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Industrial and digital innovations research group

Hybrid Workshop

Twin Digital and Green Transition to a Resilient Economy

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Process Modelling and Simulation for Industrial Cognitive Digital Twins

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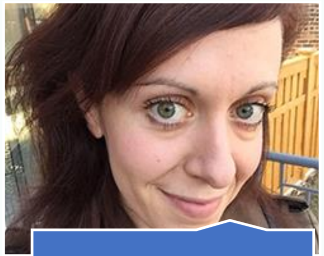
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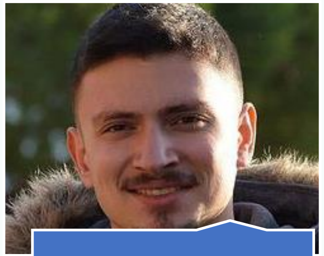
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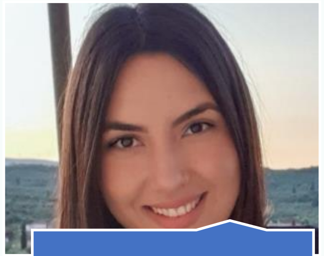
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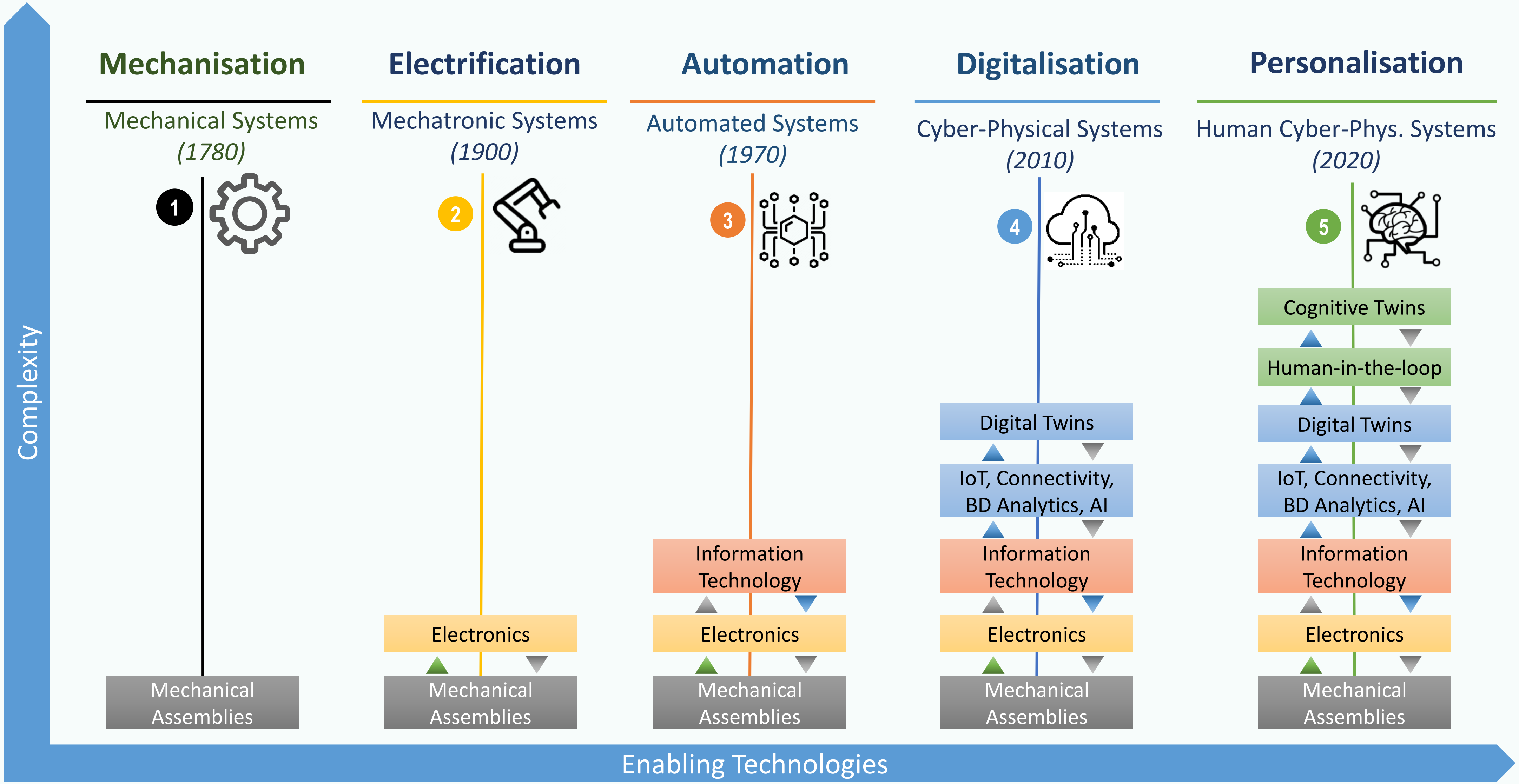
Presentation Outline

1. Twin Transition of Industry

Industrial Evolutions



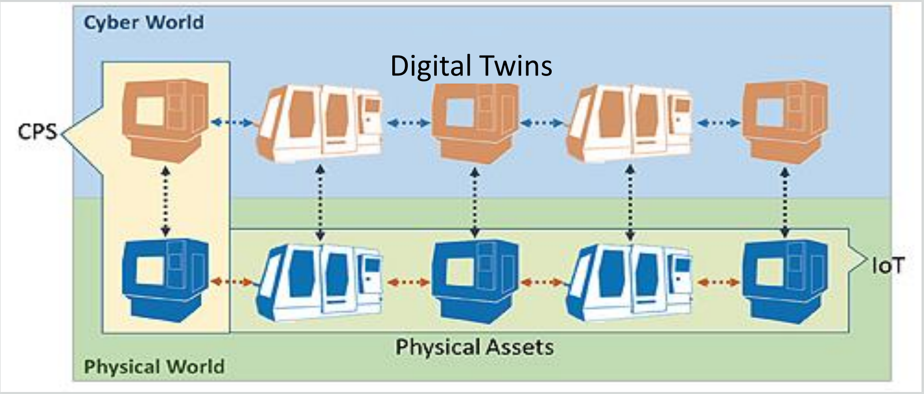
Pressure Factors that Create Challenges

Pushing Industry Towards Increased Digitalisation

1. Pressure for environmental **sustainability** and minimization of the consumption of non-replaceable resources
   - Drives a trend for accountability, assessment and prognosis of the use of resources and any parameter, factor, condition and contingency related to the maximisation of resource efficiency
2. Pressure for quick and economically sustainable adaptation to changing technologies, market conditions and trends (**agility**)
   - Targets value chain connectivity, interoperability, supply & demand balancing, cost minimisation, production/product optimisation, marketability of products and social acceptance of production and supply chains

