Digital Twins in the Chemical Industry: Enhancing Efficiency and Innovation

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Gemelos digitales en la industria química: mejora de la eficiencia y la innovación

Bessons digitals a la indústria química: millora de l'eficiència i la innovación

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ABSTRACT

Digital twins have emerged as transformative tools in the chemical industry, revolutionizing traditional manufacturing methods and driving innovation. By creating virtual representations of physical assets and processes, digital twins enable real-time monitoring, simulation, and optimization of complex chemical systems. This review synthesizes findings from peer-reviewed literature and industry reports to provide a comprehensive analysis of digital twin applications, integration with advanced technologies like the Internet of Things (IoT), artificial intelligence (AI) and machine learning (ML) and an evaluation of challenges and opportunities in the chemical sector. The study highlights the significant impact of digital twins on process optimization, predictive maintenance, safety management, and product development. However, the adoption of this technology faces challenges related to data quality and integration, cybersecurity concerns, skill gaps, and high initial investments. Despite these limitations, the review provides a roadmap for chemical industries to harness digital twins effectively, emphasizing strategies for overcoming challenges and leveraging opportunities for innovation, efficiency, and sustainability. The integration of digital twins with emerging technologies like blockchain, extended reality (XR), and cross-industry collaboration is expected to further enhance their capabilities and drive the digital transformation of the chemical industry. As the sector embraces the digital future, digital twins are poised to play a crucial role in redefining operational dynamics and ensuring a competitive advantage in an increasingly complex global marketplace.

Keywords: Digital Twins; Chemical Industry; Internet of Things, Artificial Intelligence

RESUMEN

Los gemelos digitales han surgido como herramientas transformadoras en la industria química, revolucionando los métodos de fabricación tradicionales e impulsando la innovación. Al crear representaciones virtuales de activos y procesos físicos, los gemelos digitales permiten la monitorización en tiempo real, la simulación y la optimización de sistemas químicos complejos. Esta revisión sintetiza hallazgos de literatura académica revisada por pares e informes de la industria para ofrecer un análisis integral sobre las aplicaciones de los gemelos digitales, su integración con tecnologías avanzadas como el Internet de las Cosas (IoT), la inteligencia artificial (IA) y el aprendizaje automático (ML), así como una evaluación de los desafíos y oportunidades en el sector químico. El estudio destaca el impacto significativo de los gemelos digitales en la optimización de procesos, el mantenimiento predictivo, la gestión de la seguridad y el desarrollo de productos. Sin embargo, la adopción de esta tecnología enfrenta retos relacionados con la calidad e integración de los datos, preocupaciones sobre ciberseguridad, brechas

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de habilidades y altas inversiones iniciales. A pesar de estas limitaciones, la revisión proporciona una hoja de ruta para que las industrias químicas adopten los gemelos digitales de manera efectiva, haciendo hincapié en estrategias para superar los desafíos y aprovechar las oportunidades de innovación, eficiencia y sostenibilidad. Se espera que la integración de los gemelos digitales con tecnologías emergentes como la cadena de bloques (blockchain), la realidad extendida (XR) y la colaboración intersectorial potencie aún más sus capacidades y acelere la transformación digital de la industria química. A medida que el sector adopta el futuro digital, los gemelos digitales están llamados a desempeñar un papel crucial en la redefinición de las dinámicas operativas y en garantizar una ventaja competitiva en un mercado global cada vez más complejo.

Palabra clave*:* Gemelos digitales; Industria química; Internet de las Cosas, Inteligencia Artificial

RESUM

Els bessons digitals han esdevingut eines transformadores en la indústria química, revolucionant els mètodes tradicionals de fabricació i impulsant la innovació. Mitjançant la creació de representacions virtuals dels actius físics i els processos, els bessons digitals permeten la monitorització, simulació i optimització en temps real de sistemes químics complexos. Aquesta revisió sintetitza resultats de literatura científica revisada per parells i informes del sector per oferir una anàlisi completa de les aplicacions dels bessons digitals, la seva integració amb tecnologies avançades com l'Internet de les Coses (IoT), la intel·ligència artificial (IA) i l'aprenentatge automàtic (ML), així com una avaluació dels reptes i oportunitats en el sector químic. L'estudi destaca l'impacte significatiu dels bessons digitals en l'optimització de processos, el manteniment predictiu, la gestió de la seguretat i el desenvolupament de productes. No obstant això, l'adopció d'aquesta tecnologia afronta reptes relacionats amb la qualitat i la integració de dades, preocupacions de ciberseguretat, mancances de competències i elevades inversions inicials. Malgrat aquestes limitacions, la revisió proporciona una guia perquè les indústries químiques aprofitin els bessons digitals de manera eficaç, posant èmfasi en estratègies per superar els obstacles i aprofitar les oportunitats d'innovació, eficiència i sostenibilitat. S'espera que la integració dels bessons digitals amb tecnologies emergents com la blockchain, la realitat estesa (XR) i la col·laboració entre sectors potenciï encara més les seves capacitats i impulsi la transformació digital de la indústria química. A mesura que el sector adopta el futur digital, els bessons digitals estan destinats a jugar un paper clau en la redefinició de la dinàmica operativa i en garantir un avantatge competitiu en un mercat global cada vegada més complex.

