

## Digital Twin for Optimization in the Hydrocarbon Energy Supply Chain

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### Introduction

In refining and petrochemical industries, optimizing production processes is critical to improving product yields and minimizing operational costs. Digital twins, virtual representations of physical processes linked to real-time data, enable continuous optimization and dynamic decision-making. These models offer insights into current operations, predict future outcomes, and suggest optimal strategies for both short- and long-term operations.

The integration of process simulation, data-driven models, and real-time optimization within a unified framework provides a powerful tool for refining and petrochemical operators to make more informed decisions, mitigate risks, and adapt to changing operational conditions.

## Key Components of the Digital Twin

The digital twin is built around several key components:

- Process Models: These are the backbone of the digital twin and can be based on first principles (physical and chemical properties) or data-driven methods such as machine learning.
- Real-Time Data Integration: Sensor data from the physical process is continuously fed into the digital twin, ensuring that the model is always aligned with real-world conditions.
- Optimization and Simulation Tools: These tools provide actionable insights, allowing operators to perform "what-if" scenarios, predict future outcomes, and optimize operations across different time horizons.
- Data Reconciliation: Advanced algorithms like Kalman filters or Moving Horizon Estimation ensure the process model remains dynamically aligned with real-time data, enabling accurate representation of the physical process.





Hybrid Models - Combine AI with Conventional Process Simulation

## **Example Applications**

#### **Refinery-Wide Optimization**

A refinery-wide digital twin optimizes various processing units, including distillation columns and reaction units. By providing real-time feedback, it enables operators to optimize feedstock selection and product yields, reducing give-away and maximizing profit margins. The model reconciles data across the facility, providing a real-time mass and energy balance that improves decision-making.

#### **Olefins Process Optimization**

In a steam cracker, a digital twin is used to optimize furnace operations and manage feedstock fluctuations. The model integrates feedstock supply forecasts with furnace operation dynamics, allowing real-time adjustments in feed and process conditions to ensure continuous and efficient production.

#### Olefins Furnace Scheduling

Furnaces used in olefin production must undergo periodic decoking to maintain efficiency. A digital twin helps optimize decoking schedules, feed allocation, and operational conditions to maximize furnace run length and minimize downtime, improving overall plant efficiency and profitability.

#### Supply Chain Optimization

A digital twin of an integrated hydrocarbon energy supply chain, covering upstream, midstream, and downstream operations, facilitates real-time monitoring of operational conditions across the entire asset. By leveraging precise process models and thermophysical properties, it can track individual molecular components, such as hydrogen, methane, and CO2, from the wellhead to the end user or emission point. This technology allows energy companies to improve performance, monitor environmental impact in real time, reduce costs, and strengthen supply chain resilience, ultimately increasing operating margins and optimizing return on capital employed.



A dynamically reconciled digital twin model provides the basis for a range of operations optimization and decision support applications.

## Dynamic Data Reconciliation and Optimization

A key feature of the digital twin is its ability to reconcile real-time data with the process model continuously, a process often referred to as model calibration, adaptation, or data reconciliation. This calibration aligns the virtual model with actual plant data to validate measurements and improve model accuracy. Discrepancies between the physical process and the digital twin can stem from sensor errors, missing or noisy data, or modelling inaccuracies, requiring adjustments to the virtual model to account for these inconsistencies.

During calibration, model parameters and measurement biases are fine-tuned to provide the best fit between real-world data and the model. This real-time updating capability ensures that the digital twin accurately reflects the current state of the process, even during dynamic conditions like changes in feed composition or maintenance activities. By continuously aligning the model with live data, the digital twin remains a reliable tool for monitoring and optimizing operations.



# Benefits of Digital Twins in Refining and Petrochemical Processes

- Enhanced Flexibility: Digital twins provide dynamic insights into process operations, enabling real-time adjustments that maximize operational efficiency and flexibility.
- Improved Product Quality: Continuous optimization of feed and process conditions helps reduce variability in product quality, leading to higher yields and reduced waste.
- Cost Reduction: By improving process efficiency and reducing downtime, digital twins help minimize operating costs, including energy consumption and maintenance expenses.
- Risk Mitigation: Predictive analytics allow operators to foresee potential issues, such as equipment failures, and take proactive steps to mitigate these risks.
- Sustainability: The ability to optimize energy consumption and minimize emissions also contributes to achieving environmental sustainability goals.



Example of a Refinery Middle Distillate Optimizer

## **Challenges in Digital Twin Implementation**

While digital twins offer significant benefits, there are challenges to consider:

- Model Accuracy: Ensuring the digital twin is accurate requires continuous calibration and high-quality data.
- Scalability: As refineries and petrochemical plants are highly complex, building scalable models that can handle all processes, and their interactions is difficult.
- Data Integration: Integrating data from multiple sources, including sensors, process simulators, and legacy systems, is critical for the digital twin's success.



## Conclusion

Digital twin technology offers a powerful tool for optimizing refining and petrochemical processes by providing real-time insights, optimizing operations, and improving decision-making. By integrating process models with real-time data, digital twins enable operators to enhance flexibility, reduce costs, improve product quality, and mitigate risks. Although challenges remain in implementing these systems at scale, the potential benefits make digital twins a key enabler of future process optimization in the refining and petrochemical industries.

## Reference

A Dynamically Reconciled Digital Twin for Operations Optimization and Decision Support. Paper presented at the ADIPEC, Abu Dhabi, UAE, October 2022.

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