Core Digitalisation Concepts

Paradigms Characterising Industrial Digitalisation

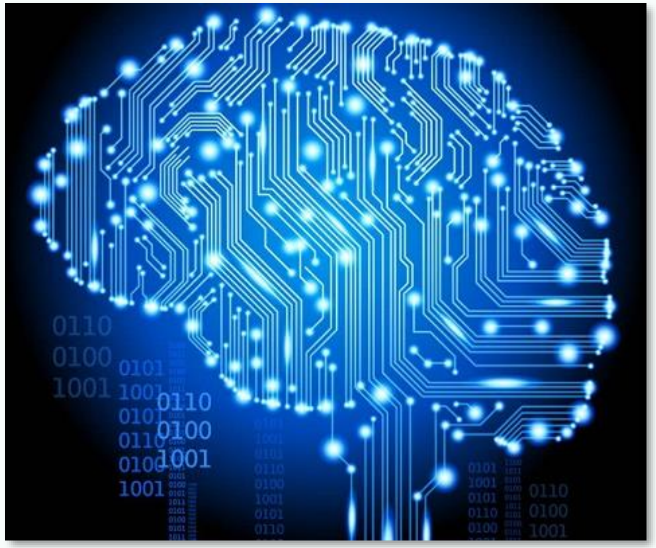


- **Cyber-Physical Systems (CPS)**: Networked systems with embedded sensors, processors, and actuators that can sense and interact with the industrial environment (including human) and provide real-time services
  - General Directive: The tighter the coupling of the digital part of the CPS to its physical system (production, supply chain), the better
  - Necessities: (i) Accurate and holistic modelling and representation of the physical system in CPS' digital part; (ii) Dynamic representation, i.e. follow in time closely the physical system's evolution, state and behavior
- **Industrial Digital Twins (DT)**: Replicates digitally a production process, production line, factory and/or supply chain, accurately modeling it and its entities and simulating uniquely its state and behavior at any instance by being connected to it and updating itself in response to system changes

Why Cognition and Cognitive Models are Needed

Is the Future of Production Systems Cognitive?

- A cognitive entity is an entity that can process thought, acquire input knowledge and use it to solve problems all by itself
- A cognitive DT (or cognitive CPS) must analyse and “understand” the physical system’s state and behavior, so as to respond to its needs
  - At the factory level, digital cognition can enable proactive and reactive response to contingencies and optimize packaging, materials and logistics
  - At a higher level (supply chain), it can be used to monitor virtual production lines by connecting all involved stakeholders [and enable agile connected supply chains.



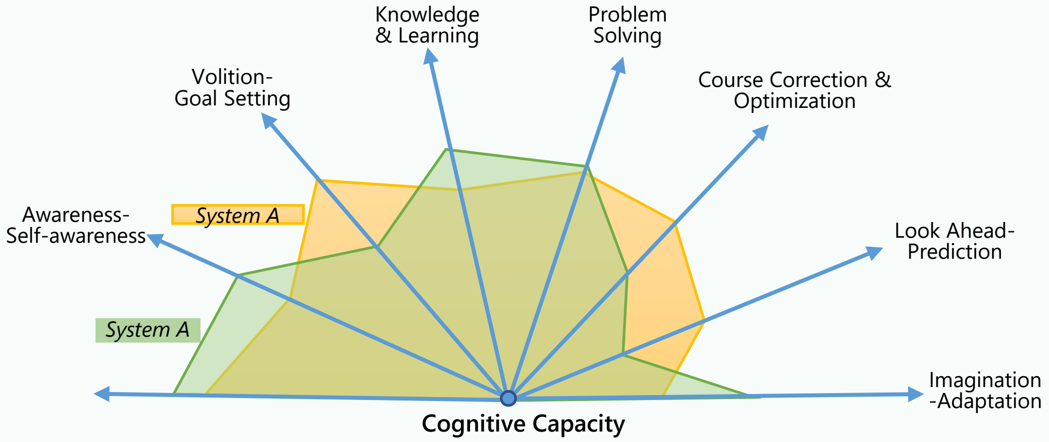
In order to support digital cognition, a cognitive modelling paradigm shift is needed to define novel system models with more complex structure and enhanced attributes

2. Cognitive Manufacturing

Semantics of Cognition

Cognitive Behavioural Vector (Attributes)

Cognitive technologies are ones that **mimic human brain functions**



1. Dynamic sensing provides comprehensive, concurrent and continuous views of environment and self, distinguishing between the two, with immediate recognition of changes
2. Awareness of self and others, as well as internal & external situations and events relevant to them
3. Volition motivated by setting/pursuing goals and evaluating/ assessing status against them
4. Memory of past **experiences** and learning, i.e. converting experiences into active new **knowledge**
5. Identification of problems, dangers, opportunities, unexpected events and finding **responses/solutions**
6. Improvement/optimisation of course towards a position or goal while minimizing risks and/or effort
7. Looking ahead to anticipate the **future**, even plan for resources, sustainability or contingencies
8. Adapting to changes in environment or own capacities/needs, using knowledge & imagination

Mapping Biological to Digital Cognition

Digital Cognition follows the Paradigm Human Cognition

#	Cognition Attributes	Map	Digital Cognition
1	**Senses/Views** *Self vs Environment*	→	Real-time monitoring enabling Dynamic behavior, Security, Edge analytics, Process calibration
2	**Awareness** *Situation vs Self*	→	Systemic & Value chain view, System dynamics, Big data analytics, Statistics & Visualization
3	**Volition – Goal Setting** *Understanding (set) vs Assess (pursue)*	→	Dynamic assessment & Self-assessment, Benchmarking, Business rules & Decision support
4	**Knowledge (past)** *Remember vs Learning*	→	Semantics, Knowledge engineering/representation, Databases, Machine learning
5	**Problem Solving (now)** Identifying vs Responding	→	Anomaly detection, AI inference & Root-cause analysis, Proactive & Reactive responses
6	**Course Correction/Optimization (now)** *Minimize Risk vs Effort*	→	Optimization algorithms and tools, Self-calibration, Expert rules
7	**Looking Ahead (future)** *Sufficiency vs Contingencies*	→	Prediction of inputs/outputs/key factors, Capacity planning, Production rescheduling
8	**Adaptability (to change)** *Environment vs Needs*	→	What-if evaluations, Scenario building & Simulation, Self-adaptation

Challenges

- (1–4) Environmental Sustainability ↓ Resource Efficiency
- (5–8) Economic Sustainability ↓ Agility