Paraules clau*:* Bessons digitals; Indústria Química; Internet de les coses, intel·ligència artificial

1. INTRODUCTION: THE DIGITAL REVOLUTION IN CHEMICAL MANUFACTURING

The emergence of digital twins has transformed multiple sectors, particularly the chemical industry, presenting significant opportunities for improving efficiency and encouraging innovation. The virtual representations of tangible assets or processes facilitate real-time observation, simulation and enhancement of complex systems (Murugan, 2024). In the chemical sector, the application of digital twins can enhance production processes, improve energy efficiency and increase overall operational performance (Table 1) (Figure 1).

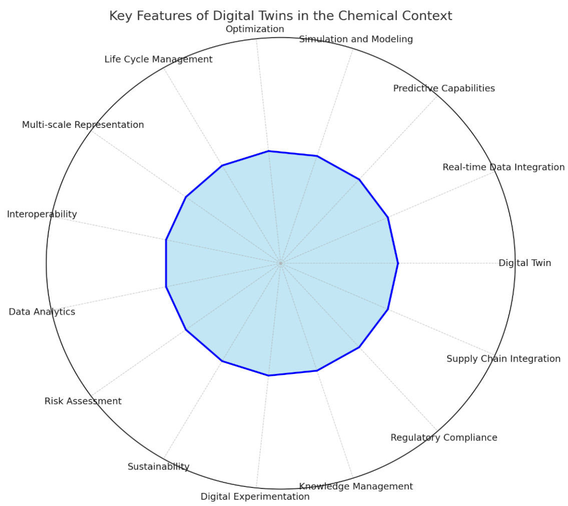

Figure 1. *Key points on understanding Digital Twins in the chemical industry*

Table 1. *Key Applications of Digital Twins in the Chemical Industry*

Application Area	Description	Example Technologies/Tools	Benefits
Process Optimization	Real-time monitoring and control	Aspen Plus, Honeywell Forge	Reduced waste, energy savings
Predictive Maintenance	Early detection of equipment issues	AI-based predictive models	Lower downtime, cost savings
Design and Simulation	Virtual prototyping of plants/processes	ANSYS, COMSOL	Reduced design cycle time
Supply Chain Management	Integration of production and logistics	IoT platforms, Digital Twins	Improved delivery times, cost management
Safety Management	Risk analysis and hazard prediction	Hazard modeling tools	Enhanced safety, regulatory compliance

Table 2. *Comparison of Conventional vs. Digital Twin Approaches*

Feature	Conventional Approach	Digital Twin Approach
Data Handling	Manual and periodic	Real-time and automated
Process Simulation	Static	Dynamic and interactive
Fault Detection	Reactive	Predictive
Cost Implications	Higher operational costs	Lower with efficient resource usage
Implementation Complexity	Moderate	High (initial setup)

Through the creation of virtual models for chemical facilities and processes, organizations can conduct simulations of various scenarios, predict outcomes and make data-driven decisions to enhance productivity and reduce costs (Iliuța et al., 2024; Bortolini et al., 2022; Zhang et al., 2023). This technology facilitates predictive maintenance, reduces downtime and enhances asset utilization. The integration of digital twins with advanced technologies like the Internet of Things (IoT), Artificial Intelligence (AI), Machine Learning (ML) and Extended Reality (XR) significantly amplifies their capabilities within the chemical industry (Kolekar et al., 2023). These integrations enhance simulations, enable immediate data analysis, and improve the visualization of complex chemical processes. Nonetheless, tackling the cybersecurity challenges linked to the integration of physical and virtual realms is crucial for maximizing the benefits of digital twin technology within the chemical industry (Gupta et al., 2023) (Table 2).

