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Intelligent digital operations -
incorporating deep process knowledge within plant automation systems

Chris Leingang | APAC 2019 | Manchester

Evolution of a Digital Twin for a Steam Cracker

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***Abstract*—A digital twin is composed of many software elements that are already state of the art. New perspectives are opened by the integration of individual models and simulation tools to a holistic, semantically integrated system, integrated across different hierarchy levels of the plant, and integrated along all phases of plant lifecycle. The application example of a steam cracker shows which parts of this vision can be implemented now already.**

***Keywords*— digital twin, simulation, steam cracker**

I. Living with a Digital Twin

The term „digital twin" triggers a lot of associations. Human twins share a common genetic makeup, similar character traits and often surprising parallels of their path of life. Today there is still a large gap between the attraction of the term "digital twin" (more than 500 million links at Google) and the number of real-world applications. However, "digital twin" is already more than a buzzword for process industries. There are already a lot of different technical concepts, and there are already the first steps of real implementations. The intention of this paper is to explain terminology, functions and benefits of digital twins in context of process industries, and to demonstrate practical use cases along several phases of plant lifecycle. Although there are different concepts of digital twins in discrete manufacturing industries, they share the main general idea.

At a first glance, the number of different types of digital twins is confusing. Typical terms like

- Digital product twin
- Digital automation twin
- Digital production twin
- 3D digital twin
- Asset digital twin

The digital twin includes planning data from design and engineering phase, plant data from operation phase, and description of plant behavior in form of models. The individual simulation models, that are part of the digital twin, are dedicated to their specific purpose and fulfill the precision requirements of this purpose. The digital twin evolves – in parallel to the real twin – along the lifecycle of the plant, and it integrates in each phase the actual data and the actual knowledge. It does not only allow to describe plant behavior, but it also allows to develop solutions for the real plant [1].

Many individual parts of the digital twin are already state of the art. New perspectives are now opened by the idea to integrate the individual models and simulation tools to a holistic, semantically integrated system, integrated across different hierarchy levels of the plant, and integrated along all phases of plant lifecycle.

A. Models and Simulation along the Lifecycle of a Process Plant

Each simulation can be considered as a virtual experiment, with the aim to achieve a better understanding of the real system. The system is modelled with its relevant properties such that finally a mathematic description is realized that is sufficiently precise to run a computer simulation. The development of a simulation model is driven by a specific purpose and is in this sense context-specific, i.e. it serves to answer specific questions. A model can describe the physical, chemical, energetic and/or the information technological behavior of the plant.
Today, simulations are used in all phases of plant lifecycle more or less frequently. Simulations can be classified into the following groups:

- Design simulations
- Simulations for virtual commissioning
- Simulations for operator training systems (OTS)

Pfeiffer, B.; Oppelt, M.; Leingang, C. (2019): Evolution of a Digital Twin for a Steam Cracker

A single integrated modelling environment ACROSS the PROCESS LIFECYCLE

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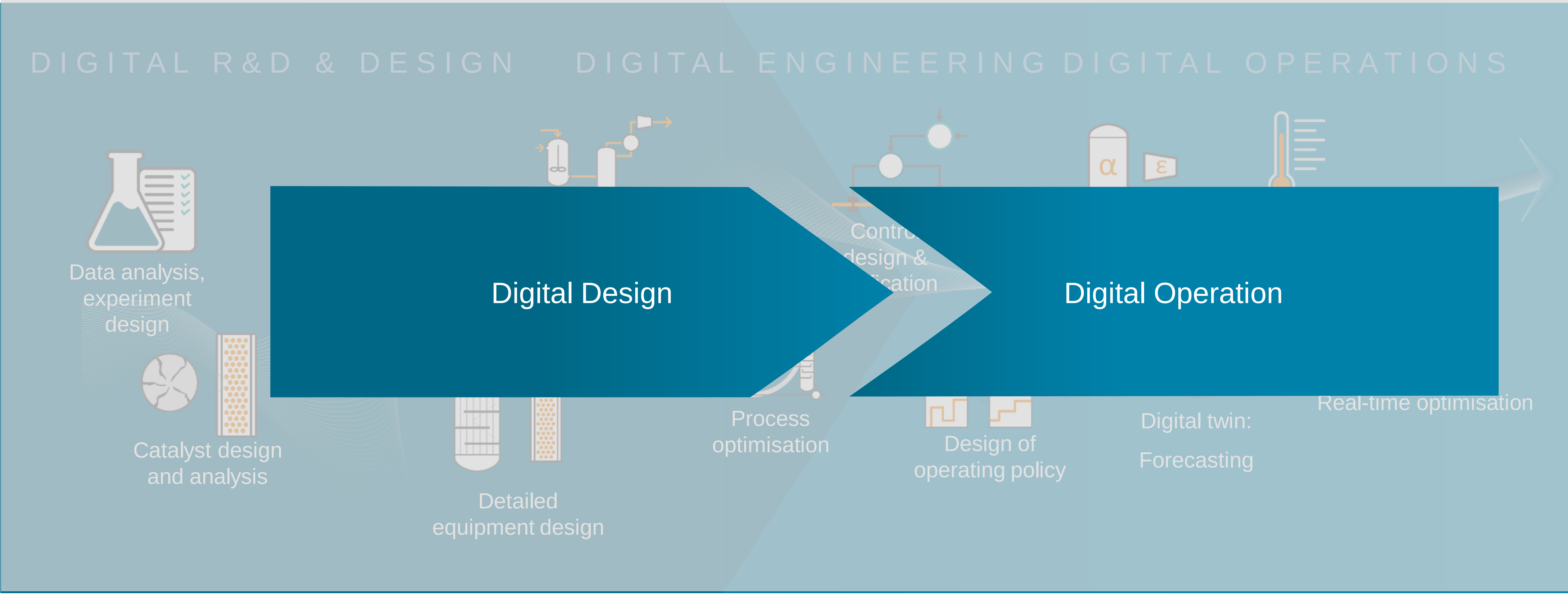

