Applying Comprehensive Digital Twins to Optimize Production and Reduce Carbon Footprint

Paper No. PCIC energy EUR26_19

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Abstract - Sustaining competitive advantage in the energy and chemical industries requires simultaneous advancement of operational excellence, decarbonization metrics, and strategic workforce development.

This technical paper proposes a novel approach to address these multifaceted challenges by leveraging comprehensive digital twins, powered by advanced artificial intelligence (AI). By creating high-fidelity virtual replicas of physical assets, processes, and entire facilities, comprehensive digital twins integrate real-time sensor data, historical operational records, and predictive models. AI algorithms, including machine learning, are then applied to analyze this rich dataset, enabling proactive identification of inefficiencies, prediction of equipment failures, and dynamic optimization of process parameters. This integrated framework facilitates real-time decision-making, leading to substantial improvements in production yield, asset utilization, and energy consumption. Furthermore, the digital twin's predictive capabilities allow for the simulation and evaluation of various operational scenarios, including the impact of alternative feedstocks, and process modifications, thereby enabling the identification and implementation of strategies to minimize greenhouse gas emissions. This approach drives both operational excellence and economic benefits while supporting the sector's transition toward a more sustainable and environmentally responsible future.

I. INTRODUCTION

Today's volatile markets, along with geopolitical shifts, confront companies in the energy and chemical industry with cost pressures, supply chain disruptions, and requirements for faster time-to-market. Simultaneously, all applications in a process plant must comply with the latest safety requirements and environmental regulations. In such a disruptive and demanding environment, agility is key to business success, and these challenges can only be addressed with a data-centered and knowledge-driven approach.

Traditionally, engineering, operations, and maintenance information has resided in silos, making it difficult to achieve a comprehensive, real-time understanding of operations and asset conditions. This has led to inefficient processes, reactive maintenance, long downtimes, and significant hurdles in personnel training. Moreover, the increasing focus on Environmental, Social, and Governance (ESG) criteria by investors, regulators, and the public adds another layer of complexity, pushing companies to demonstrate tangible commitments to sustainability.

Transformation into a truly digital enterprise provides opportunities to address these challenges. The concept of applying comprehensive digital twins has emerged as a cornerstone of this transformation, offering a powerful paradigm shift in how industrial assets and processes are managed and optimized.

This paper explores how comprehensive digital twin implementations can be strategically leveraged to optimize production workflows and significantly reduce the carbon footprint of industrial operations.

II. UNDERSTANDING THE COMPREHENSIVE DIGITAL TWIN

A digital twin is a virtual representation of a physical object or system - in this specific case, a process plant.

A comprehensive digital twin goes beyond simple 3D models or basic simulations. It is a dynamic, data-rich virtual replica that integrates multi-domain data throughout the entire lifecycle of an asset or process - continuously updated with real-time data, enabling comprehensive analysis, prediction, and control.

Key characteristics include:

- **High-fidelity representation:** Accurate virtual models that mirror the behavior and characteristics of their physical counterparts, achieving exceptional fidelity to real-world conditions.
- **Interoperability:** Seamless integration with various engineering tools, operational systems, and business platforms, reducing data silos and improving decision-making speed.
- **Real-time data integration:** Continuous flow of operational data from sensors and control systems to keep the digital twin synchronized with the physical world, ensuring decisions are based on the most current information.
- **Closed-loop optimization:** The ability to feed insights and recommendations from the digital twin back into the physical system for continuous improvement, enabling autonomous or semi-autonomous adjustments that maintain optimal performance.
- **Predictive analytics and AI:** Utilization of advanced algorithms and artificial intelligence to forecast performance, identify potential issues days or weeks in advance, and optimize outcomes.