2. UNDERSTANDING DIGITAL TWINS IN THE CHEMICAL INDUSTRY

2.1 Definition and Core Concepts

In the chemical industry, digital twins act as virtual representations of physical entities or processes, facilitating real-time monitoring, visualization and prediction of system states (Eckhart & Ekelhart, 2019). The virtual counterparts utilize advanced technologies like artificial intelligence, the Internet of Things (IoT) and data analytics to improve operations and promote innovation in chemical manufacturing processes (Dayneko et al., 2024; Vetrivel et al., 2024). The essential elements of digital twins in the chemical industry include:

- Real-time data collection and analysis: Sensors and IoT devices gather information from physical systems, which is then processed and analyzed to yield insights into process performance (Dayneko et al., 2024; Zhang et al., 2023).
- Simulation and forecasting: Digital twins utilize advanced modeling techniques to replicate and anticipate system behavior, enabling proactive decision-making and optimization (Billey & Wuest, 2024; Vetrivel et al., 2024).
- Collaboration with Industry 4.0: Digital twins leverage various technologies associated with the fourth industrial revolution, such as big data analytics, blockchain, augmented reality and machine learning, to improve their functionalities and foster innovation (Dayneko et al., 2024).

It is important to highlight that, despite the swift integration of digital twins in multiple sectors, their role in advancing sustainability, especially in the context of lowering carbon emissions, is still a developing field of inquiry (Zhang et al., 2024). This offers a chance for the chemical sector to explore the application of digital twins in enhancing environmental outcomes and operational effectiveness.

2.2 Key Components of Chemical Digital Twins

The chemical manufacturing sector is undergoing a significant transformation with the adoption of digital twins, which are improving operational efficiency and driving innovation. These digital representations of tangible systems or processes integrate crucial components like extensive data, sophisticated analytics, interconnected devices, simulation modeling and machine intelligence (Dayneko et al., 2024). Through the facilitation of real-time monitoring, analysis and optimization of chemical manufacturing processes, digital twins are transforming the industry. The combination of sensors, 5G networks and AI-driven predictive models facilitates the gathering and analysis of essential parameters such as stirring speeds, water usage and air pressure in production processes (Zhang et al., 2023). This leads to enhanced energy efficiency, optimized production and reduced costs. While digital twins have been quickly embraced in multiple industries, their capacity to improve sustainability, especially in terms of lowering carbon emissions, is still an emerging field of investigation (Zhang et al., 2024). This offers a chance for the chemical sector to leverage digital twin technology for enhancing operations as well as promoting environmental responsibility.

3. APPLICATIONS OF DIGITAL TWINS IN CHEMICAL MANUFACTURING

3.1 Process Optimization

In the manufacturing industry, digital twins have emerged as significant tools for enhancing efficiency and driving innovation, particularly in the realm of process optimization. These digital representations of tangible entities or processes enable comprehensive testing, analysis, and optimization before actual implementation (Alfred et al., 2024). Chemical manufacturers have the opportunity to leverage this technology to model product behavior and performance, facilitating the early detection of inefficiencies and the potential for cost savings in production (Alfred et al., 2024; Vetrivel et al., 2024).

Digital twins are utilized in multiple facets of optimizing chemical manufacturing processes, including the modeling and enhancement of reactor conditions, forecasting product quality, and improving energy efficiency (Mohamed et al., 2023). Utilizing artificial intelligence and machine learning methods such as Support Vector Machine (SVM) optimization, digital twins can analyze data from various interconnected sources to enhance digital transformation processes in chemical plants (Alfred et al., 2024; Vetrivel et al., 2024).

The integration of digital twins with Industry 4.0 technologies has significantly broadened their capabilities in chemical manufacturing. The virtual models facilitate automated real-time process analysis among interconnected machines and data sources, enhancing the speed of error detection and correction in chemical production lines (Zhihan, 2023). Furthermore, digital twins can be used to improve energy efficiency in chemical processes, which may lead to significant cost reductions and increased sustainability (Billey & Wuest, 2024; Mohamed et al., 2023).

Real-time implementation of digital twins extends beyond the chemical industry. In manufacturing, they are widely adopted for predictive maintenance, production streamlining, and efficient asset management (Zhong et al., 2023). These applications illustrate the transformative impact of digital twins, enabling smarter and more agile operations. The ongoing digital transformation in the chemical industry is expected to significantly benefit from such advancements, promoting continuous improvement and innovation.

