TOWARD TRANSPARENT DECISION SUPPORT: BUILDING FULLY INTEGRATED DIGITAL TWIN FOR REFINERY OPERATIONS

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MOLGROUP

Pannon Egyetem
University of Pannonia

MOL GROUP IN BRIEF

INTEGRATED DOWNSTREAM IN CEE

PRODUCTION UNITS

6

20.9 mtpa REFINING AND
2.2 mtpa PETROCHEMICALS
CAPACITY

EMPLOYEES

15.000

SERVICE STATIONS

~1.900

IN 10 COUNTRIES

CORE ACTIVITIES

CLEAN CCS EBITDA BY SEGMENTS IN 2022 (USD MN)

KEY FIGURES

CAPITAL MARKETS

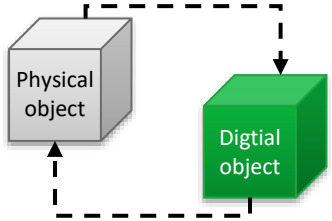
BUSINESS / ASSETS

WHY - DIGITAL TWIN (DT)

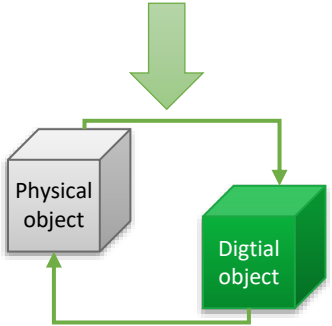
A Digital Twin:

- **cyber-physical integration** by which data can be collected, analyzed, and visualized
- to **make more informed decisions**

} to **optimize operations**

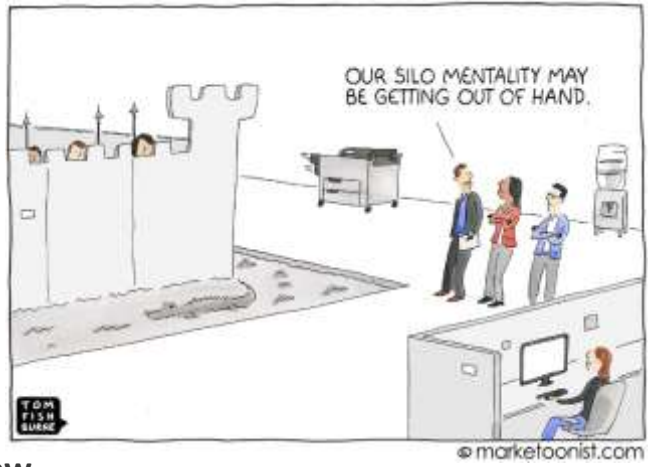


Digital model
Not automated (Silo)



Digital Twin
Fully integrated

- Separate **models** with **different scope**
  - *Simulation models,*
  - *Energy prediction, monitoring,*
  - *Quality prediction,*
  - *Crude selection,*
  - *Anomaly detection, etc..*
- Model generation ad-hoc, **problem driven**
- Models **not integrated** into one eco-system
- Models' health are not monitored -> **missing** continues **maintenance**, version control
- Simulation models are available only for a **narrow group**



A faster and continuous response to business needs could increase profitability by transitioning from siloed digital models to an integrated Digital Twin

RTO OR DIGITAL TWIN? WHAT'S THE DIFFERENCE?

RTO

- **Dynamic process control** – Continuously adjusts operational parameters to optimize the performance
- **Aim:** move the **system towards optimum**, given current **boundary conditions**