Digital Design

Integrated engineering extend by detailed process simulations

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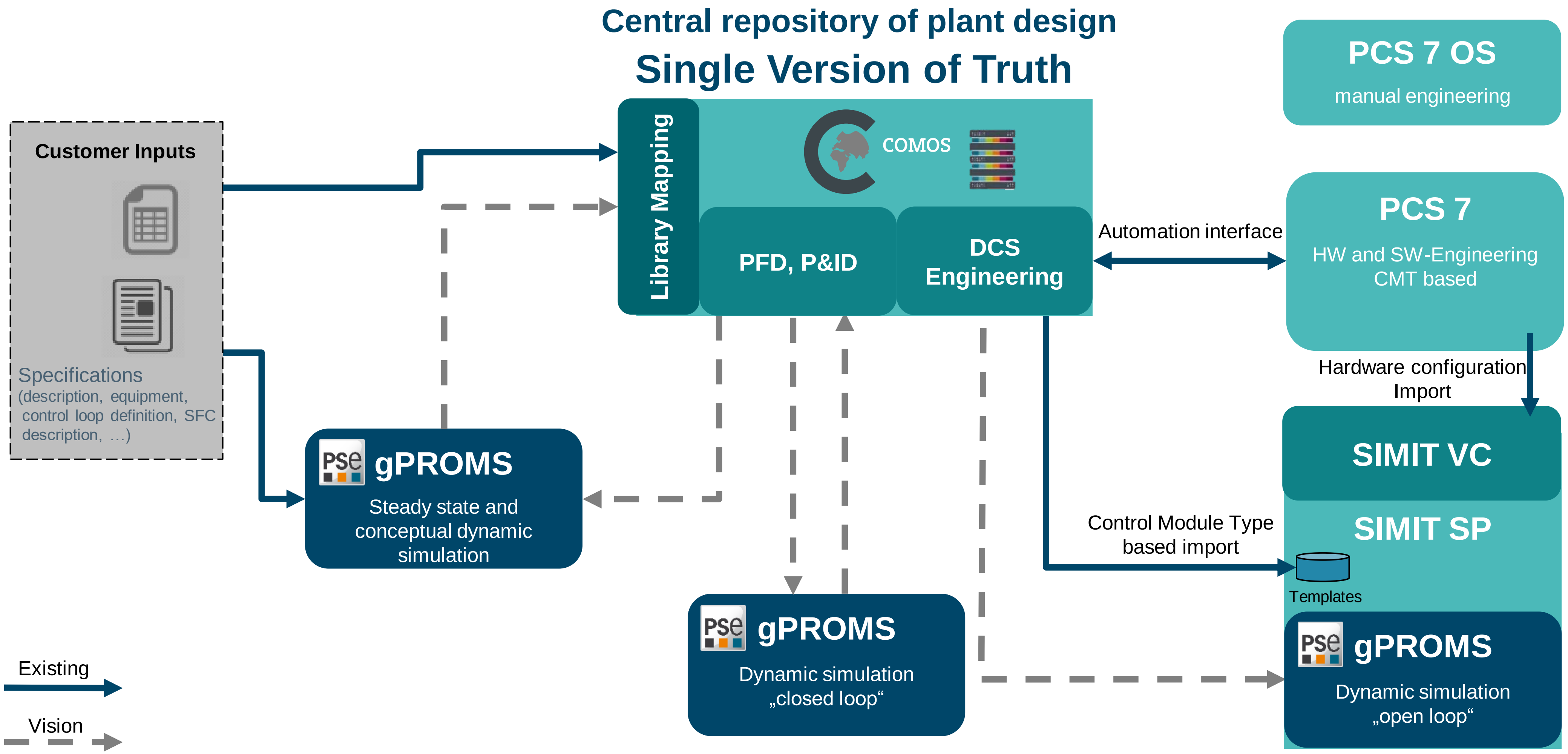

Overview of Ethylene Plant

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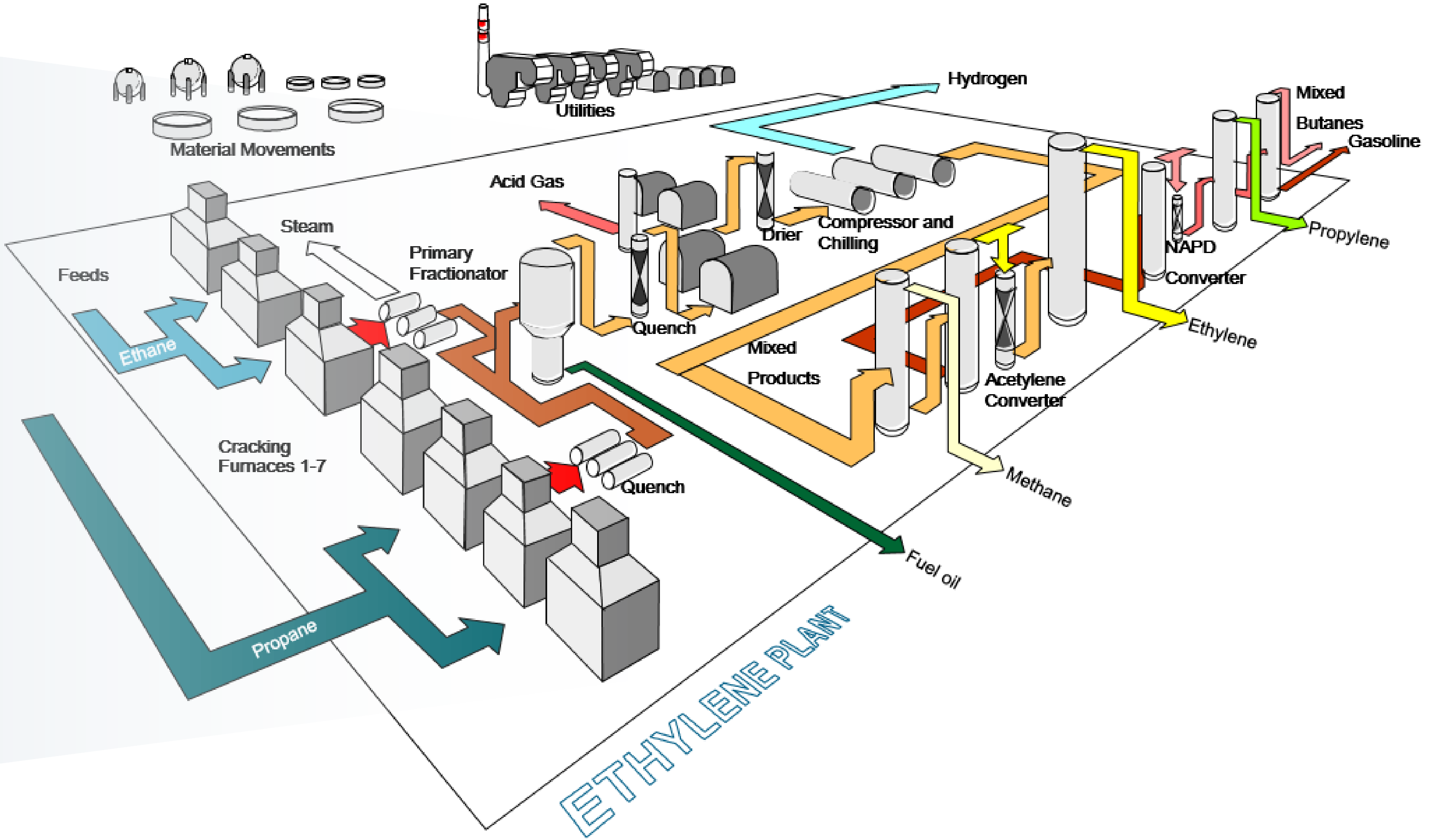
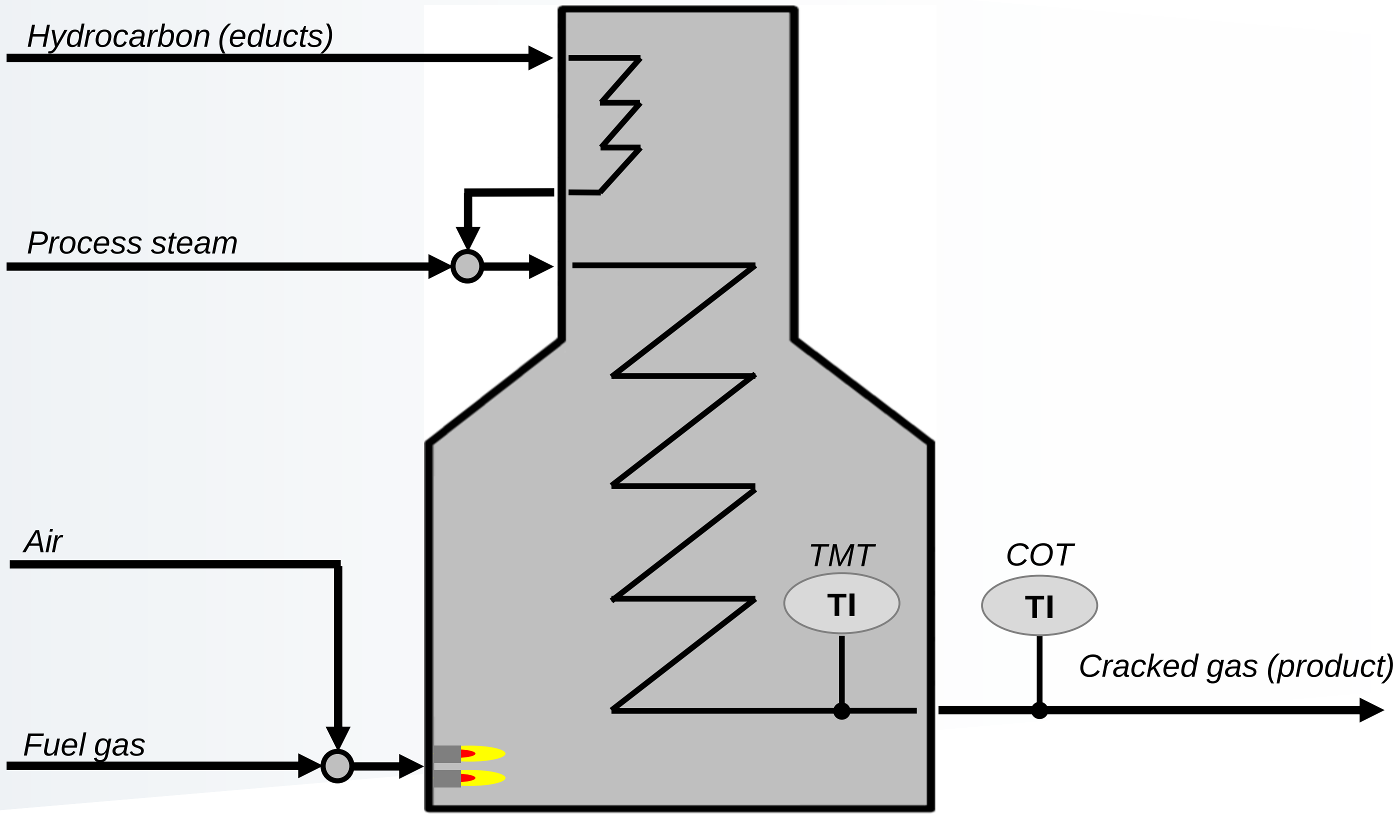
Raw materials
- Ethane, propane and/or naphtha
- Several **steam crackers** in parallel
- Multi-stage **separation process** with distillation columns, flash tanks, coolers and similar units

