1bn tonnes in 2020

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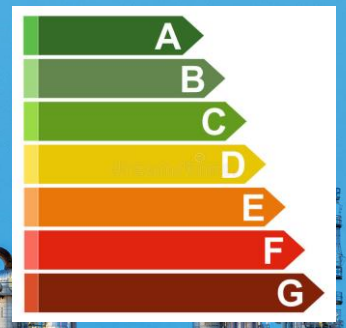
Climate change & the process industries
Addressing the decarbonization challenge

Emissions reduction
- Energy efficiency
- Process intensification
- Electrification



CCS / CCU
- CO_2 capture
- CO_2 utilization
- CO_2 storage

Sustainable feedstocks
- Recycling
- Circular economy
- Bio-based feeds

Hydrogen
- Production
- Transportation
- Storage
- Use

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Climate change & the process industries

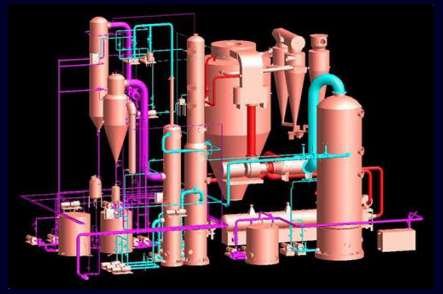
Addressing the decarbonization challenge … via digital process technologies

Multiple objectives
Complex interactions

A new golden era of innovation & opportunity

R&D

Engineering Design



Plant Operations

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“3 steps to a sustainable process industry”: a phased approach

How digital technologies help at every step

1 REDUCE: Improve the carbon efficiency of existing processes

Digital operations applications

Operational excellence
Enhanced plant efficiency
Emissions reduction applications

2 MITIGATE: capture CO_2, use and/or store it

Digital process design

Quickly analyse complexity: integration issues, operability dynamics

3 AVOID: Develop & deploy alternative low-carbon process routes

Digital process design

Accelerate innovation & manage risk using state-of-the-art model-based techniques

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Three steps to decarbonization

1. REDUCE: Improve the carbon efficiency of existing processes

There is no silver bullet for achieving net zero overnight

But you can certainly improve the CO_2 footprint of existing processes within the space of months …

… without redesign or capital expenditure.

- Digital twins of site-wide energy and utility systems can be implemented in the control room
- …to reduce emissions on a 24/7 basis using advanced monitoring & optimization techniques
- …tightly integrated within wider energy ecosystem