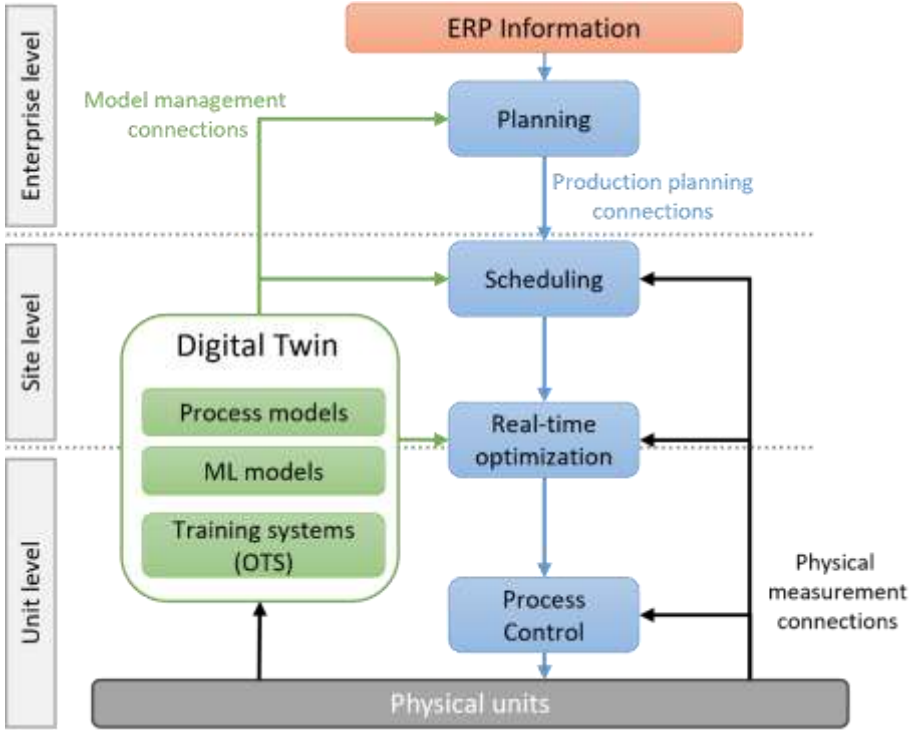
Digital Twin

- **High-fidelity virtual model** of a physical process
- Integrates available process information („White Box")
- **Can simulate various scenarios** to **analyze the impact of changes**, such as variations in catalyst activity or feedstock quality.

Objective:

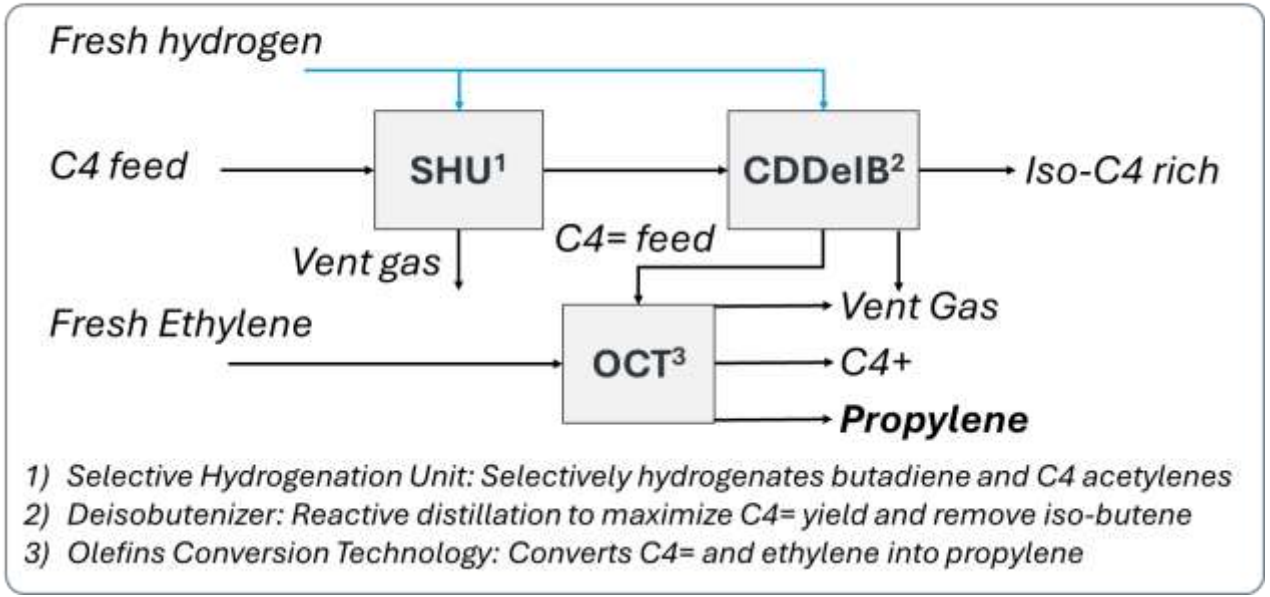
- ***RTO:*** Focuses on **continuously optimizing the current process in real-time** to achieve the best performance under existing conditions.

- ***Digital Twin:*** Aims to **provide a virtual environment for testing and analysis**, allowing for the exploration of various scenarios and their impacts without disturbing the actual process.