Cognition Supported by Modelling

Modeling Elements Needed for Providing Digital Cognition Enhancement

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Function / Cognitive Attribute	Additional Modeling Element Needed	Modelling Methodologies
1. Dynamic sensing	Ontology and related Data Model	▪ Knowledge Engineering
2. Awareness	System Entities' Relations and Agent-Based Modelling	▪ Knowledge Engineering
3. Volition – Goal Setting	Teleology and Performance	▪ Mathematical Modeling
4. Knowledge	Knowledge & Learning Representation	▪ Knowledge Engineering
5. Problem Solving	Inference Model & Causal Relationships	▪ Knowledge Engineering ▪ AI inference
6. Correction/Optimisation	Optimisation Problem Modeling	▪ Mathematical Modeling
7. Looking ahead	Modeling of Market Drivers & Trends	▪ Mathematical Modeling
8. Adapting	Systemic Simulation Modeling	▪ Mathematical Modeling

However, all cognitive attributes would need to be solidly based on a model of the dynamic, distributed and concurrent, processes of the production system

3. Modelling Methodology

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Mathematical Process Modelling Space

Continuous and Discrete Production Systems

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Industrial Process Modelling

Model Types

- Continuous Process Modelling
- Discrete Process Modelling

Model Components

Continuous Process Modelling

- Processes
- Production stages
- Resource stocks / warehouses
- Inputs – outputs
- Material / energy flows

Discrete Process Modelling

- Discrete Processes
- Buffers
- Inputs–outputs (with different multiplicities)
- Resource allocation
- Transfer equipment (cranes)
- Material / energy & information flows
- Priorities – conflict resolution policies
- Control actions
- Decision making
- Random Events (e.g. machine breakdowns)

Model Extensions

Continuous Process Modelling

- Whole factory
- Whole product's value chain
- Industrial complexes, Industrial symbiosis

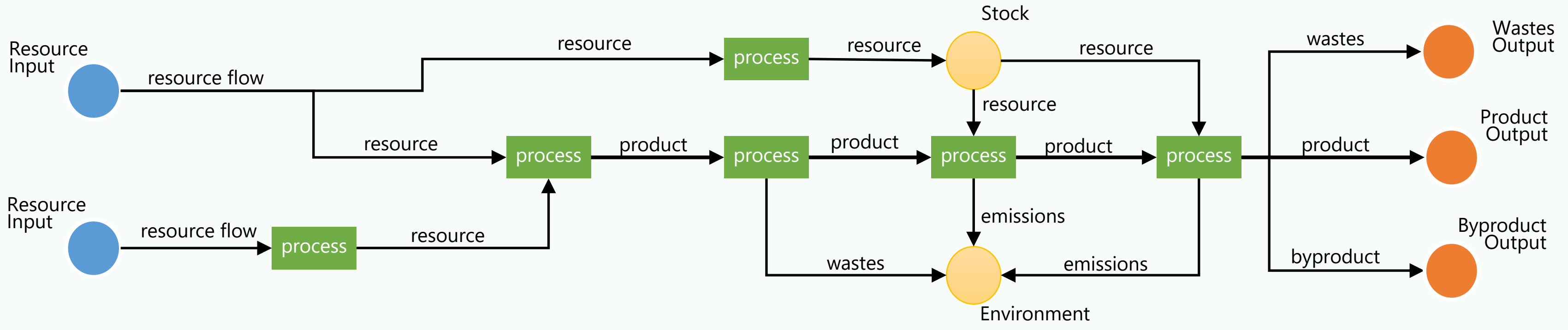
Discrete Process Modelling

- Sets of machines and equipment (e.g. cranes) that perform the same process
- Whole product's value chain

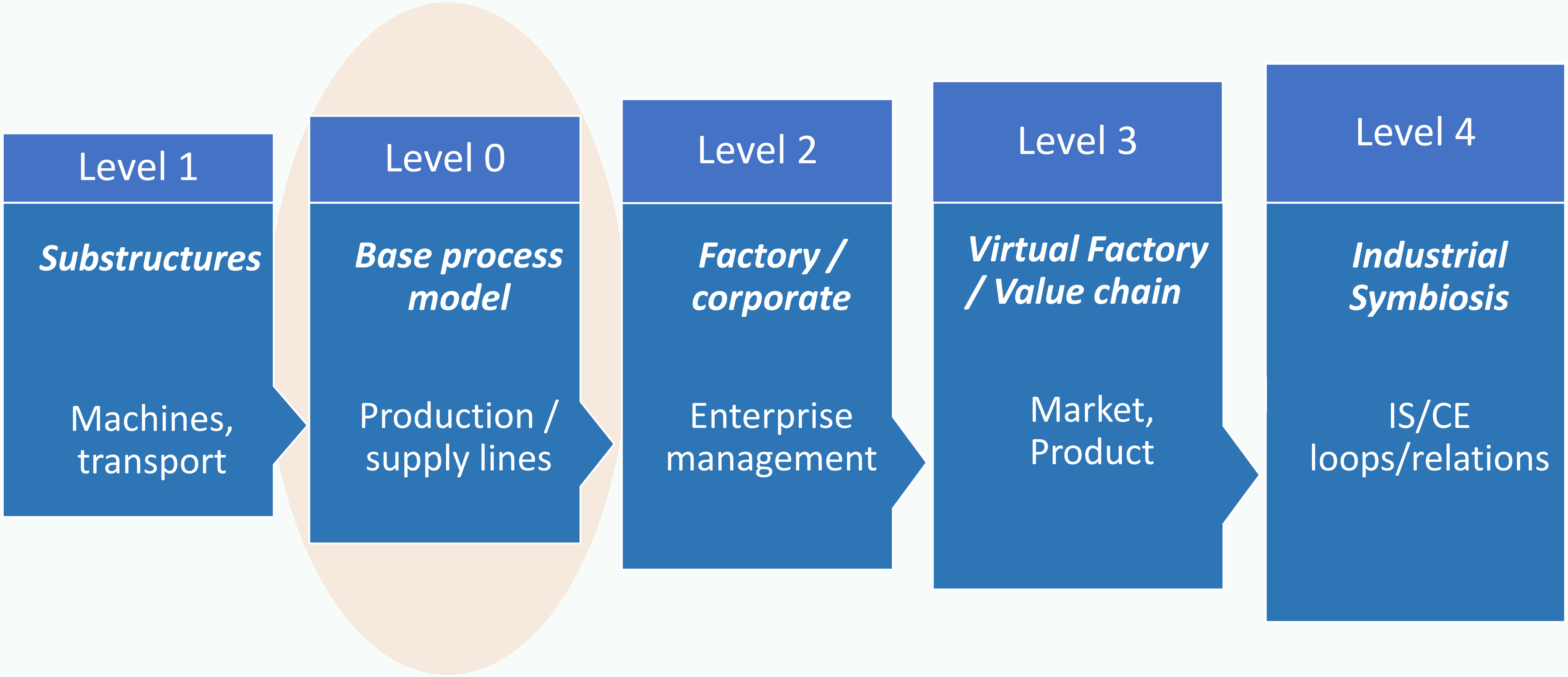
Process Modelling Schema

Representation of Production – Supply Processes

- Directed **Petri Net** process-flow representational schema
  - Production, pre-production and post-production processes are modeled mathematically as “**transitions**”
  - Systemic input or output points, stocks, warehouses, transshipments, product outlets, waste disposal, the physical environment, etc. are modeled as “**places**”
  - Material, energy, financial and/or informational flows as modelled as “**arcs**”
- Simplicity and strict mathematical definition, enabling easy implementation of simulations, optimizations and other computational procedures