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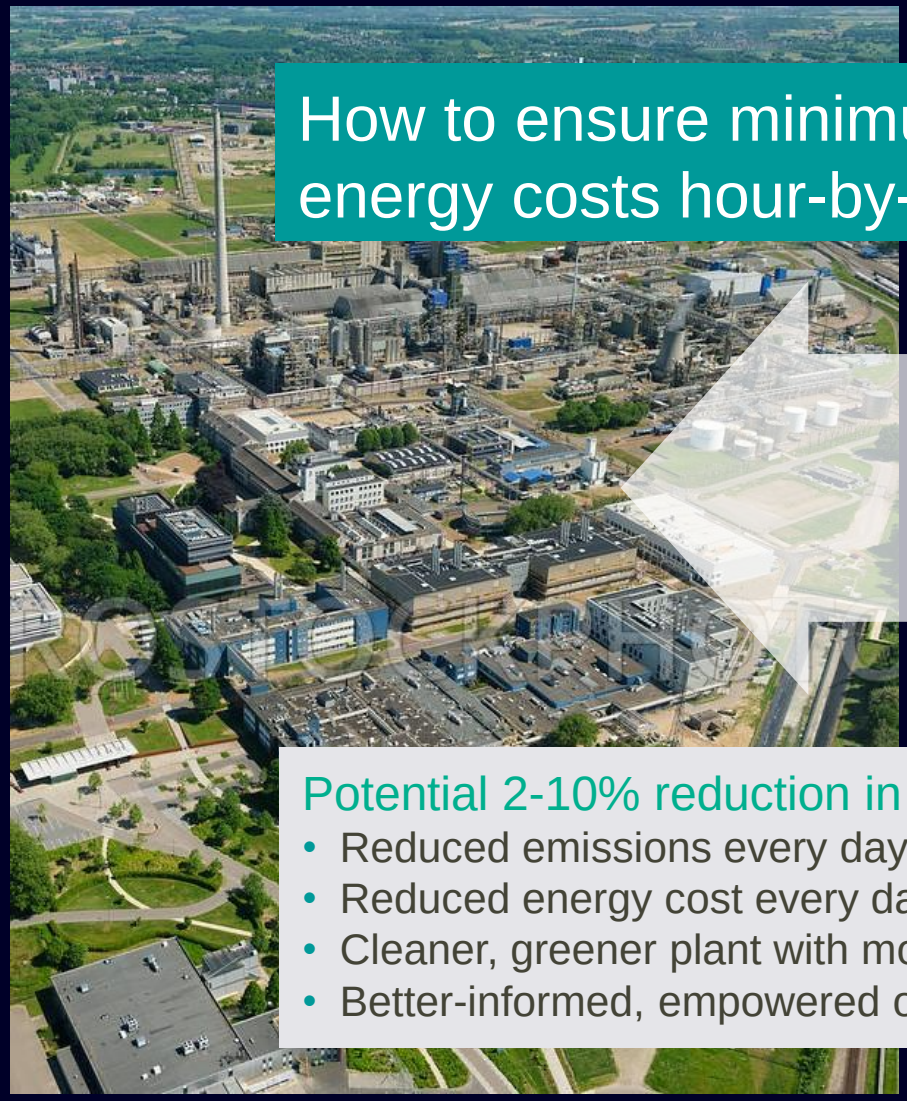
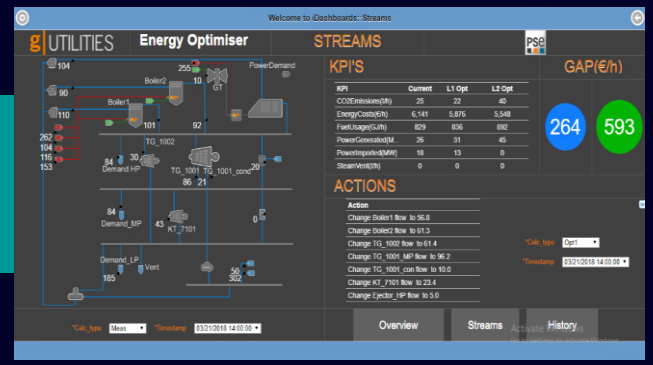
Digital Operations use cases
Reducing site utilities emissions and energy costs



How to ensure minimum emissions and energy costs hour-by-hour



gPROMS Utilities operations decision support

- **Site-wide utilities optimizer** implemented in control room
- **Operators** see current **'profits gap'** and **actions to reduce it**
- **Hour-by-hour** decision support
- **Instant optimal recovery** to **upsets and disturbances**

Potential 2-10% reduction in emissions & cost

- Reduced emissions every day
- Reduced energy cost every day
- Cleaner, greener plant with more flexible operation
- Better-informed, empowered operators

> gPROMS Utilities gives us significant base-line savings on our refinery site.
> – Galp Energia, Portugal.

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Three steps to decarbonization
2. MITIGATE: Capture CO_2, use and/or store it

Carbon capture is a key technology – proven and available now – in the transition to a decarbonized economy.
It may also be one of few practical options for hard-to-decarbonize sectors such as steel and cement.

- Carbon capture needs to be tightly integrated with main processing systems
- Digital process twins help minimize the energy penalty and ensure operability and controllability of the entire carbon chain
- Digital technology is essential for development of new concepts for capture (e.g. Direct Air Capture) and storage (e.g. mineralization)

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gPROMS Process: digital design and digital operation for process systems with carbon capture, utilization and storage

Map out **system interactions**, design **control systems** and **operating procedures**, design for **dynamic operation**

Integrated environment for

Design: optimize heat integration, explore alternatives, predict transient response

Operation: process digital twin for on-line decision support, real-time optimization

Scope: detailed predictive models for power generation, capture unit, compression, transportation and storage + many more other process units

Key projects

Optimizing start-up and shutdown of gas treatment plants [Shell]