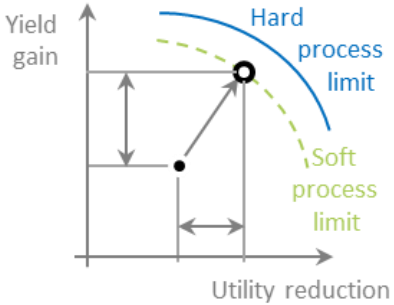


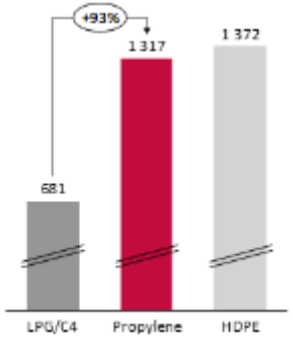
USE-CASE OLEFIN CONVERSION UNIT (OCU)

Metathesis of 2-Butene and Ethene: $C_4H_8 + C_2H_4 \rightarrow 2C_3H_6$

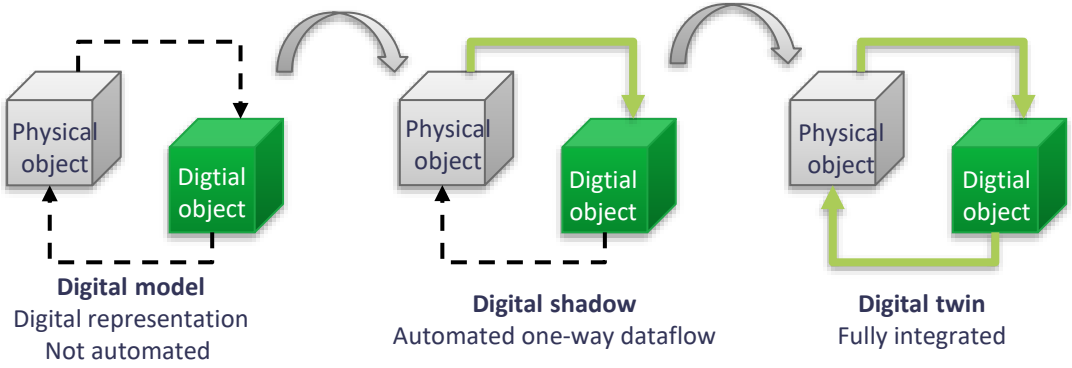


1) *Selective Hydrogenation Unit: Selectively hydrogenates butadiene and C4 acetylenes*
2) *Deisobutenizer: Reactive distillation to maximize C4= yield and remove iso-butene*
3) *Olefins Conversion Technology: Converts C4= and ethylene into propylene*