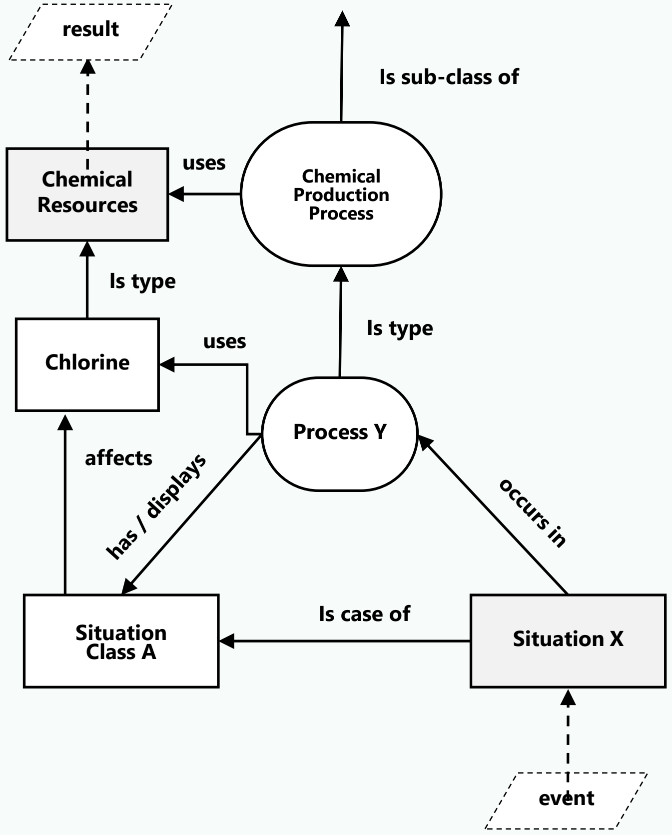
Systemic Extensions to Process Modeling



Modeling System Knowledge

Operational and Enterprise Procedures and Rules

- Knowledge Graph (KG) combines advantages of both expert systems and knowledge bases
  - Defined as a semantic data network that integrates knowledge into an ontology, which becomes its schema layer.
  - A collection of interlinked semantic descriptions of all relevant entity types of the industrial system and their relations are stored in a graph topology, with entities as vertices and their associations as edges.
- A KG represents knowledge in a semantic form that can be readily utilised by AI reasoning that can be integrated with the outlined process model



Simulation of Industrial Production Systems

- Simulation Engine implemented on top of the process model
  - Emulates certain cognitive functions of the human brain, such as the evaluation of consequences of considered actions, or the understanding of causes of past events
- The engine uses the underlying models as a test-bed
  - able to run simulations of very different spaces (system-wide or focusing on part of the system, or a single process) and time frames (just-in-time, product batch, hourly, daily)
  - use a hybrid simulation engine, able to select continuous, discreet and dynamic/agent-based simulation techniques, in any combination
- Executes scenarios, i.e. a complete virtual run of the production/supply system's model or part of it, with an optional set of modifications, for a sufficient or predefined virtual time period, starting from the current system state or a custom predefined state (e.g. a stored past state)
- Model flows, process state changes (optionally other system events also, e.g. contingencies, maintenance) are estimated and system status statistics are synthesised and aggregated to produce KPIs for assessment

4. Process Simulation Modelling Tools

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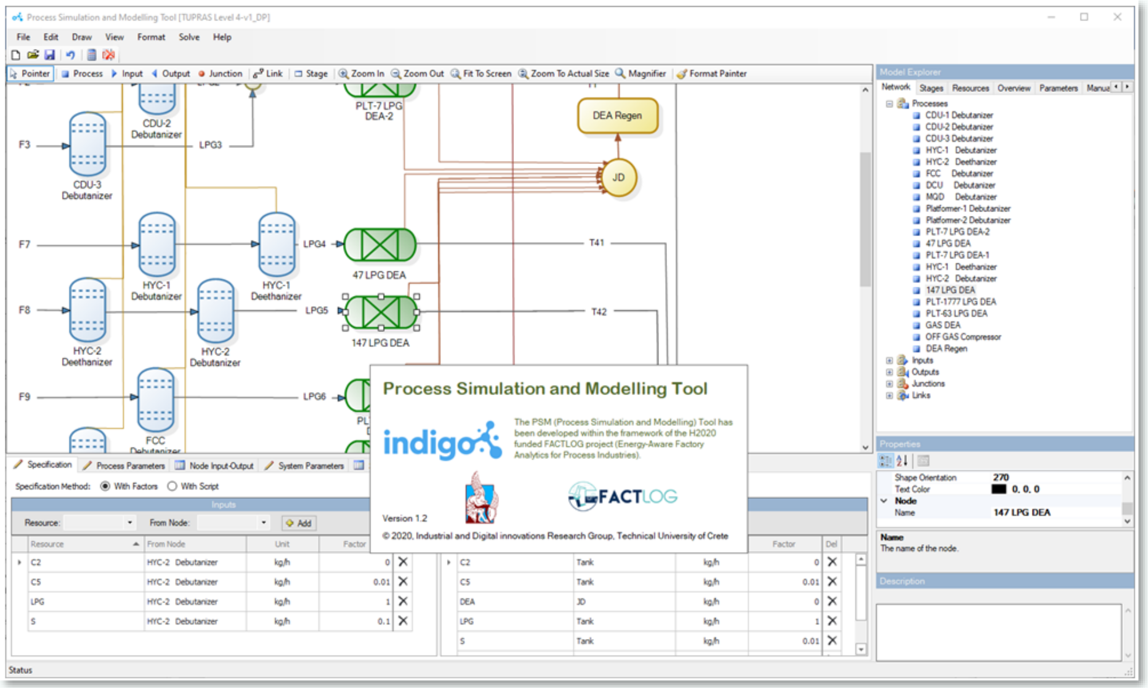
Process Simulation Modelling (PSM) Tool

- Tool developed by the TUC in order to address the requirements of FACTLOG and AquaSPICE research project
- Main functionalities :
  - model design, namely the representation of stages and processes taking place
  - process mapping, which includes the specification of resource flows to and from each process as well as the relations between input/output flows
  - calculation of the resources flow, with the simulation of the production process according to the specified parameters and constraints,
  - presentation and reporting of the results at different levels of the system