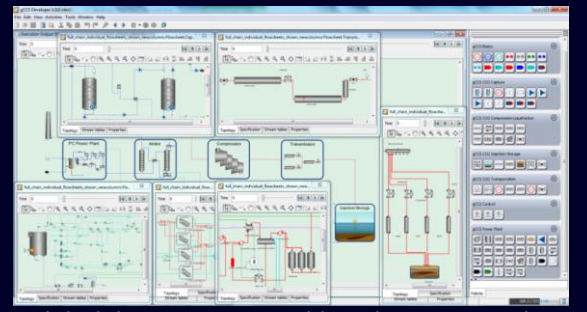
CCS chain and network studies [Energy Technologies Institute]

Major benefits include

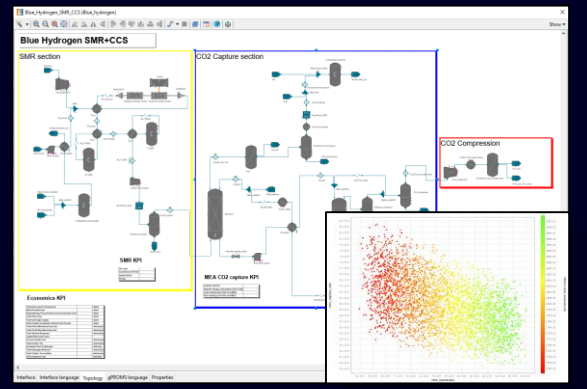
Better design, increased confidence when scaling up

Better heat integration → reduced energy penalty

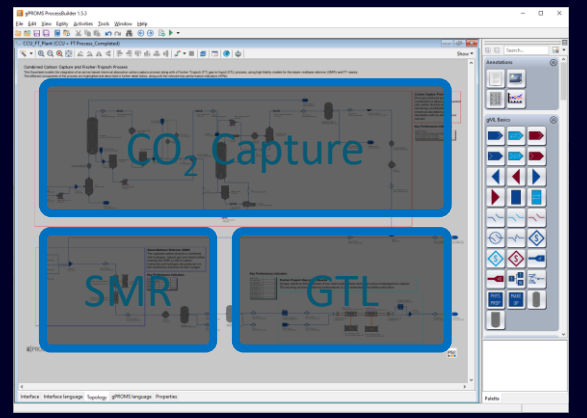
Faster startup/shutdown, better response to process disturbance



Whole-chain capture process model covering power generation, CO_2 capture, compression, transportation and storage



Blue hydrogen process model including SMR unit, CO2 capture unit and heat integration, used for sensitivity analsyis



Carbon capture and utilization process model covering CO_2 capture, methane reforming and hydrocarbon (C5+) synthesis

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Three steps to decarbonization
3. AVOID: Develop alternative low-carbon process routes

The hydrogen economy is driving much new process development.

However, getting new equipment & processes to market rapidly and reliably poses many challenges – particularly if they need to be designed for variable feed rates.

Digital process development is helping reduce time-to-market and cost by

- …enabling rapid and informed evaluation of alternatives
- …quantifying uncertainty and managing risk in innovation
- …maximizing effectiveness & efficiency of experimental R&D programmes