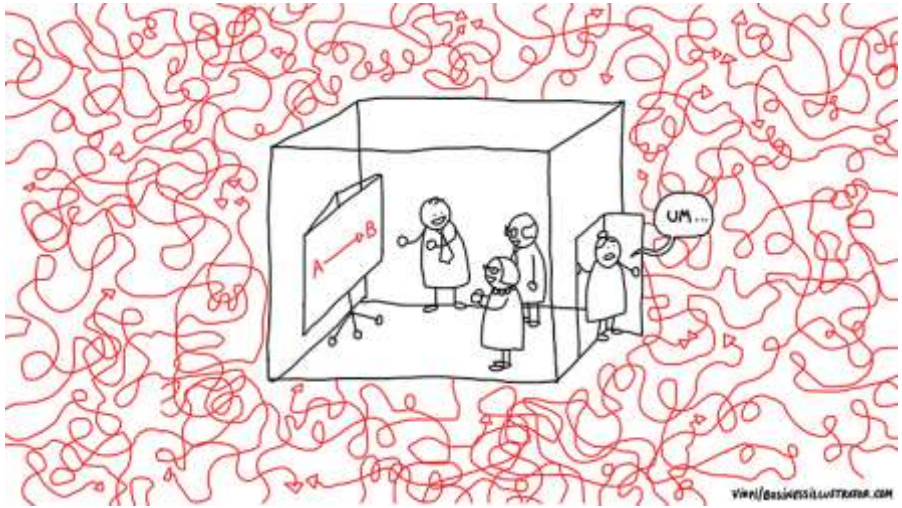
MOVING TOWARDS DIGITAL TWIN SEEMS TO BE SIMPLE…



Digital model
Digital representation
Not automated

Digital shadow
Automated one-way dataflow

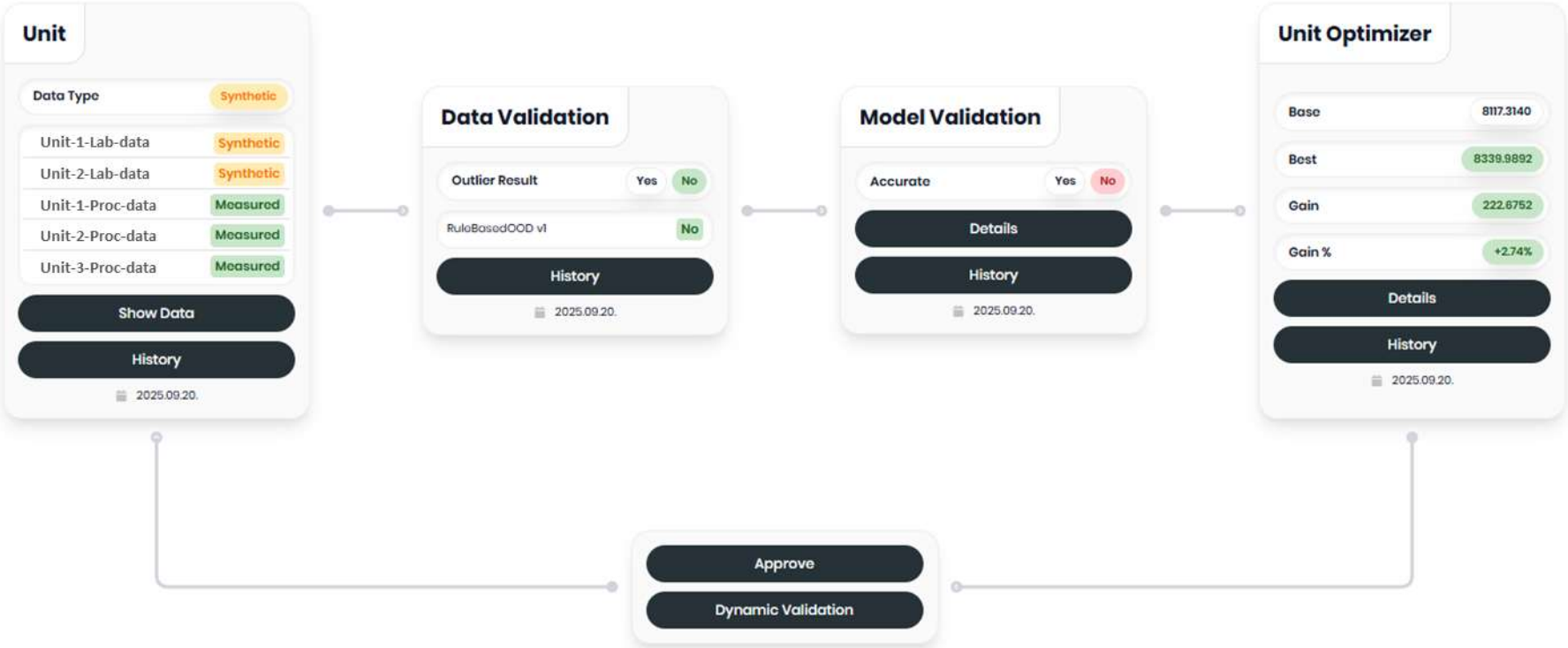
Digital twin
Fully integrated



Challenges

- Real-time automated connection adds **excessive** system **complexity**.
- **Multi-model integration** (first-principles + ML).
- **Model management** – monitoring, continuous calibration, and version control.
- Poor **data quality** → poor model output.
- Siloed models instead of **multi-purpose use**.
- Weak/missing **validation**.
- **Low trust** – caused by **complex** and **hard-to-interpret** solutions.