Model Based Cognitive Digital Twin Engine

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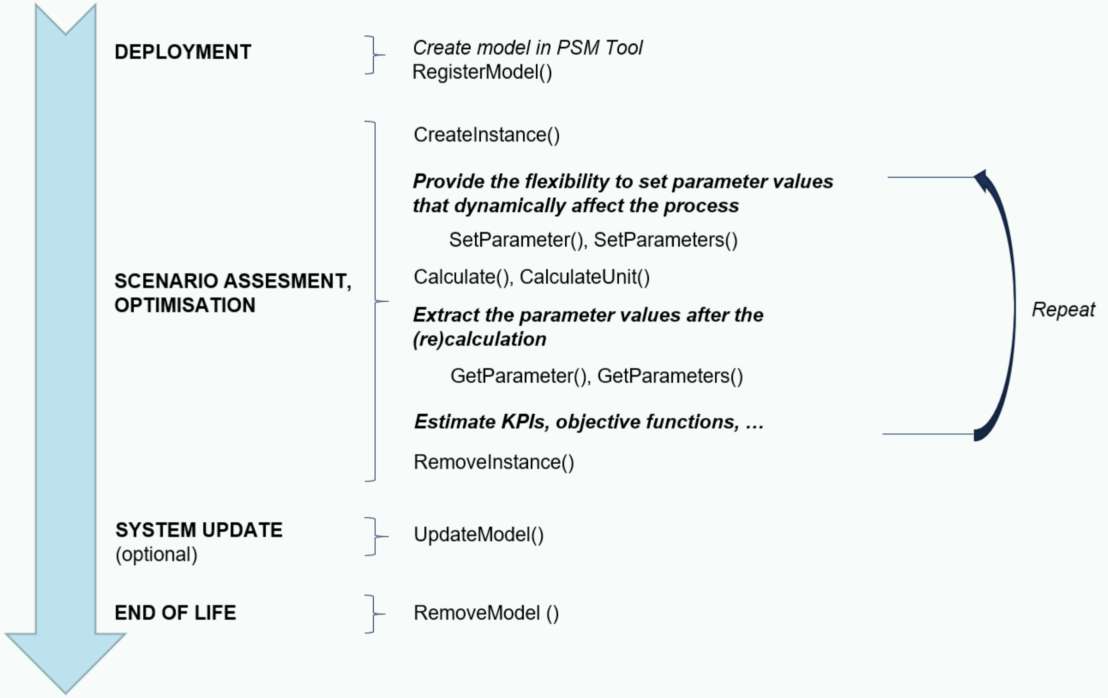
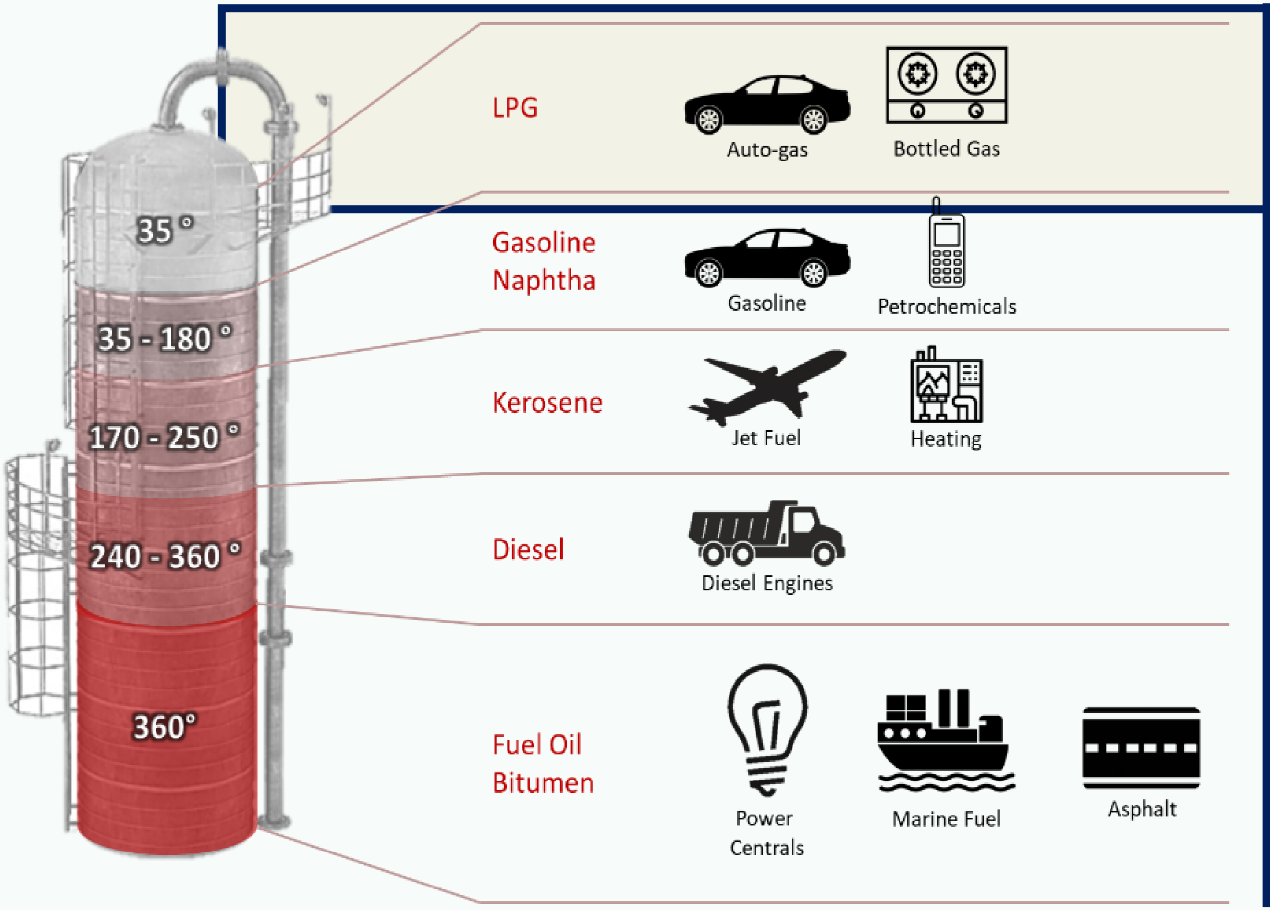
- The model is created using the PSM stand-alone Tool
- With the help of model management services, it is registered in the system
- Next step concerns definition of an instance at the specific time frame important for the specification, assessment or optimisation effort
- API provides the flexibility to set parameter values that dynamically affect the process
- When the values are set, we can run the simulation and read the calculated values
- With these results KPIs or objective functions can be calculated
- When calculations regarding the specific instance are finished, we can discard it
- Update of the system model is possible if necessary
- When experimentation is finished, the model can be completely removed from the system

Model Life-Cycle (methods exposed by API)