Products
- Ethylene, propylene, methane, hydrogen
- are used to produce intermediates for polymers (e.g. polyethylene), varnishings, solvents or herbicides



Steam Cracker

- Steam cracker: tubular reactor with numerous coils, belongs to the most complex unit operations in petrochemicals
- Educts are mixed with steam and heated to temperatures of about 840°C
- Long-chain hydrocarbon molecules are transformed in seconds by thermal cracking
- High throughput, high economic value → **any optimization potential has to be exploited!**



Steam Cracker: Challenges

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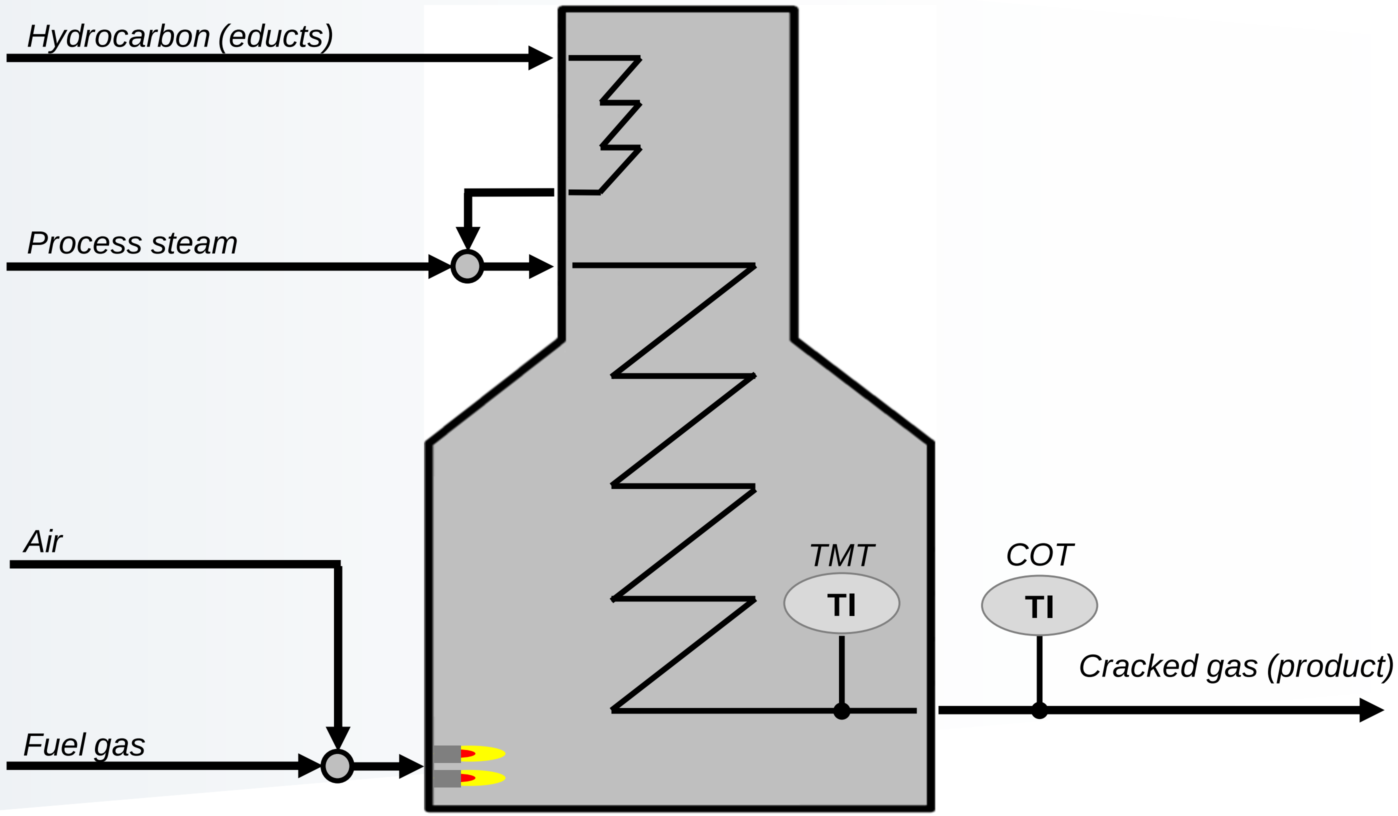
Yield

