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

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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 shown, which parts of this union can be implemented now already.

Keywords—digital twin, simulation, steam cracker

1 LIVING WITH A DIGITAL TWIN

The term "digital twin" triggers a lot of association. 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 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 modeled with its relevant properties such that finally a mathematical 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 operation training systems (OTS)

...
A single integrated modelling environment ACROSS the PROCESS LIFECYCLE

Digital Design

- Data analysis, experiment design
- Catalyst design and analysis
- Detailed equipment design
- Digital twin: Health monitoring
- Digital twin: Soft-sensing
- Digital twin: Forecasting
- Digital twin: Real-time optimisation
- Digital twin: Health monitoring
- Digital twin: Soft-sensing
- Digital twin: Forecasting
- Digital twin: Real-time optimisation
- Process optimisation
- Design of operating policy
- Control design & verification

Digital Operation

- Digital twin: Real-time optimisation
- Design of operating policy
- Control design & verification
- Process optimisation
- Detailed equipment design
- Catalyst design and analysis
- Digital twin: Soft-sensing
- Digital twin: Forecasting
- Digital twin: Health monitoring
Digital Design
Integrated engineering extend by detailed process simulations

Central repository of plant design
Single Version of Truth

Customer Inputs
Specifications (description, equipment, control loop definition, SFC description, …)

Library Mapping
PFD, P&ID
DCS Engineering

PCS 7 OS
manual engineering

PCS 7
HW and SW-Engineering
CMT based

SIMIT VC
Hardware configuration
Import

SIMIT SP
Templates

Control Module Type
based import

PCS 7 OS

Automation interface

gPROMS
Steady state and conceptual dynamic simulation

gPROMS
Dynamic simulation „closed loop“

gPROMS
Dynamic simulation „open loop“

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Overview of Ethylene Plant

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

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

**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
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
2. Gas-to-air ratio control: "GARC"

3. Model Predictive Control

1. Ratio control educt feed and process steam
Multi-Level Solution Concept

- Monitoring & Optimization Level (gPROMS Digital Applications)
  - RTO: Real-time optimization
  - NLMP: Nonlinear MPC
  - LMG: Linear model generation
  - DAP: gPROMS Digital Applications Platform
- HMI Level (PCS 7 OS)
- Automation Level (Linear MPC, Advanced Control & Logic)
- Field Level (Actors and Sensors)
- Process Level (Plant Behavior)

Plant Automation System

Digital Instrumentation Twin

Digital Process Twin

Real Plant

Virtual Plant

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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

![MPC Diagram](image-url)
Multi-Level Solution Concept

HMI Level
(PCS 7 OS)

Automation Level
(Linear MPC, Advanced Control & Logic)

Field Level
(Actors and Sensors)

Process Level
(Plant Behavior)

Monitoring & Optimization Level
(gPROMS Digital Applications)

Optimal CV set-points
Linearized model update for linear MPC

Real-time optimization
Nonlinear MPC
Linear model generation

Plant measurements
Soft-sensed real-time values

Future scenarios

Digital Instrumentation Twin

Digital Process Twin

Real Plant

Virtual Plant

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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

- 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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