3.2 Predictive Maintenance

In the industrial sector, digital twins serve as essential instruments for enhancing efficiency and fostering innovation, particularly in the area of predictive maintenance. These virtual representations of physical assets and processes facilitate real-time monitoring, simulation, and optimization of chemical manufacturing operations (Vetrivel et al., 2024). In the context of predictive maintenance, digital twins leverage AI and machine learning algorithms to analyze data from multiple interconnected sources, such as IoT devices, to anticipate equipment failures and inefficiencies (Alfred et al., 2024; Rane & Shirke, 2024). This approach results in notable reductions in downtime, lower production expenses, and extended asset lifespans.

The integration of digital twins with IoT devices enables continuous data collection and transmission from various components of chemical processing equipment (Golovan et al., 2024). This ongoing stream of information enhances the accuracy of maintenance forecasting, optimizes resource allocation, and increases operational effectiveness.

Additionally, digital twins facilitate scenario simulation, allowing chemical manufacturers to test and refine maintenance strategies without halting actual production (Cespedes-Cubides & Jradi, 2024). This method has also proven effective across other sectors. For instance, in construction, digital twins are applied for lifecycle management and operational efficiency, integrating IoT data for predictive analytics and resource planning (Mousavi et al., 2024). These real-time capabilities underline the cross-industry potential of digital twins in maximizing uptime and system reliability.

3.3 Safety and Risk Management

Digital twins have emerged as a significant resource in the chemical industry, especially for enhancing safety and risk management within manufacturing processes. These digital replicas enable comprehensive simulations and evaluations of multiple operational scenarios, allowing for early hazard detection and enhanced safety protocols (Alfred et al., 2024; Vetrivel et al., 2024). Real-time observation and analysis of interconnected data sources support proactive maintenance and risk mitigation strategies.

The ability of digital twins to forecast equipment failures, identify inefficiencies, and simulate emergency conditions contributes directly to improving safety standards and reducing the likelihood of accidents (Alfred et al., 2024; Zhihan, 2023). The integration of AI further strengthens these capabilities by enabling faster and more informed decision-making in response to potential threats (Elbouzidi et al., 2023; Vetrivel et al., 2024).

Digital twins also contribute to sustainability by minimizing waste and environmental impact, thus supporting broader risk management goals (Abu-Hassan et al., 2024; Alfred et al., 2024). By enabling virtual testing prior to physical implementation, they reduce the need for hazardous experiments and prototypes (Bassey, 2022).

Beyond chemical manufacturing, supply chain management has also embraced digital twins to identify disruptions, enhance predictive risk management, and improve sustainability (Enyejo et al., 2024). These cross-sector applications highlight the growing role of digital twins in establishing safer and more resilient operational systems.

3.4 Product Development and Innovation

Digital twins have become transformative tools in the chemical sector, opening new avenues for efficiency and innovation in product development. These virtual models allow for the simulation and testing of chemical products and processes before physical deployment (Alfred et al., 2024). This capacity enables the early identification of inefficiencies, thereby reducing production costs and accelerating product timelines (Alfred et al., 2024; Ocaña et al., 2024).

In chemical manufacturing, safety and precision are paramount. Digital twins support these needs by allowing virtual product simulations that ensure optimal design and performance. They are also instrumental in advancing sustainability initiatives by reducing resource waste and environmental impact throughout the production lifecycle (Mohamed et al., 2023).

The integration of intelligent systems, such as Intelligent Digital Twin Systems (IDTS), further enhances these capabilities. These systems leverage AI, sensor data, and 5G connectivity to monitor key indicators