- Depends on a lot of influencing factors → multi-variable control problem
- Cannot be measured directly at cracker outflow, but only in summary and with large delay after cooldown

Severity

- Describes the actual degree of thermal cracking, quantified by the ratio of certain concentrations
- Not directly measurable either

→ Online estimation by **soft sensor**



Steam Cracker: Challenges

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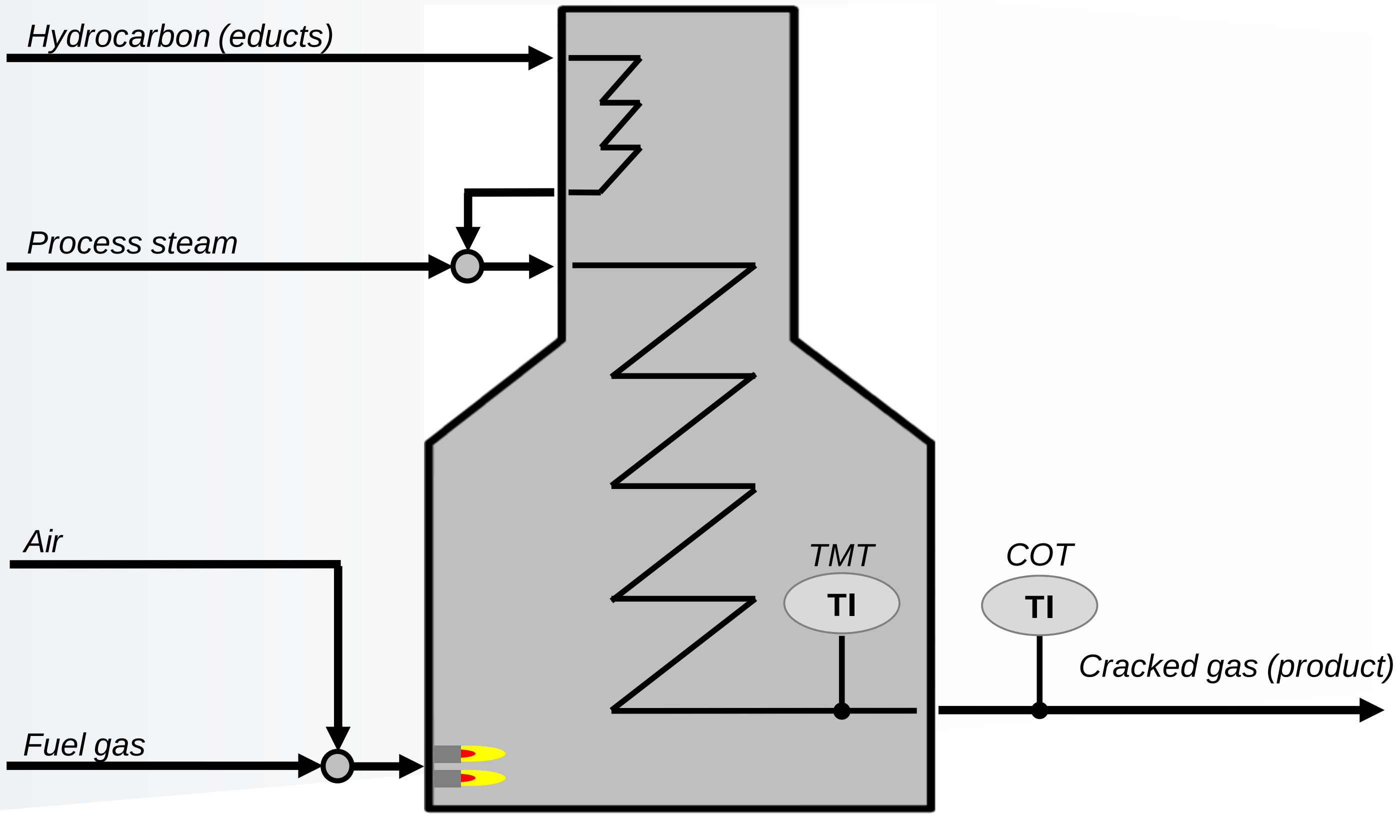
Coking