In essence, comprehensive digital twins combine data from all lifecycle phases, functions and levels, helping users to understand, manage, and predict the performance of the corresponding process or plant and thereby laying the groundwork for informed data-based decisions. The digital twin cube illustrates the three-dimensional structure of the digital twin framework, linking lifecycle phase, use cases, and focus areas into a unified model:

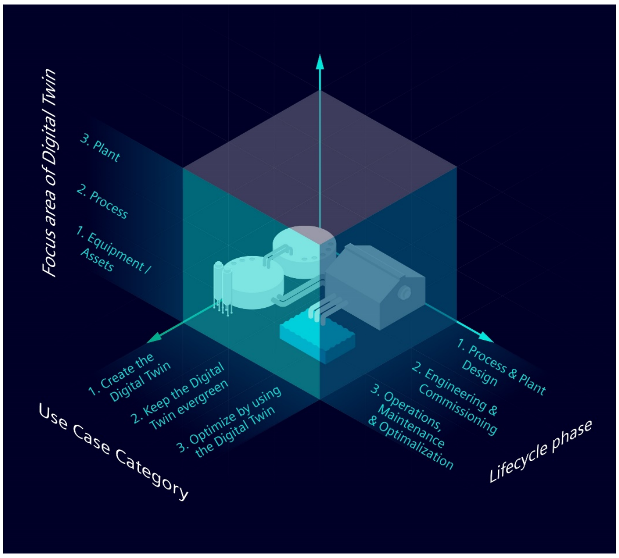

Fig. 1: Digital twin cube (based on the IoT Analytics Research study 2020)

III. IMPLEMENTING AND MAINTAINING THE DIGITAL TWIN

The digital twin is suitable for greenfield and brownfield applications. In many cases, the starting point is an existing plant requiring the transformation of diverse data sources—such as paper-based records and fragmented digital data—into reliable, structured information. This information originates from all phases of the plant lifecycle, from process design over engineering up to operations, maintenance and modernization. Upon collection, the data is digitized, cleaned, and contextualized according to dynamic interoperable data management principles. The digital twin is not only consistently updated and adapted according to the changes made in the plant, but also continuously validated against operational data.

Creating the Digital Twin:

- **Integrated engineering design:** In the design phase, steady-state process models are used to design the production process for specific operating points. The results are the Process Flow Diagrams (PFD), Piping and Instrumentation Diagrams (P&ID), and data sheets for the equipment. In this phase, only partially dynamic process models are used, which can represent transient behavior of the process, like start-up and shutdown processes.
- **Virtual prototyping and simulation:** Before physical construction, digital twins allow for extensive simulation and validation of designs, identifying potential bottlenecks, safety hazards, and inefficiencies. This can significantly reduce engineering design time and cut commissioning costs by minimizing rework and accelerating time-to-market.
- **Modular plant concepts:** Facilitate the design and integration of standardized, pre-validated modules, streamlining project execution and enhancing flexibility, often leading to measurable project schedule reductions.
- **Legacy data:** Creating a holistic digital twin from legacy data represents an enormous challenge as large amounts of information must be merged from different systems. Standardized and open interfaces (e.g., DEXPI, OPC UA, NOA, eCl@ss) allow the integration of data from various sources. However, this process requires contextualizing data and solving conflicts in information.
- **Use of artificial intelligence:** AI-based services can recognize and extract important information and its context from sources such as tags, properties as well as relations between tags. These services aim at digitizing and further accelerating engineering data preparation and integration. They are also intended for (semi-) automated cleansing of 1D brownfield data as well as extraction services for 2D schematic drawings and can be integrated into a common knowledge graph management framework.

Digital twin applications can be operated via cloud as well as on premise or even in a hybrid way, empowering users to choose the setup best suited for their individual data policy in terms of performance, availability, budget and level of required security.

Keeping the Digital Twin "Evergreen"

The long-term value and reliability of a digital twin are fundamentally dependent on its "evergreen" status, meaning it accurately reflects the current state and behavior of its physical counterpart throughout its lifecycle. As physical assets undergo modifications, experience wear and tear, or operate under varying conditions, an outdated digital twin rapidly loses its predictive accuracy and decision-support capabilities. An evergreen approach, characterized by continuous data synchronization, model updates, and recalibration, ensures that the digital twin remains a faithful, high-fidelity representation. Without this ongoing maintenance, the initial investment in digital twin technology diminishes, leading to suboptimal operational decisions, inaccurate predictions, and a failure to realize potential benefits in efficiency, sustainability, and risk management. Therefore, an evergreen strategy is not merely an operational overhead but a fundamental requirement for unlocking and sustaining the full transformative potential of digital twins.

In many plants, engineering, automation, simulation and software systems are not interconnected, which makes exchanging data between the different systems and relevant stakeholders difficult. To facilitate this, an interoperable tool landscape for engineering, automation and simulation is advisable, allowing users to keep their digital twin "evergreen".