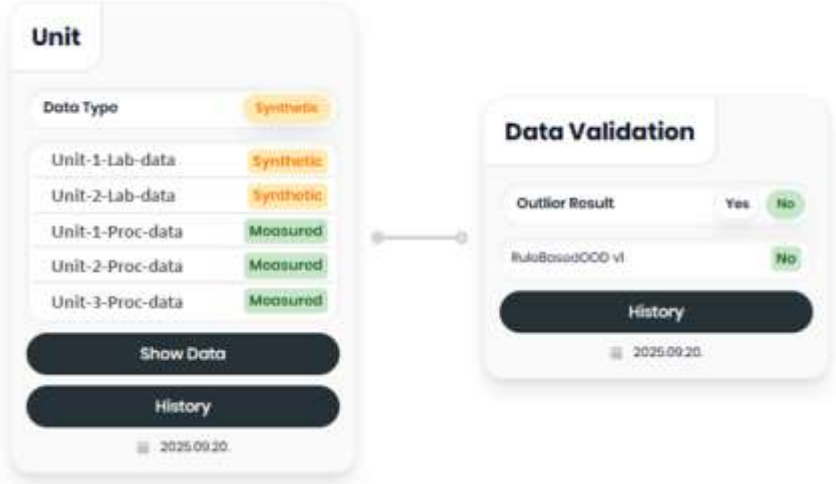
KEY ELEMENTS OF DEVELOPED FULLY INTEGRATED DIGITAL TWIN FRAMEWORK



DATA VALIDATION & INTEGRATION

Reliable decisions require **trusted data:**

- **Filter by operating range** – apply models only where they are valid.
- **Validate data** – remove outliers, correct errors, ensure consistency.
- **Integrate sources** – merge sensor, system, and database inputs.
- **Harmonize** – align units, formats, and timestamps for clarity.
- **Explain with visuals** – clearly show what was changed, removed, or corrected, and why.

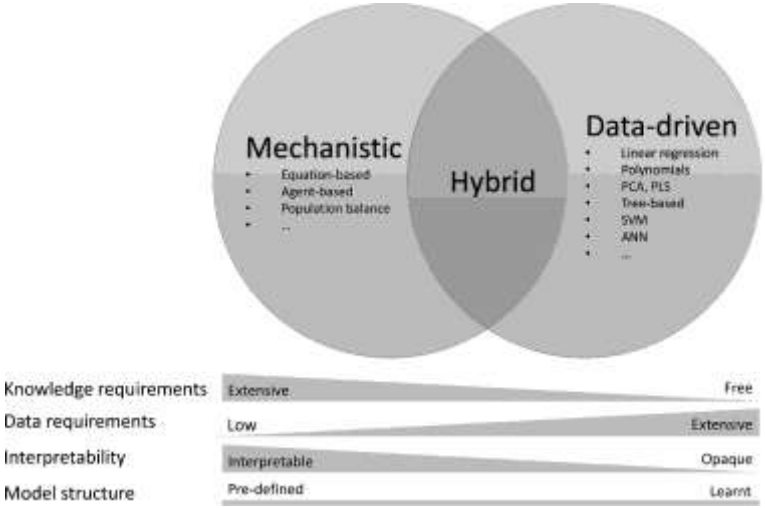


Poor quality or out-of-range data can lead to inaccurate results, limiting the model's effectiveness and compromising decision-making.

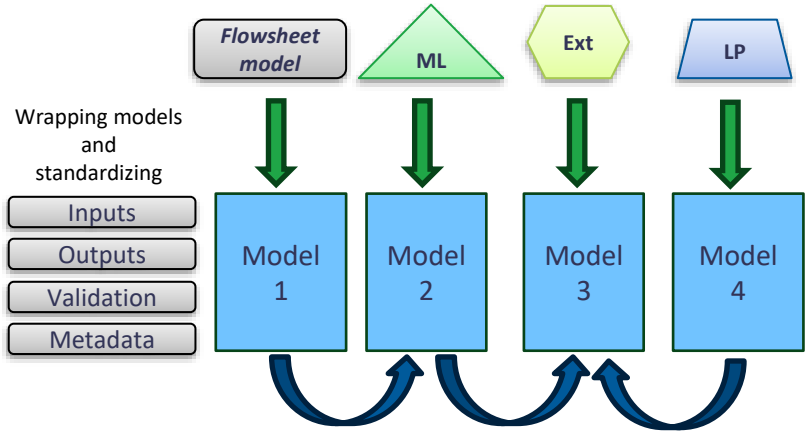
THE HEART OF A DIGITAL TWIN: MODELS

Within Digital Twin the model(s) can **vary in type**, **level of detail**, and **granularity**. These models:

- Simulate physical system behavior
- Coherent multi-layered view of the system (interconnectedness).



How can we seamlessly integrate diverse models in a digital twin?