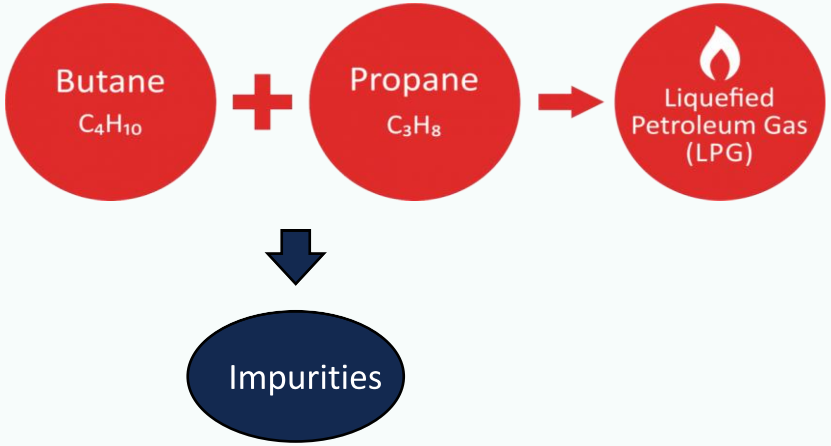
5. Application Example

Refinery – The LPG Value Chain



LPG – Liquified Petroleum Gas

	Total Impur.	Vapor Pressure	C5	C2	Sulphur
Spec's	%5 mol/mol	1430 kPa	%2 mol/mol	%0.5 mol/mol	50 mg/kg



LPG Purification Plant

10 LPG Debutanizer Units

6 LPG Sulphur Absorption Units

1 GAS Sulphur Absorption Unit

1 LPG Recovery Compressor

1 DEA Regeneration Unit

110 process sensor (temp., pres., flow, level)

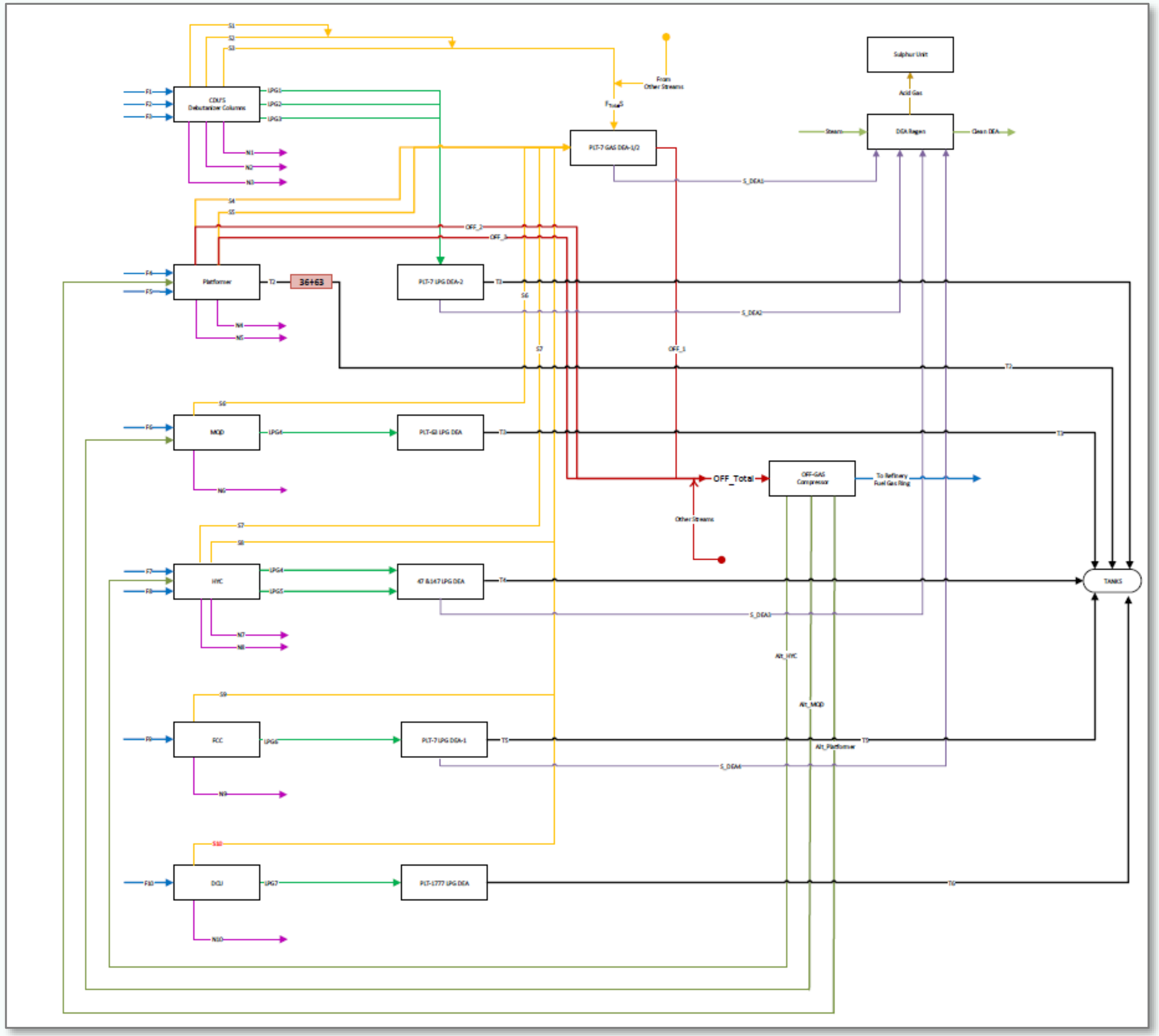
40 tank sensor (temp., level, flow)

4 online analyzer (Gas Chromatography, H2S)

35 lab analysis (H2S, sulphur, GC analysis)