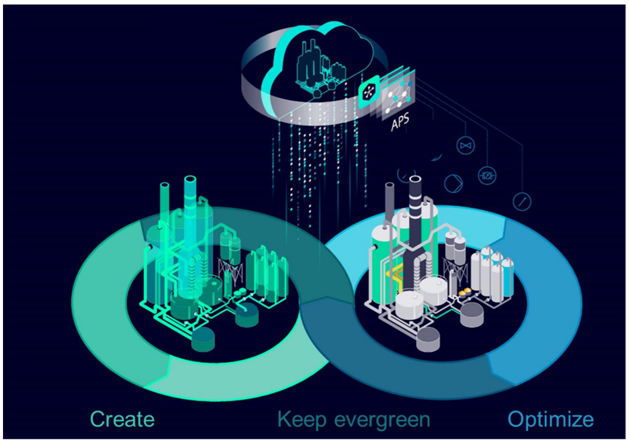

Fig. 2: Digital twin lifecycle – creating the digital twin, keeping it evergreen, and optimizing a plant with it

IV. BENEFITING FROM THE DIGITAL TWIN ACROSS THE LIFECYCLE

Although the benefits of using a digital twin start in the engineering phase, the main benefits materialize during operations.

Operational Excellence:

- **Real-time monitoring and diagnostics:** Operators gain a comprehensive, real-time view of plant performance, enabling proactive identification of deviations and rapid troubleshooting. This can reduce unplanned downtime by up to 25%.
- **Advanced Process Control (APC):** Digital twins can host advanced control strategies that continuously adjust operational parameters to maintain optimal performance, maximize production by up to 5%, while minimizing energy consumption, and improving product quality consistency. Typical return-of-invest rates of APC systems are well below 12 months.
- **"What-If" scenario planning:** The ability to simulate alternative operational scenarios allows for risk-free experimentation to identify optimal strategies for production changes or maintenance activities. This enables optimized decision-making and significantly reduces operational intervention.
- **Operator Training Systems (OTS):** High-fidelity digital twins can serve as immersive training environments, allowing operators to practice complex procedures and emergency responses without impacting live operations, improving safety and operational readiness, and potentially reducing human error-related incidents.

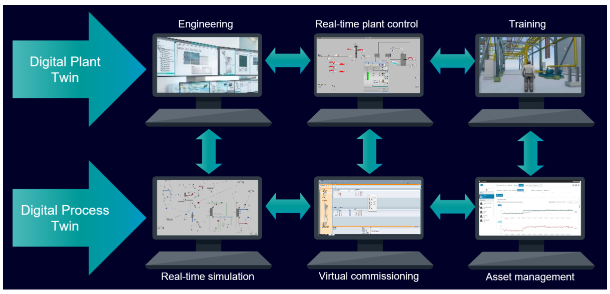

Fig. 3: Applying the digital twin concept across the lifecycle

Maintenance and Asset Performance Management:

- **Predictive maintenance:** By analyzing data from digital twins, potential equipment failures can be predicted well in advance, enabling scheduled maintenance interventions rather than costly reactive repairs. Applying artificial intelligence and machine learning to improve diagnostics can significantly extend asset lifespan and reduce maintenance costs by 15-20%.
- **Performance benchmarking:** Continuous comparison of actual performance against the digital twin's optimal model helps identify performance gaps and areas for improvement, leading to continuous efficiency gains.
- **Mobile worker concepts for integrated maintenance:** Unique identification of assets, equipment, and material along with access to documentation and experts.

Fig. 4: Mobile worker concepts for integrated maintenance

V. BENEFITING FROM THE DIGITAL TWIN FOR CARBON FOOTPRINT REDUCTION

Beyond production efficiency, comprehensive digital twin technology is a powerful enabler for sustainability initiatives and carbon footprint reduction:

Energy Consumption Optimization:

- **Utility systems optimization:** Specialized digital applications can model and optimize site utility systems (e.g., steam, power, cooling), identifying opportunities to reduce hydrocarbon fuel consumption and associated emissions. These systems can provide real-time recommendations for optimal operational settings, leading to energy savings of 5-15% and a direct reduction in associated CO_2 emissions.
- **Advanced Process Control for energy efficiency:** By precisely controlling process parameters, digital twins minimize energy waste in various industrial processes, from chemical reactions to material processing, often resulting in specific energy consumption reductions of 3-7%.