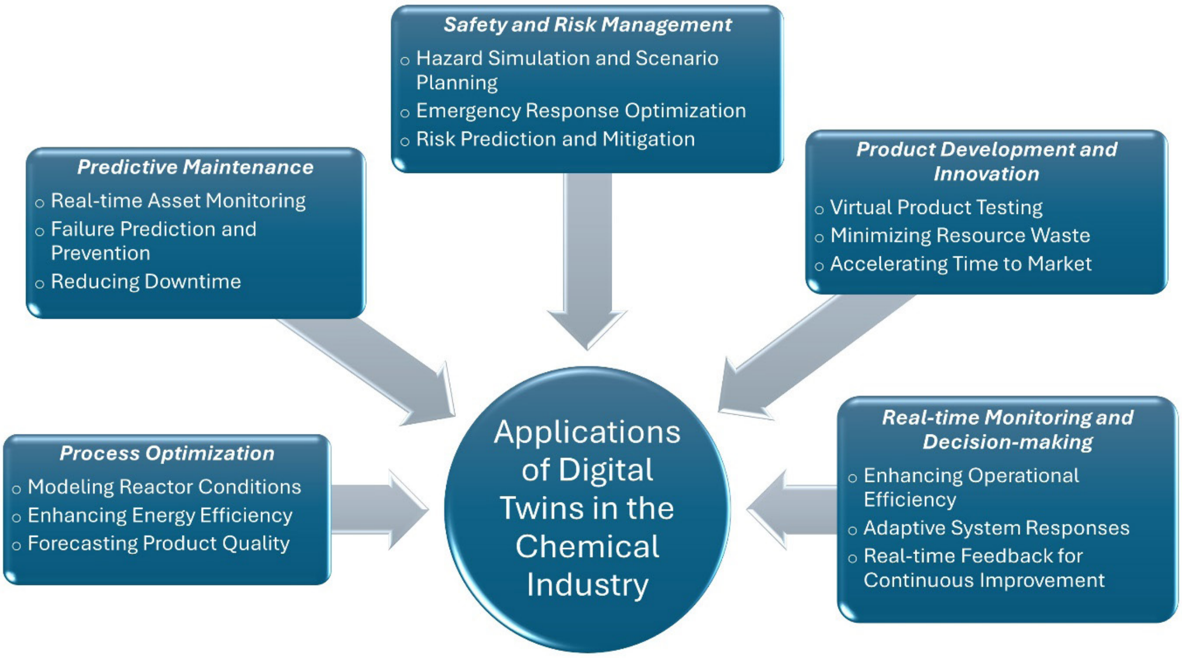

Figure 2. *Applications of Digital Twins in the Chemical Industry*

and optimize energy usage (Zhang et al., 2023; Lim et al., 2021).

Importantly, the application of digital twins is not confined to the chemical sector. In real-world, real-time applications, industries such as manufacturing, construction and supply chain management are reaping similar benefits. These sectors use digital twins to innovate faster, reduce waste and enhance operational control (Zhong et al., 2023; Mousavi et al., 2024; Enyejo et al., 2024). These examples demonstrate how digital twins are driving not only product innovation but also broad operational improvements across global industries (Figure 2).

4. BENEFITS OF IMPLEMENTING DIGITAL TWINS

4.1 Operational Efficiency

The operational efficiency of the chemical industry can be greatly enhanced by implementing digital twins. The virtual representations of physical assets and processes facilitate real-time monitoring, analysis and optimization of chemical operations (Alfred et al., 2024). Implementing this technology allows companies to pinpoint inefficiencies at an early stage, reduce production costs and speed up product launches (Alfred et al., 2024). In chemical plants, digital twins serve to model and optimize production processes, monitor equipment performance and predict maintenance needs. The incorporation of real-time data from sensors and IoT devices enables digital twins to deliver continuous insights into plant operations, facilitating proactive decision-making and reducing downtime (Golovan et al., 2024). This method improves predictive maintenance abilities, optimizes resource distribution and ultimately increases the overall operational efficiency of chemical facilities (Golovan et al., 2024). It is important to highlight that, although digital twins have been thoroughly examined across different industrial domains, their application in current industrial environments, like chemical plants, poses significant challenges due to the intricate nature of these settings (Kamali et al., 2024). Future studies should focus on creating automated data validation methods, real-time processing techniques and advanced 3D visualization approaches to maximize the potential of digital twins in the chemical industry (Kamali et al., 2024).

4.2 Cost Savings

The chemical industry is poised to realize significant financial advantages through the adoption of digital twins, which improve operational efficiency and promote innovation. Although the given context does not specifically target the chemical sector, valuable insights can be drawn from applications observed in other industries. The creation of virtual representations of physical assets facilitates predictive maintenance and process optimization, leading to substantial cost savings. These virtual replicas enable organizations to simulate and monitor essential components, reducing downtime and enhancing resource allocation (Liu et al., 2023). This innovative strategy for maintenance enhances the longevity and efficiency of assets, leading to a reduction in operational costs (Bassey, 2022). The chemical industry is likely to face challenges akin to those experienced in other sectors during the implementation of digital twins. The dependence on Building Information Modeling (BIM) and the necessity for advanced data acquisition systems can present limitations, especially in existing facilities that do not have digital information (Cespedes-Cubides & Jradi, 2024). Nonetheless, these challenges also offer avenues for innovation in creating methodologies that do not solely rely on BIM data.