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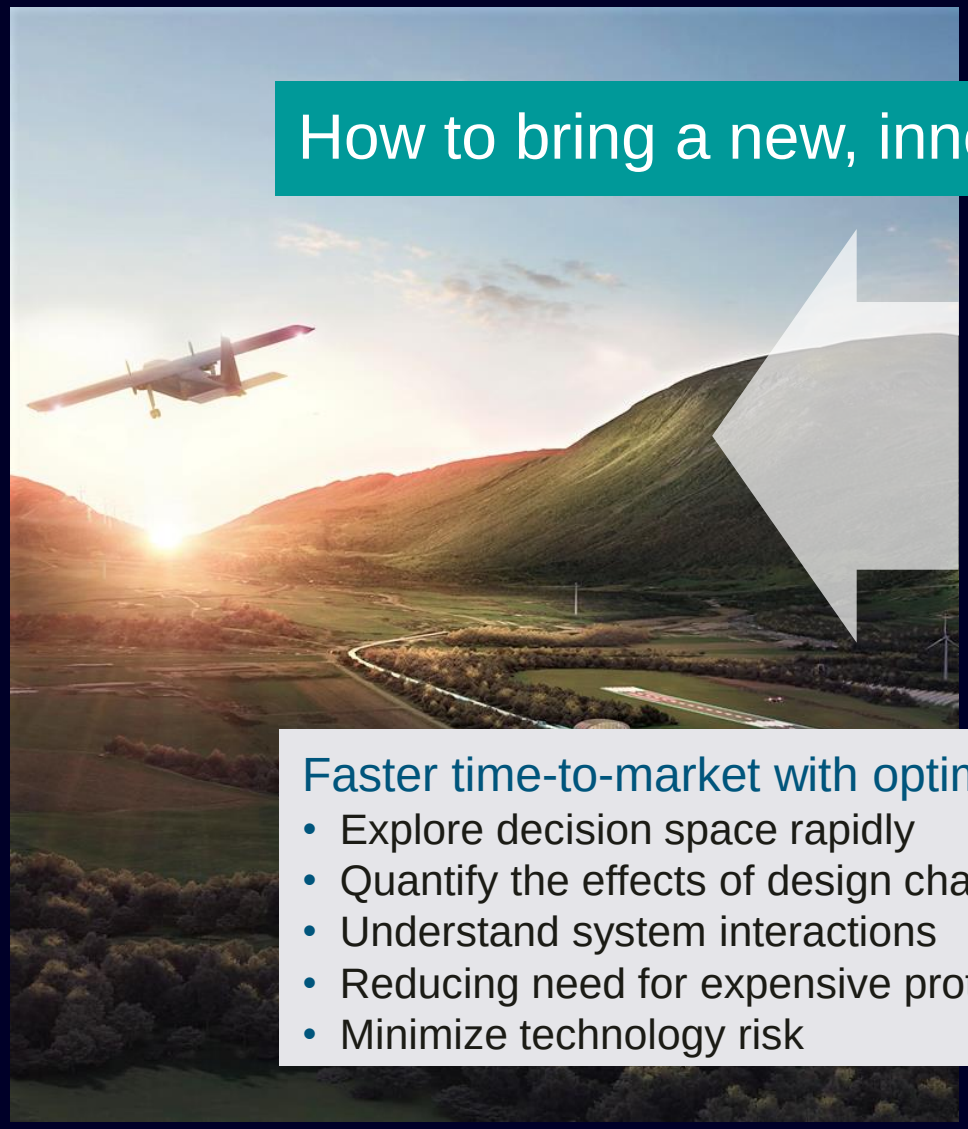
Digital Design use cases

Protium: helping enable Zero-Emissions Flight (ZEF)



How to bring a new, innovative process to market rapidly

gPROMS Process decision support for rapid hydrogen refuelling

- System for **rapid hydrogen refuelling** of aircraft
- Digital twin technology used to **accelerate the development, design, testing**
- Refuelling system model used to
  - **explore the decision space** and **optimize system design**
  - simulate and optimize **real-world performance**
- Contributes towards the UK government 2050 **net zero emissions target**.

Faster time-to-market with optimized design

- Explore decision space rapidly
- Quantify the effects of design changes accurately
- Understand system interactions
- Reducing need for expensive prototyping
- Minimize technology risk

> The digital twin approach to designing refuelling systems increases confidence and understanding in the capabilities of emerging hydrogen technology
>
> DR JEN BAXTER, DIRECTOR OF INNOVATION, PROTIUM