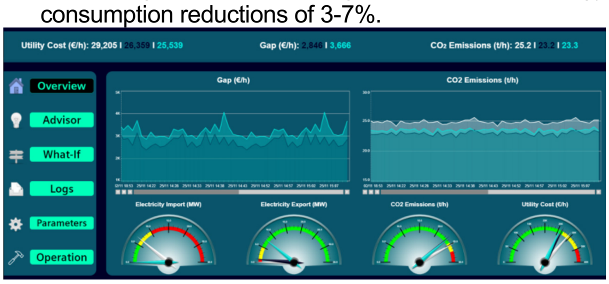

Fig. 5: Example of an advisory system for carbon management

Emissions Reduction Strategies:

- **Process optimization for lower emissions:** Digital twins can simulate the impact of different operating conditions on emissions, allowing operators to identify and implement strategies that reduce greenhouse gas releases without compromising production quality or quantity. This can lead to direct emissions reductions of 5-10% from process improvements.
- **Waste minimization:** By optimizing material flows and process efficiencies, digital twins help reduce waste generation, which indirectly contributes to a lower carbon footprint associated with waste treatment and disposal.

Integration of Green Technologies:

- **Hydrogen production optimization:** Digital replicas, such as those used for hydrogen performance, can optimize the production and utilization of green hydrogen, a key component in decarbonization strategies, leading to optimized energy input and reduced operational costs for hydrogen production.
- **Renewable energy integration:** Digital twins can model and optimize the integration of renewable energy sources into industrial grids, ensuring stable and efficient operation while reducing reliance on and usage of fossil fuels.

ESG Reporting and Compliance:

- **Soft sensing:** Physical measurements can be complex, expensive and unreliable. The solution can be data based virtual measurements derived by an AI model, a high-fidelity physical first-principle model or a combination of both.
- **Data-driven insights:** The comprehensive data collected and analyzed by digital twins provides robust evidence for environmental, social, and governance (ESG) reporting, demonstrating tangible progress in sustainability efforts. This enhances reporting accuracy and transparency, potentially improving ESG ratings.
- **Regulatory compliance:** By continuously monitoring and optimizing processes, digital twins help ensure compliance with environmental regulations and emission standards, reducing the risk of non-compliance penalties.

VI. CONCLUSIONS

The comprehensive digital twin is more than a technological advancement; it is a strategic asset for the energy and chemical sector achieving peak operational performance and sustainability targets.

By providing an integrated, data-driven view of physical assets and processes, it empowers organizations to make informed decisions that optimize production efficiency, minimize resource consumption, and significantly reduce their carbon footprint. Real-world applications demonstrate quantifiable benefits, including double-digit percentage improvements in production efficiency, energy savings, and emissions reductions. The incorporation of AI into these toolboxes will further revolutionize this development.

As industries continue to evolve, the digital twin will remain an indispensable tool in navigating the complexities of modern manufacturing and achieving a sustainable future. The deployment of artificial intelligence will further advance engineering assistance, contextualization of data, and data-driven decision-making.

VII. REFERENCES

References to gains in efficiency and reduction in emissions can be found from various sources and typically cover a wide range. Percentages provided in this document intend to reflect a reasonable average of the reviewed sources, combined with experience made by Siemens Digital Industries in executed projects.

Literature used in the preparation of this document includes among others:

[1] Siemens AG 2023, “Digital Twin for chemical industries – how an interoperable tool landscape paves the way into a sustainable future”

[2] T. Harrison, S. Chen, “Lifecycle Financial Assessment of Digital Twin – Enabled Optimization in Downstream Oil Operations”, University of Texas / MIT Sloan School of Management

[3] S. Kurhe, D. Chandre, N. Dukare “Digital Twin Technology for Sustainable Chemical Process Monitoring: An Integrated AI and IoT Perspective”, Savitribai Phule Pune University, Maharashtra, India

VIII. VITAS

Bernd Kalusche holds a master’s degree in chemical engineering from University of Stuttgart in Germany and builds on more than 25 years of experience with Siemens AG in various positions in Germany and the US. As Head of Business Development for the chemical and energy sector at Siemens Digital Industries, Bernd leads an organization serving customers around the globe with electrification, automation, and digitalization needs to master the digital transformation, and the energy transition.
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