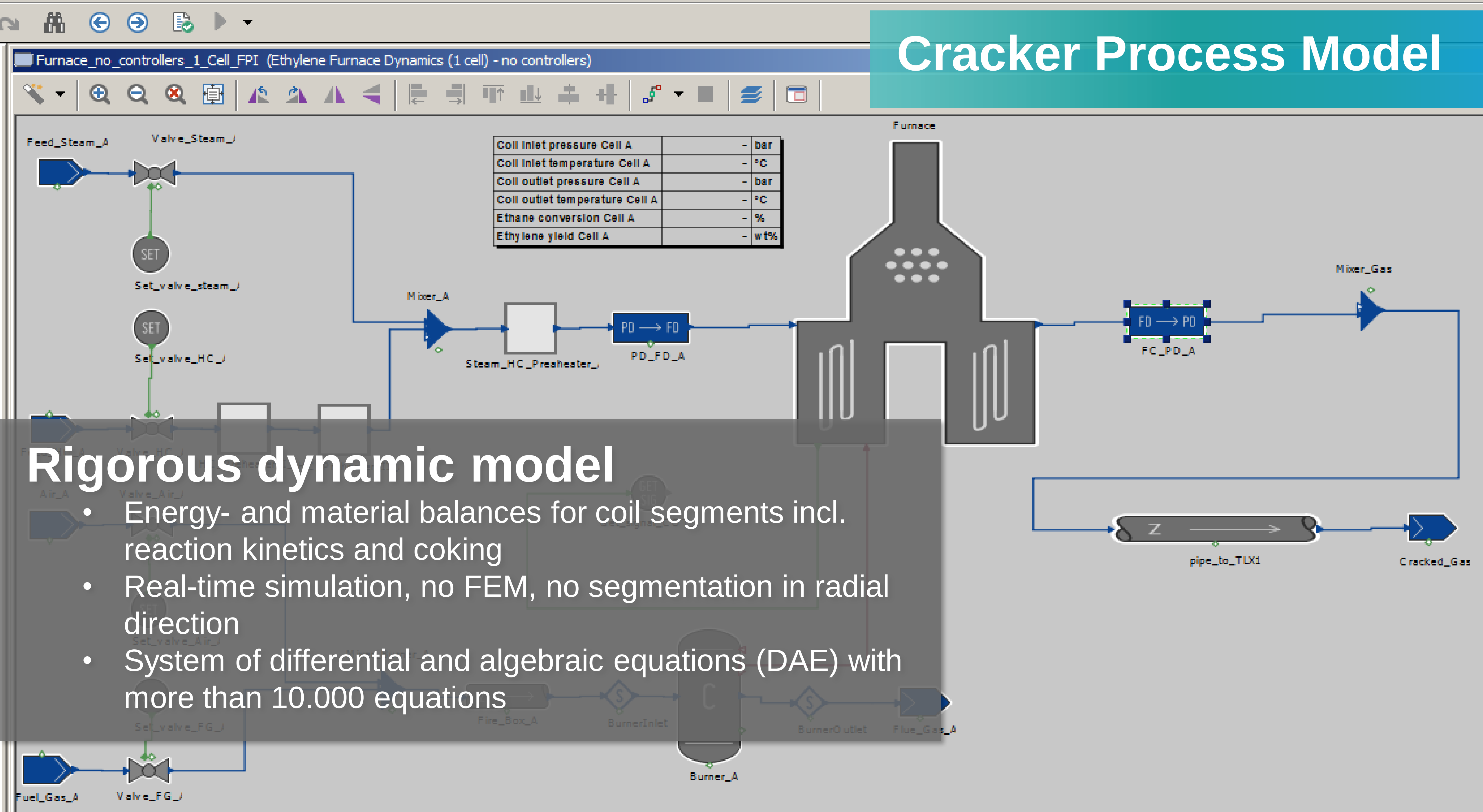
- Builds up at inside of coils
- Reduces heat transfer
- Reduces yield
- Planning of maintenance works → online estimation of actual coking state

Pass-balancing

- Keep all coils (“passes”) at same COT („Coil Outlet Temperature“) despite different state of coking



Cracker Process Model



Rigorous dynamic model

- Energy- and material balances for coil segments incl. reaction kinetics and coking
- Real-time simulation, no FEM, no segmentation in radial direction
- System of differential and algebraic equations (DAE) with more than 10.000 equations

Digital Operation –

Application example ethylene steam cracker

Multi-Level Solution Concept

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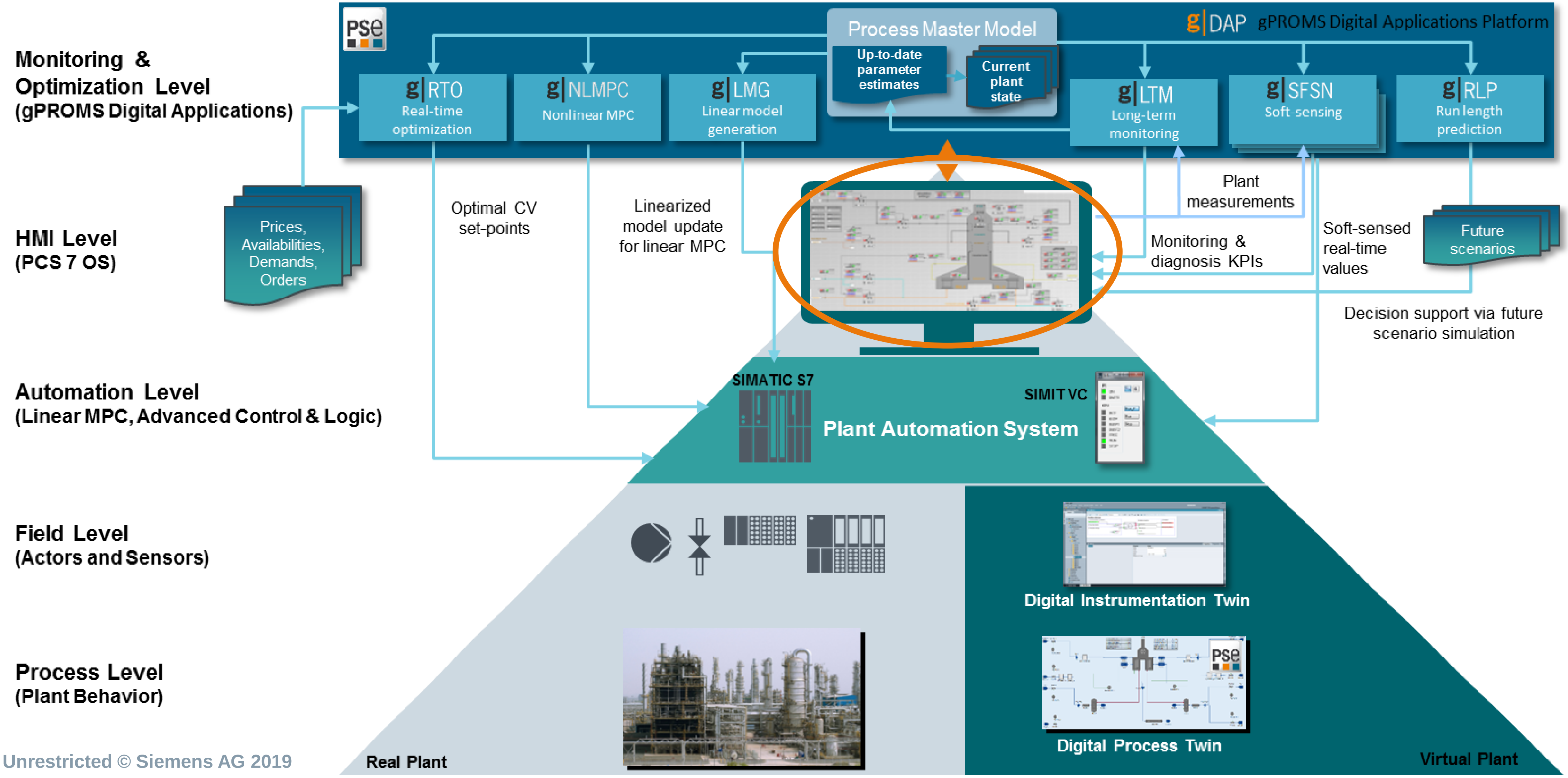