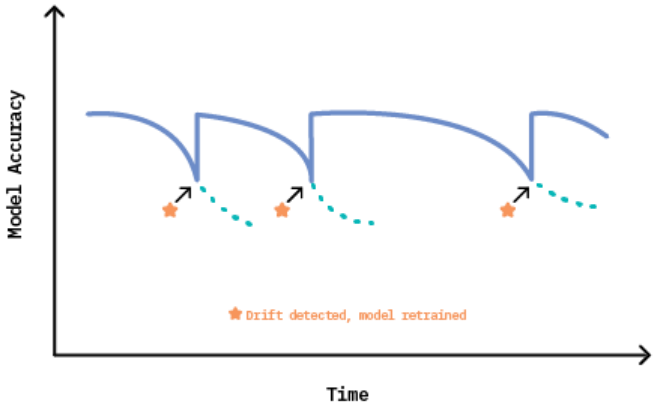


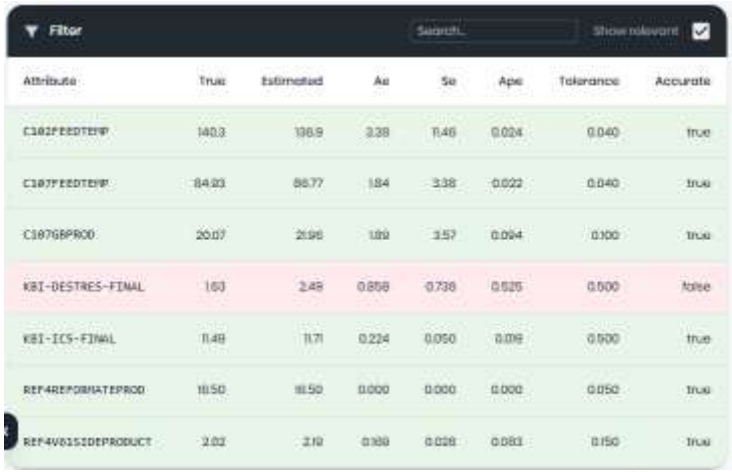
*Schneider, Mariane Yvonne, et al. "Hybrid modelling of water resource recovery facilities: status and opportunities." *Water Science and Technology* 85.9 (2022): 2503-2524.

MODEL INTEGRATION & VALIDATION

Maintaining flowsheet model performance is critical as **real-world degradation occurs**. Online connectivity demands continuous monitoring and timely intervention when drift is detected.

- **Clear ownership** – model changes are handled by subject-matter experts.
- **Performance monitoring** – detect concept drift and degradation
- **Online calibration** – use automated/semi-automated tuning to maintain accuracy.
- **Transparent validation** – track and explain model performance before and during application.