1 Process engineer

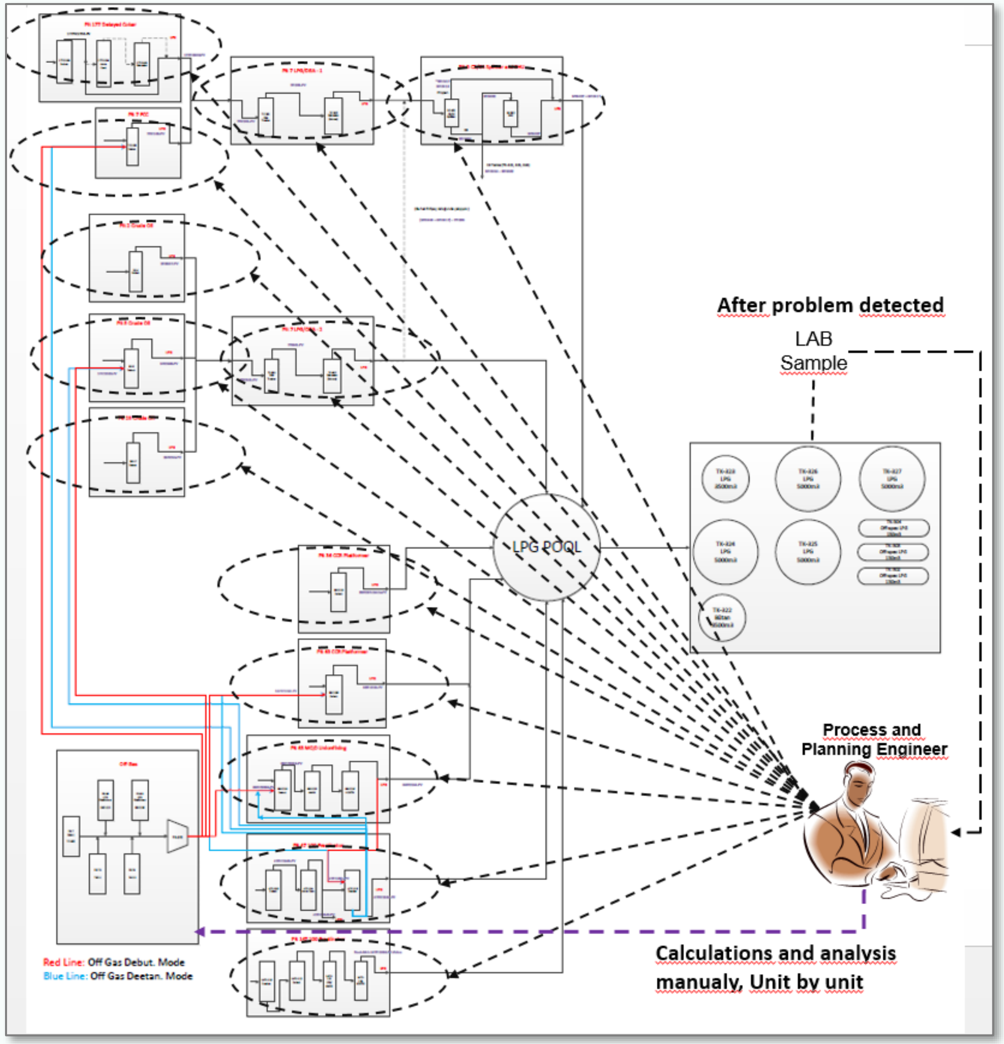
1 Planning Engineer

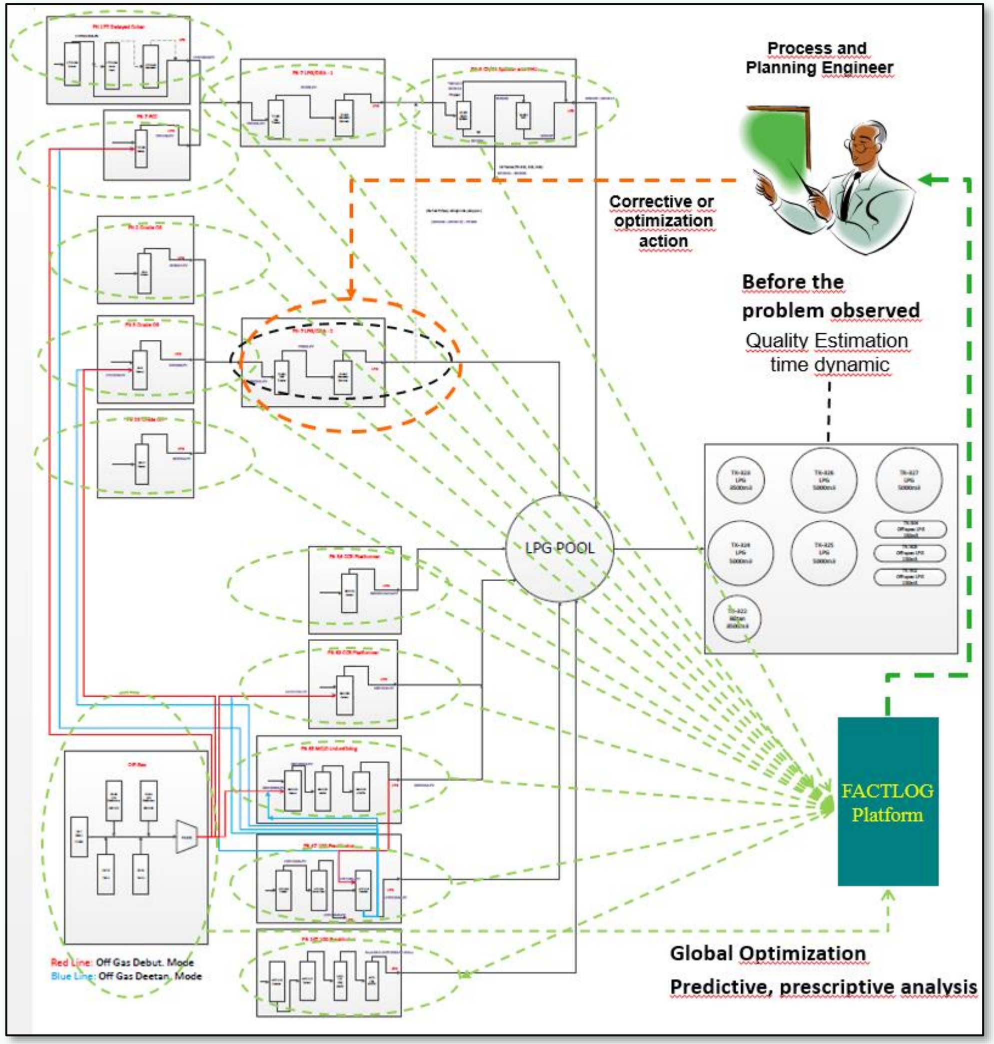


Main Business Challenges

- 24/7 production
- Lack off real time analysers, infrequent lab analysis
- Reprocess because of the off spec production
- Complex and integrated production line
- Each production unit has different dynamics
- Difficulty at troubleshooting and fault detection
- Time pressure

As-Is and To-Be Situation





Needs for Cognition

- **Monitor the production processes:**
  - All product **performance indicators** are based on **energy consumption and productivity**
- **Capture and predict events or anomalies and generate alerts:**
  - There are **event detection and prediction** based on **product qualities and energy consumption**, beyond given levels
- **Quantify the impact of identified events on the current plan:**
  - Making a **time-dependent estimation of the impact of the event** on product tanks and pattern of anomalies.
- **Provide alternatives for handling the events and evaluate these alternatives:**
  - Making **recommendations** to alleviate this impact on the final or intermediate production tanks, **globally optimizing processes** to improve energy efficiency and productivity.