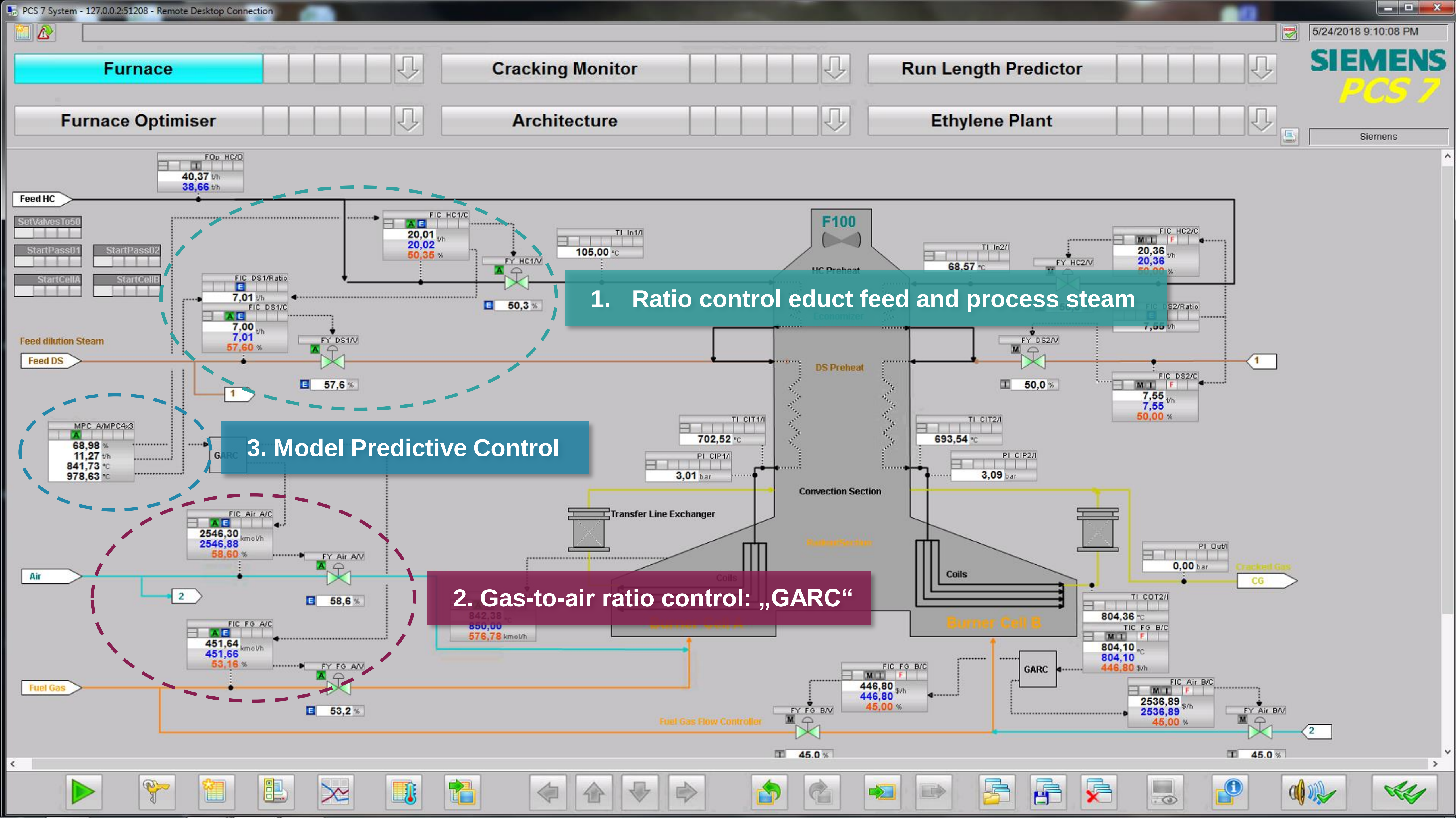
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Feed dilution Steam
Feed DS
Air
Fuel Gas
F100
DS Preheat
Convection Section
Transfer Line Exchanger
Coils
Burner Cell B
GARC
Fuel Gas Flow Controller
CG
1. Ratio control educt feed and process steam
3. Model Predictive Control
2. Gas-to-air ratio control: „GARC“