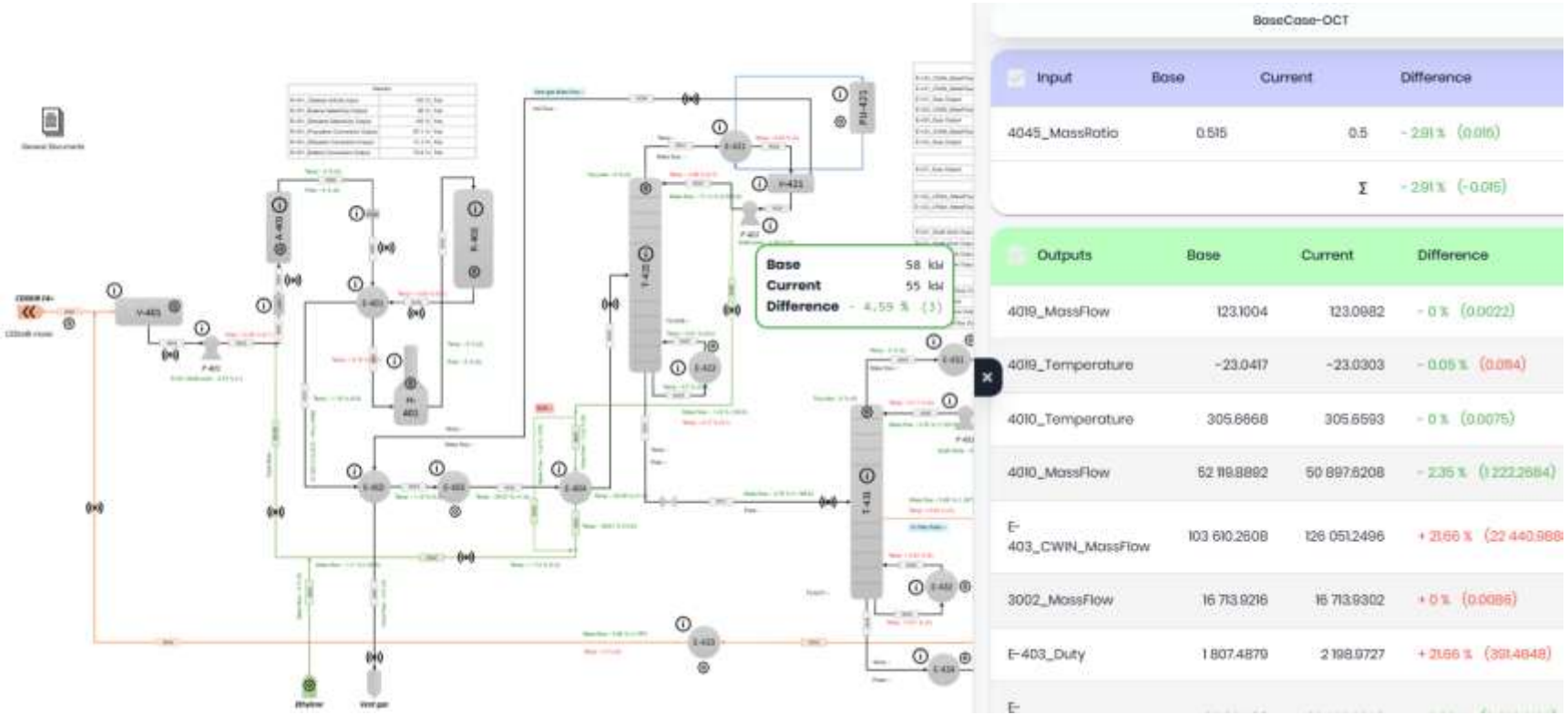




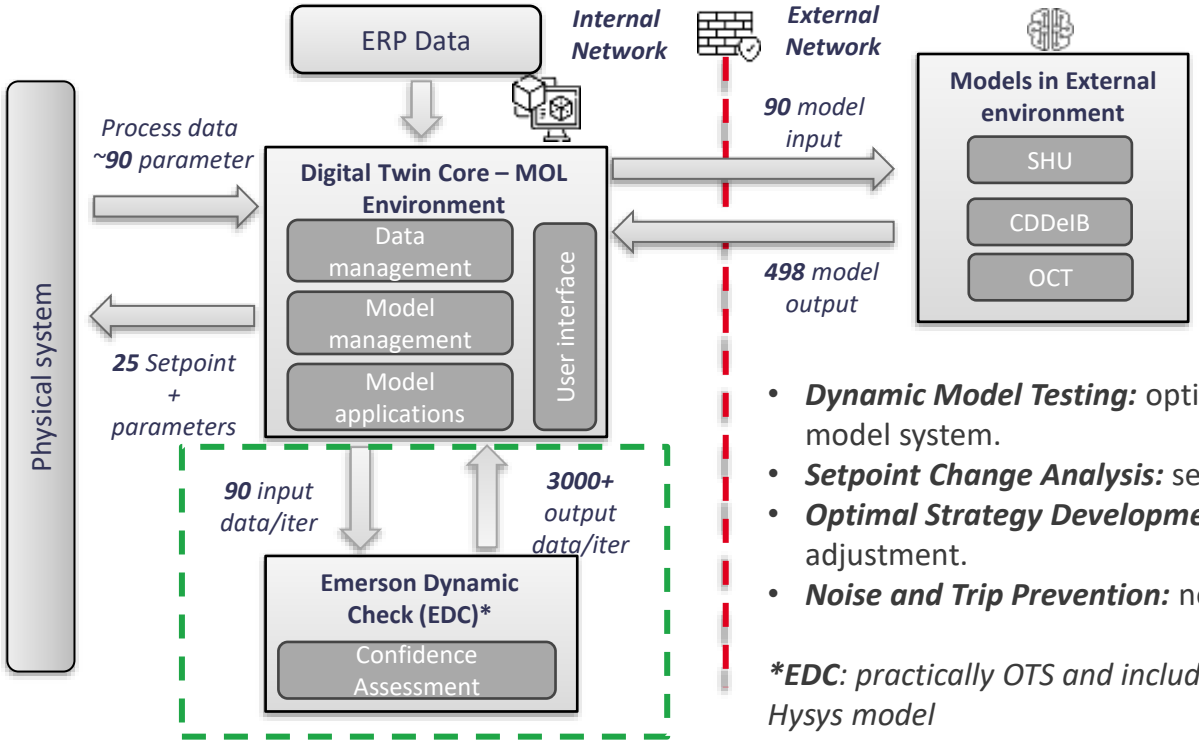
Model calibration:

- *Balázs Palotai, Gábor Kis, János Abonyi, Ágnes Bárkányi, Surrogate-based flowsheet model maintenance for Digital Twins. Digital Chemical Engineering, 15, 100228. Elsevier, 2025*
- *Balázs Palotai, Gábor Kis, Tibor Chován, Ágnes Bárkányi, Online learning supported surrogate-based flowsheet model maintenance. Digital Chemical Engineering – **Under review***

APPLICATION & PLAYGROUND



IMPORTANCE OF DYNAMIC VALIDATION IN DIGITAL TWIN



Paramount importance of Emerson Dynamic Check (EDC) is to avoid tripping the physical system and/or not losing money and credibility

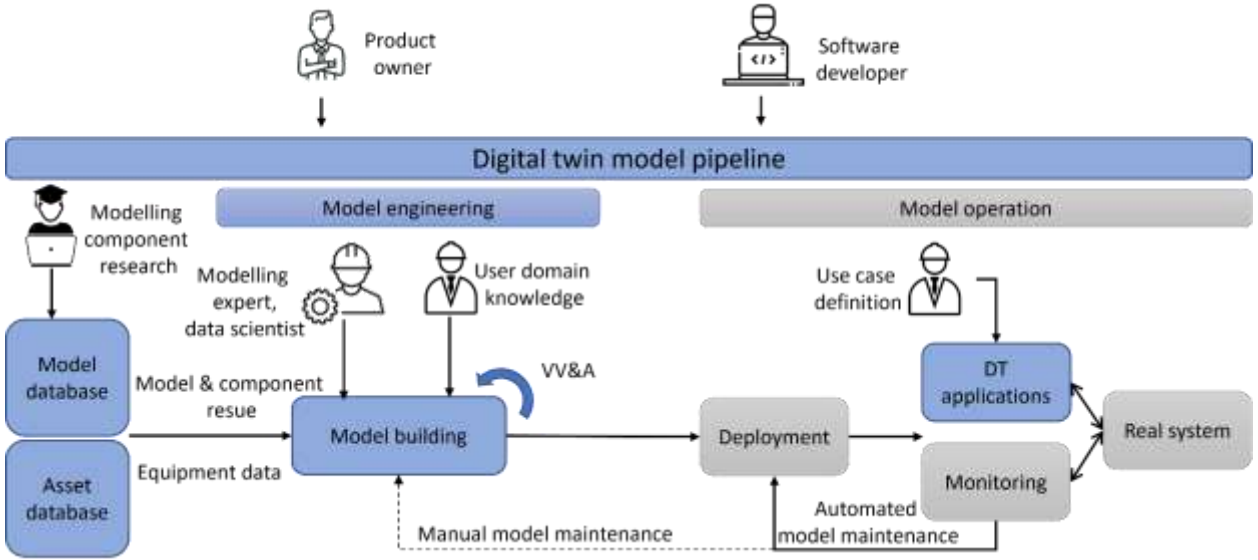
- ***Dynamic Model Testing:*** optimal operating state testing in a dynamic model system.
- ***Setpoint Change Analysis:*** setpoint change analytics and understanding.
- ***Optimal Strategy Development:*** strategy development for setpoint adjustment.
- ***Noise and Trip Prevention:*** noise and trip avoidance in the real system.

****EDC**: practically OTS and include offline DeltaV and dynamic AspenTech Hysys model*

SUMMARY

Clarity and explainability make **digital twins** trusted tools in refinery operations:

- **Clear blocks** – show how each part works and connects.
- **Explained decisions** – why data/models are valid, why optimizers choose a point.
- **Robust validation** – ensure safety and operational feasibility.
- **Flexible use** – optimization, ad-hoc analysis, advanced insights.
- **User trust** – built through clarity, visualization, and realistic testing.




THANK YOU
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