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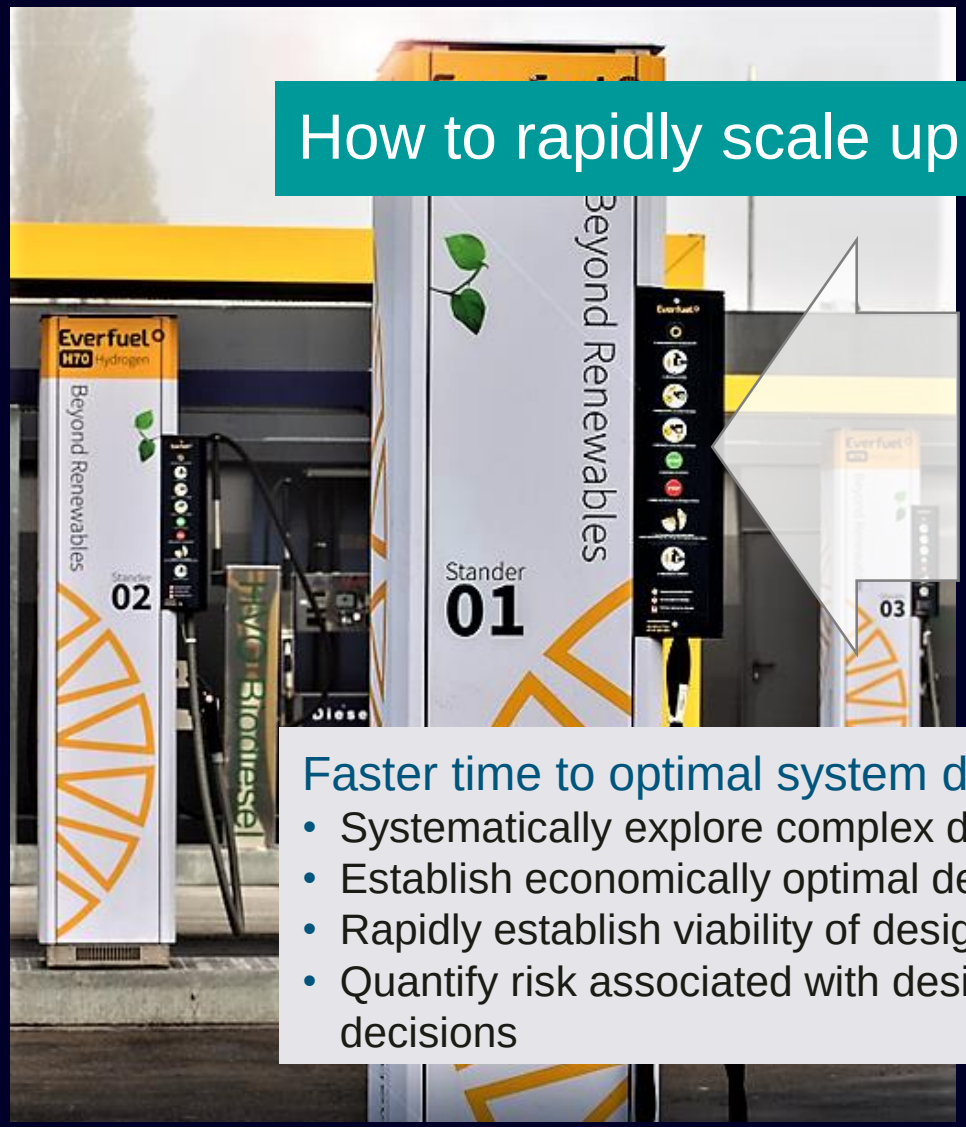
Digital Design use cases

Everfuel: developing large-scale electrolysis-based hydrogen production & storage



How to rapidly scale up of new hydrogen storage process

gPROMS Process decision support for rapid decision

- HySynergy large-scale **electrolysis hydrogen production & storage**
- Digital twin design tool **captures knowledge** of inherently complex chemical and physical processes including electrochemical cell reactors
- Used to **scale-up from initial 20 MW** to full-scale 300 MW production size
- Supports decision-making in all stages of the **project delivery** and **plant optimization** activities

Faster time to optimal system design

- Systematically explore complex decision space
- Establish economically optimal design
- Rapidly establish viability of design choices and
- Quantify risk associated with design & operating decisions

> We believe that the unmatched capabilities of gPROMS in process modelling, validation and optimization will help us secure the future of zero-emission mobility".
>
> UFFE BORUP, CTO AT EVERFUEL

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TOGETHER FOR SUSTAINABILITY (TfS) PARTNERSHIP

Activating carbon footprint transparency in the Chemical Industry

Customer Challenge

Tracking carbon emission data is difficult due to silos between different players along the value chain. This creates a challenge for product carbon footprint (PCF) and scope 3 reporting.

Solution

Partner with TfS, consisting of 47 international companies, to demonstrate the scalability of PCF data exchange across the chemical industry using SiGREEN.