Multi-Level Solution Concept

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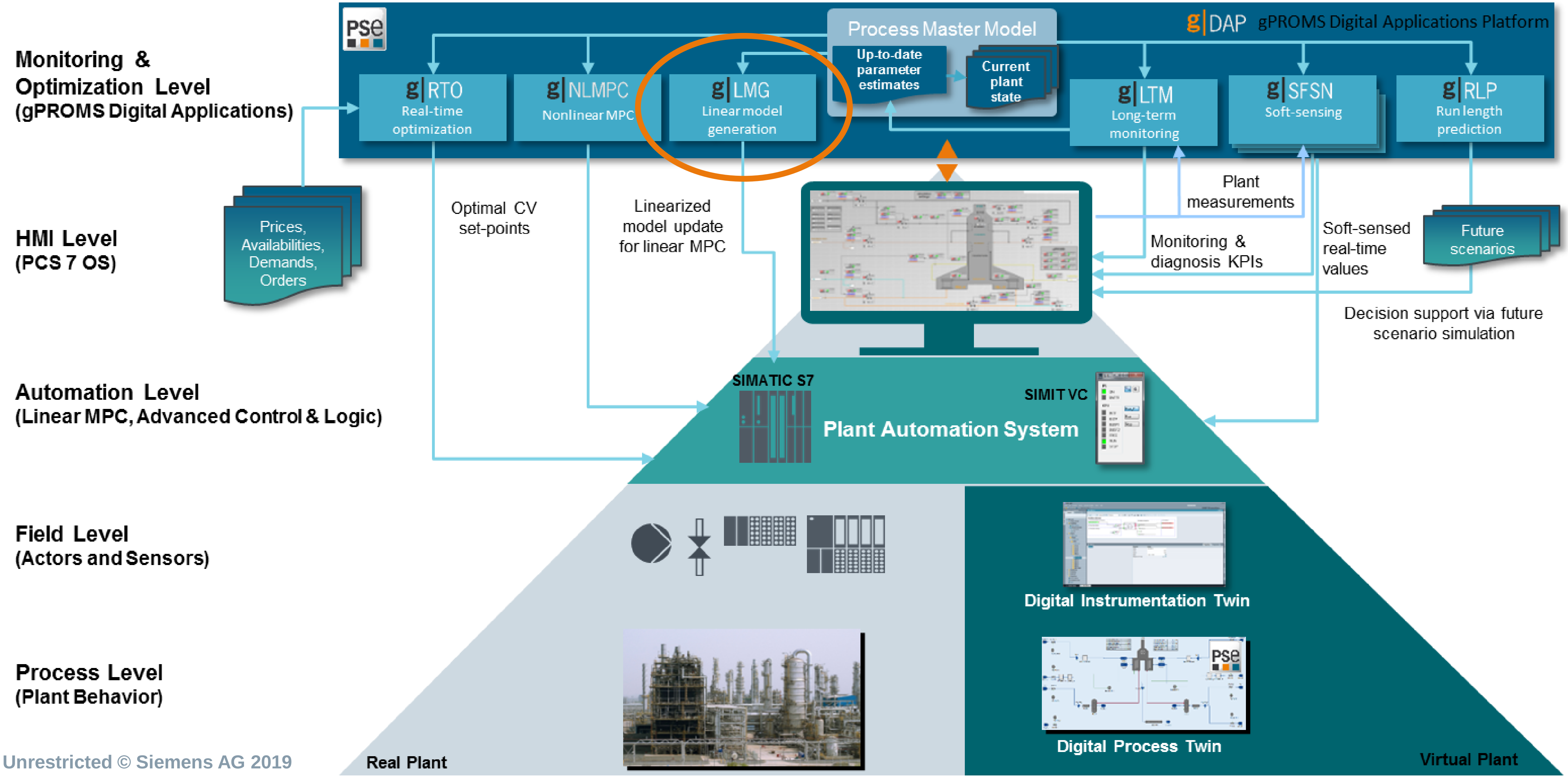
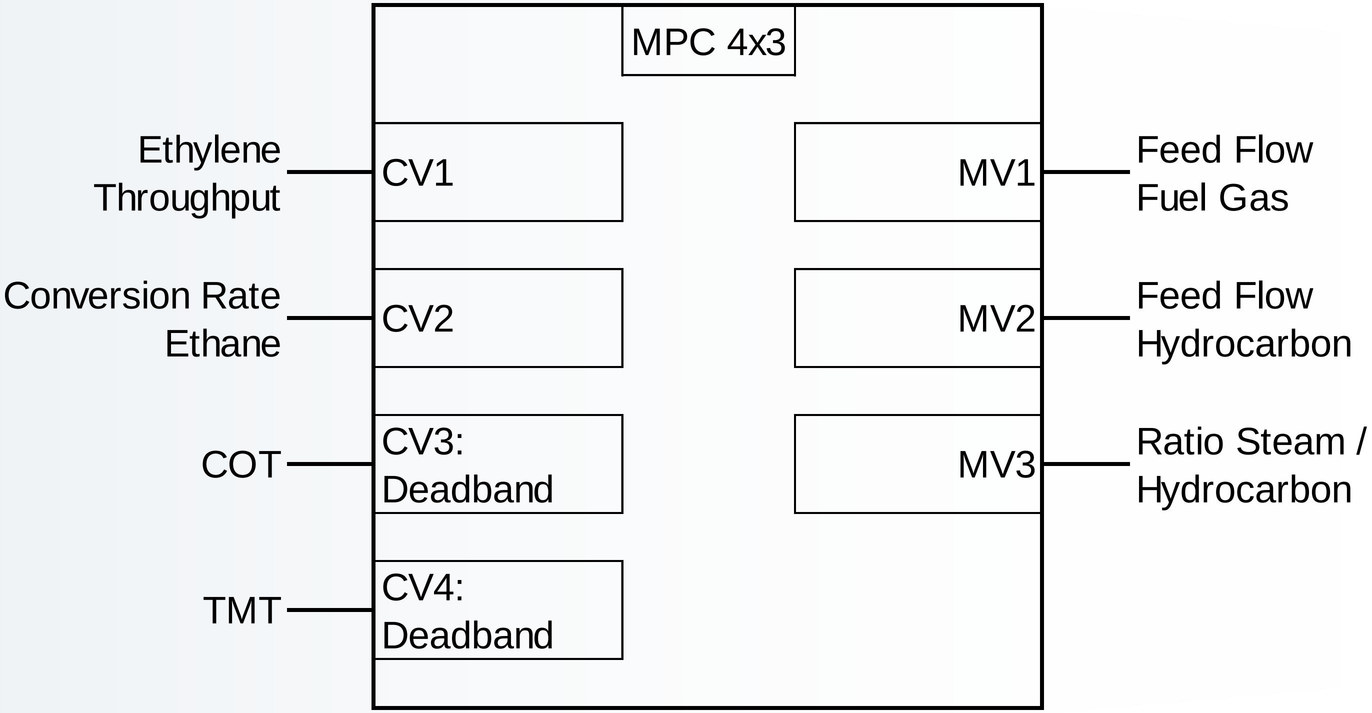


MPC Concept

Tasks to be solved by MPC

- **Production**: drive ethylene throughput to specified setpoint
- **Product quality:** keep conversion rate ethane (~ severity) at setpoint
- **Limit coking**: keep COT (Coil Outlet Temperature) in specified range
- **Safe plant operation:** keep TMT (Tube Metal Temperature) below critical upper limit
- Find **suitable combination of setpoints** for hydrocarbon feed, process steam and fuel gas