Cognition Process

1 DETECT VARIATIONS

- Detect anomalies in the LPG composition by observing variations in the sensor and laboratory result readings
  - Predict the levels of impurities from sensor readings alone. Two possible approaches:
    - Regression: predict exact value
    - Classification: predict just the likelihood of going off-specs

2 UNDERSTAND VARIATIONS

- Understand the anomalies through context knowledge provided by Industry experts

3 UNDERSTAND THE IMPACT

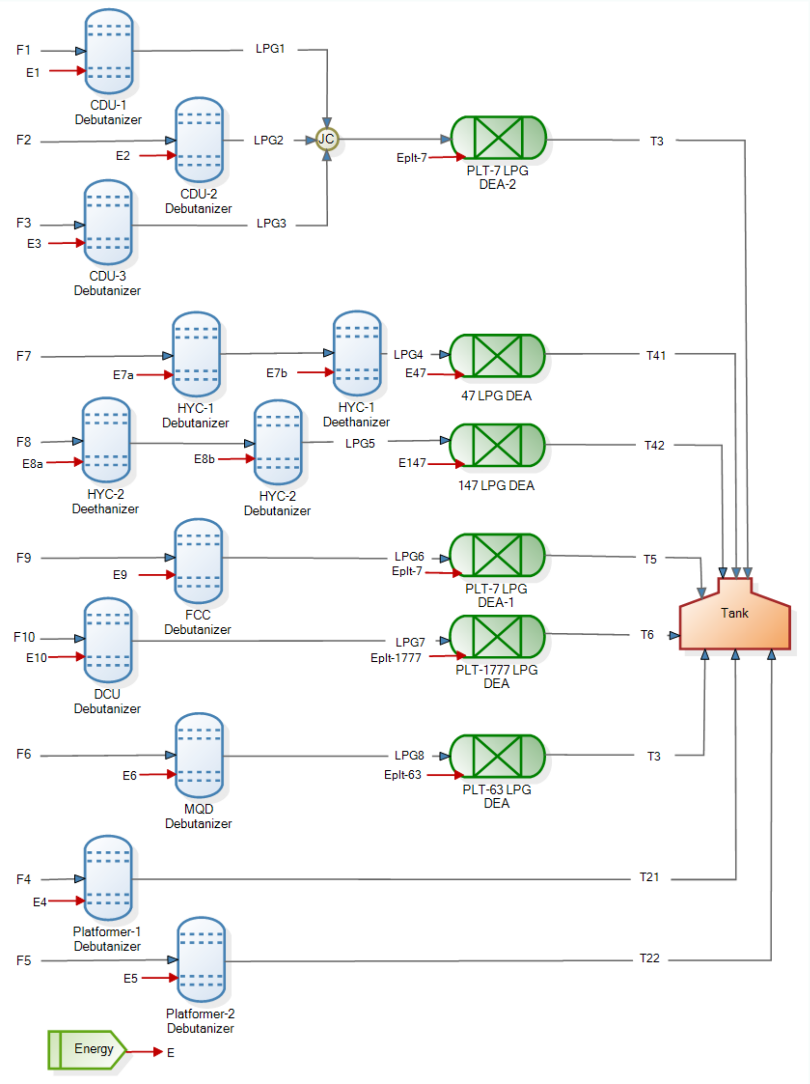
- Simulate the pipeline units to gauge impact of anomalies
  - Combination of first-principle and data driven models
  - Simulations also useful in the optimisation process

4 OPTIMISE BEHAVIOUR

- Optimize on specs recovery to LPG production

Digital Shadow Model

- Continuous process modelling
  - Processes
  - Production stages
  - Resource stocks / warehouses
  - Inputs – outputs
  - Material / energy flows
- Individual unit models:
  - First principles (mass and energy balances, thermodynamic equilibrium, chemical kinetics)
  - Regression models
  - Machine learning models



Digital Twin Platform

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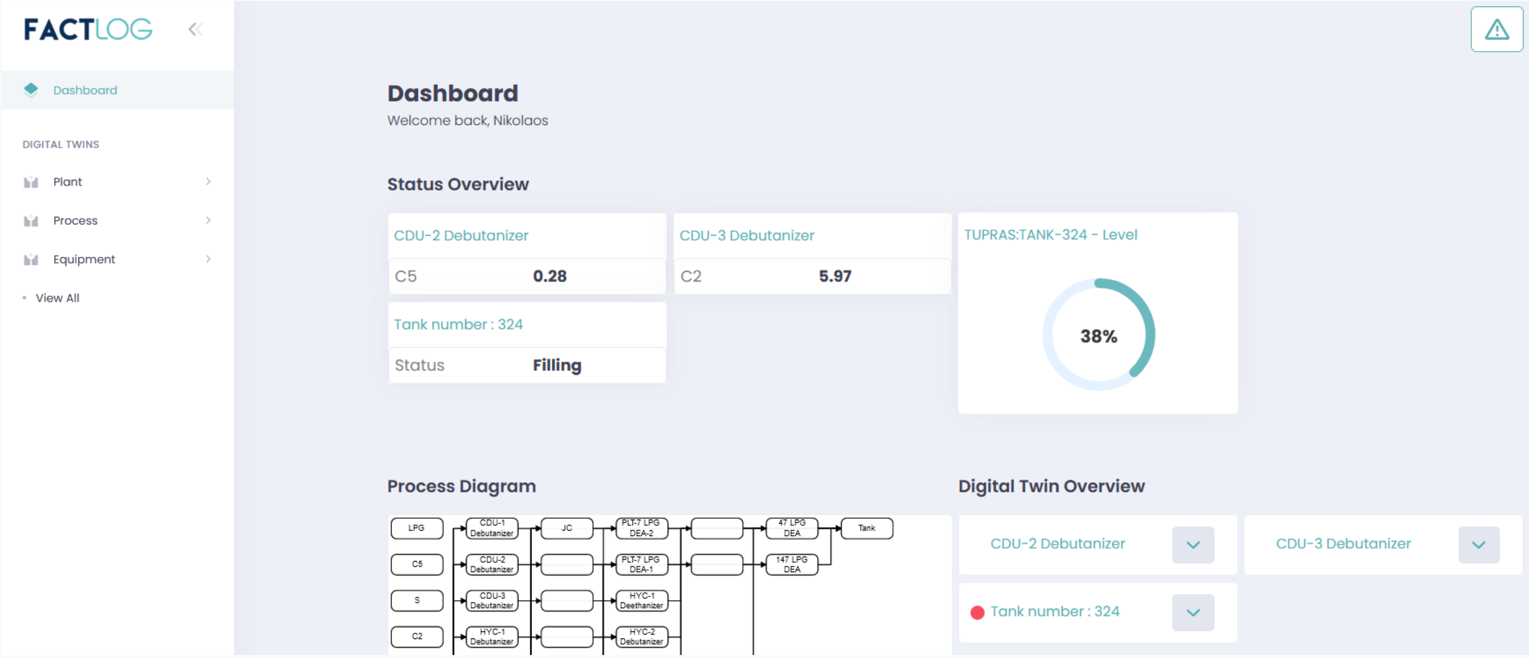

The Digital Twin of the production process can provide information about:

- Impurities on the LPG
- Storage Quantities
- Warnings and Failures
- Data Analytics
- Simulation Results
- Optimisation Results

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Thank you!

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