- Provide learnings on PCF data exchange in chemical industry
- Deploy SiGREEN to all TfS members
- Exchange PCF data securely between partners in the chemical industry supply chain

Customer Benefit

- Trustworthy and secure PCF data exchange in supply chain
- Standardized PCF guideline throughout chemical industry
- Easy identification for carbon reduction measures
- Acceleration of decarbonization in the chemical industry

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Humanity’s #1 challenge

but neither the only,
nor the most immediate one

is climate change

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Climate

Health

Energy security

Food

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Digital Process Technologies: a key part of the solution

Innovation

Product efficacy

Process efficiency

Responsiveness

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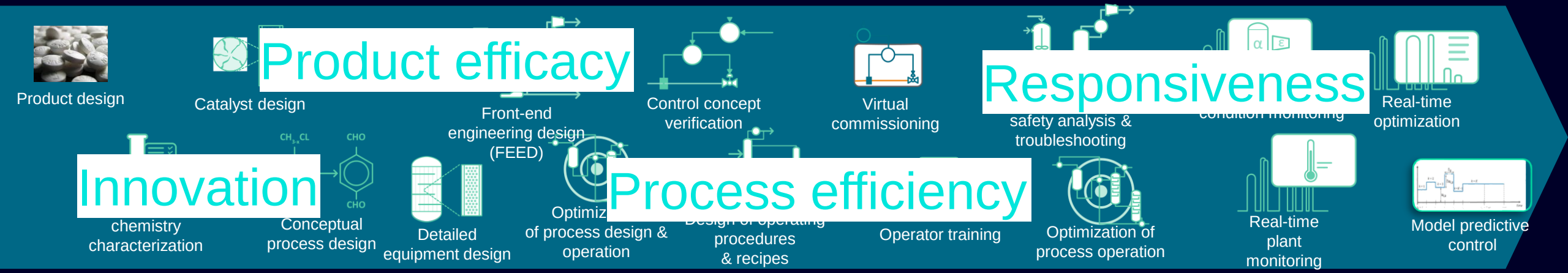
Digital process technologies across the product & process lifecycle

DIGITAL R&D

DIGITAL ENGINEERING DESIGN

DIGITAL OPERATIONS



Deep process knowledge

- captured in the form of validated models
- leveraged across the lifecycle

Significant value

- delivered at all stages of the lifecycle
- …by combining models with sophisticated mathematics & computer science

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Digital process technologies across the product & process lifecycle

DIGITAL R&D

DIGITAL ENGINEERING DESIGN

DIGITAL OPERATIONS

Product efficacy

Responsiveness

Innovation

Process efficiency

Product design

Catalyst design

chemistry characterization

Conceptual process design

Detailed equipment design

Front-end engineering design (FEED)

Optimiz of process design & operation

Control concept verification

Virtual commissioning

procedures & recipes

Operator training

safety analysis & troubleshooting

Optimization of process operation

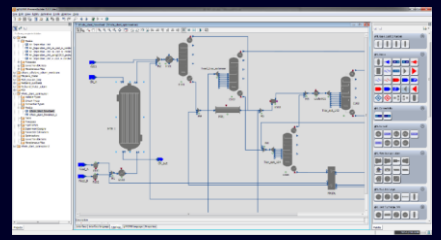
Real-time optimization

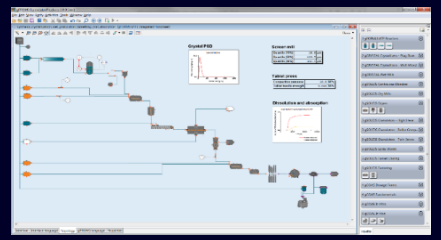
Real-time plant monitoring

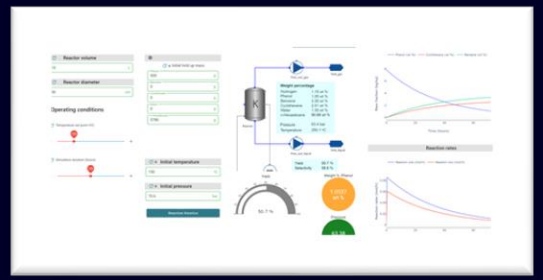
Model predictive control

gPROMS Process

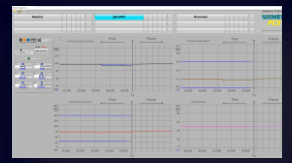
gPROMS FormulatedProducts







gPROMS Web Applications



gPROMS Digital Applications

OFFLINE ONLINE

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Thank you

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