Multi-Level Solution Concept

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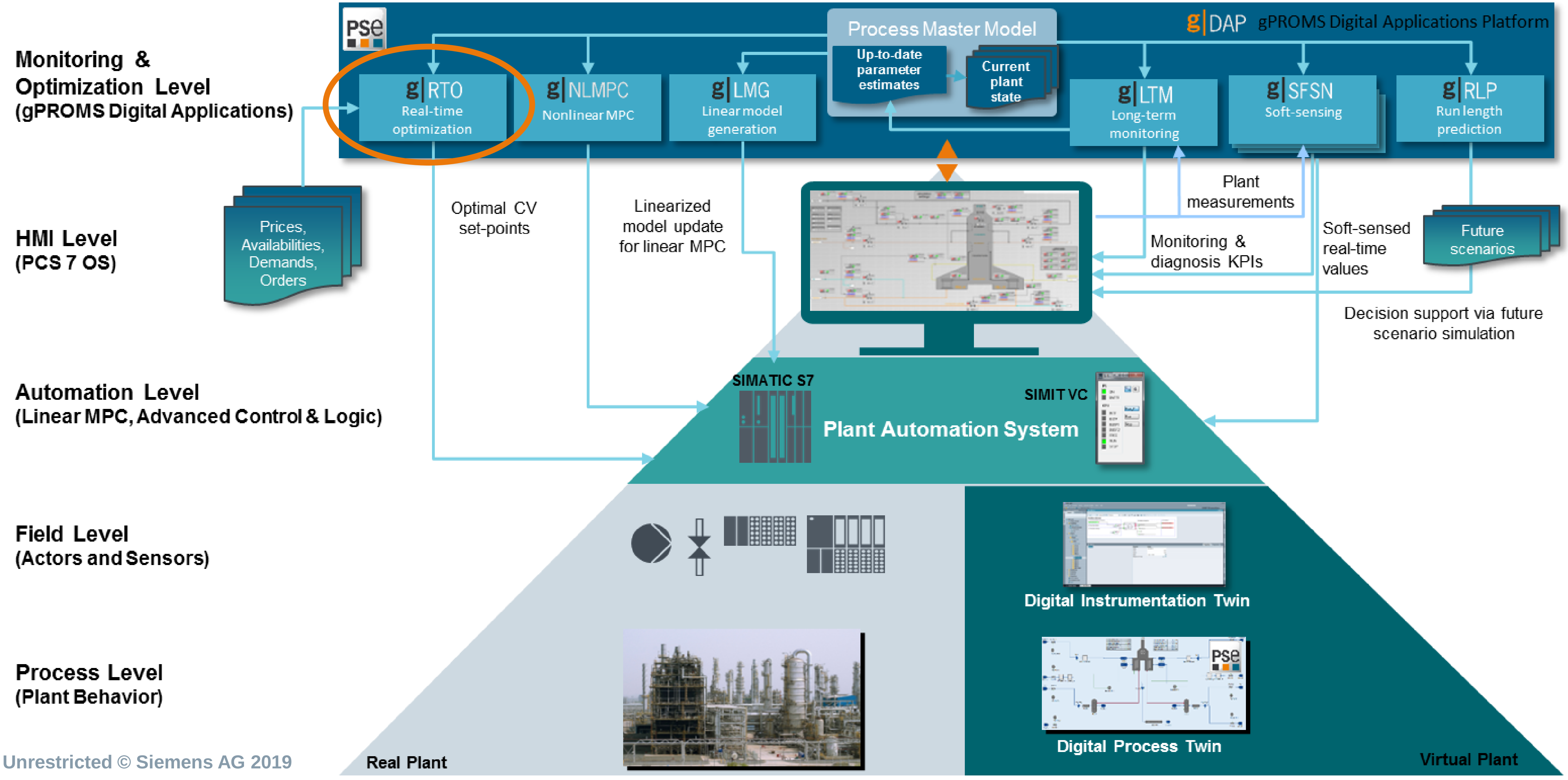
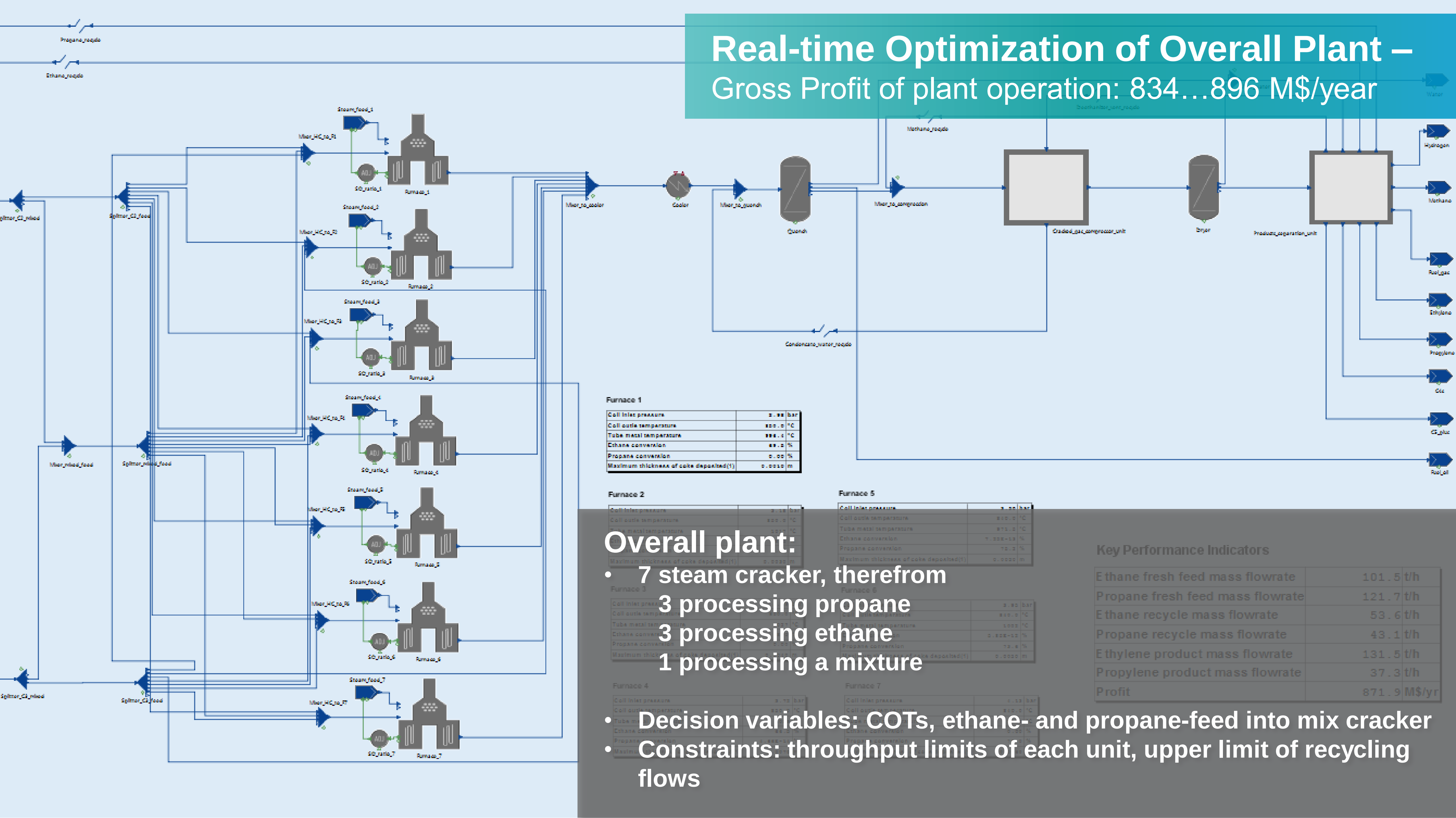


Real-time Optimization of Overall Plant –

Gross Profit of plant operation: 834…896 M$/year



Overall plant:

- 7 steam cracker, therefrom
  - 3 processing propane
  - 3 processing ethane
  - 1 processing a mixture

Key Performance Indicators

Ethane fresh feed mass flowrate	101.5	t/h
Propane fresh feed mass flowrate	121.7	t/h
Ethane recycle mass flowrate	53.6	t/h
Propane recycle mass flowrate	43.1	t/h
Ethylene product mass flowrate	131.5	t/h
Propylene product mass flowrate	37.3	t/h
Profit	871.9	M$/yr

- Decision variables: COTs, ethane- and propane-feed into mix cracker
- Constraints: throughput limits of each unit, upper limit of recycling flows

Summary

Rigorous **process model can be used**
- at different levels of solution concept
- in all phases of plant lifecycle

Digital Twin
- Integration of several models and software tools that up to now have been considered isolated: online communication and common data management
- Amortization along complete plant lifecycle, including economic benefit in plant operation phase

Digital twin for **steam cracker**
- Process model in gPROMS (PSE)
- Device model, coordination und PLC-emulation in Simit simulation platform
- Base layer automation, MPC und operator station in DCS SIMATIC PCS 7
- Soft sensor, run length prediction and plantwide RTO in gPROMS

Solution concept and **implementation** in software demonstrator are available for discussions

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