4.3 Enhanced Decision-Making

The manufacturing sector stands to gain significantly from the implementation of digital twins, facilitating enhanced decision-making via real-time analysis and the optimization of complex processes. The virtual replicas of physical assets and systems offer extensive insights that facilitate informed decision-making across multiple operational dimensions (Korepin et al., 2024; Vetrivel et al., 2024). The integration of artificial intelligence (AI) with digital twins facilitates dynamic and responsive simulations, providing real-time insights into the performance and behavior of physical assets. This combination enables decision-making based on data and enhances predictive management in facility operations (Elyasi et al., 2023; Vetrivel et al., 2024). In the petrochemical process industry, digital twins are regarded as significant business assets, enhancing a crucial aspect of decision-making referred to as 'insight value' (Mcnair, 2022). Nonetheless, in spite of the theoretical advantages that digital twins offer for improved decision-making, a gap exists between scholarly interest and real-world applications in sectors like Architecture, Engineering and Construction (AEC). This gap highlights the necessity for strong frameworks in information management and tackling organizational culture issues to fully leverage the capabilities of digital twins in decision-making processes (Elyasi et al., 2023).

4.4 Sustainability

The chemical sector has the potential to greatly improve its sustainability by implementing digital twins. The use of virtual replicas of physical environments and products allows for comprehensive testing and analysis before actual manufacturing, leading to reduced resource waste and a lower environmental impact (Alfred et al., 2024). Digital twin technology enables the optimization of resource usage, enhances energy management and encourages environmentally sustainable practices in industrial settings (Khan et al., 2024). In the chemical sector, digital twins can play a significant role in enhancing sustainability initiatives through various approaches:

- Carbon emission reduction: The application of digital twins allows for the simulation and optimization of processes, leading to a reduction in the carbon footprint associated with production (Zhang et al., 2024). This is especially important as the sector encounters increasing demand to reduce its ecological footprint.
- Enhancing resource efficiency: Through the application of AI and data analytics, digital twins can detect inefficiencies at an early stage, optimize the use of resources and promote sustainable practices (Alfred et al., 2024; Juarez et al., 2024).
- Enhancement of product lifecycle management: Digital twins have the potential to prolong product lifecycles, promote recycling and align with the principles of circular manufacturing (Juarez et al., 2024).
- Predictive maintenance facilitation: By employing continuous monitoring and diagnostics, digital twins are capable of anticipating failures prior to their occurrence, thereby minimizing downtime and decreasing waste (Bassey, 2022).

It is important to highlight that, although there has been significant growth in the use of digital twins in recent years, the majority of applications tend to prioritize enhancements in productivity, safety and management over sustainability (Zhang et al., 2024). This highlights the potential for the chemical sector to enhance its use of digital twins for environmental benefits.

5. CHALLENGES AND CONSIDERATIONS

5.1 Data Quality and Integration

The chemical field has the potential to achieve significant advantages through the implementation of digital twins, enhancing efficiency and driving innovation. However, obstacles remain, especially in relation to data quality and integration. The implementation of digital twins in chemical production processes requires strong systems for data acquisition and the integration of multiple data streams. This involves integrating process analytical technology tools and existing equipment, along with linking cloud data and simulation models (Chen et al., 2023). The precision of a digital twin representation relies fundamentally on the quality and dependability of the data involved. In the pharmaceutical sector, initiatives are being implemented to develop integrated data management and informatics tools within the Industry 4.0 framework. These efforts are focused on promoting the transition to continuous manufacturing and supporting the creation of digital twins (Chen et al., 2023). It is important to recognize that, despite the significant potential of digital twins in numerous sectors, their application in current structures encounters challenges stemming from reliance on Building Information Modeling (BIM) and the necessity for comprehensive data acquisition systems (Cespedes-Cubides & Jradi, 2024). This highlights the necessity of creating methodologies that do not solely depend on BIM data, to guarantee wider applicability.

5.2 Cybersecurity Concerns

The chemical sector is poised to gain significantly from digital twin technology, which has the potential to enhance efficiency and drive innovation. Nonetheless, the integration of this groundbreaking technology has highlighted cybersecurity concerns as significant challenges that must be addressed (Gupta et al., 2023; Mohsin et al., 2023). The integration of digital twins with advanced technologies such as IoT, AI and machine learning has led to significant improvements in the chemical sector, including heightened productivity, accelerated innovation cycles, improved safety protocols and the development of new business strategies (Dayneko et al., 2024). However, this integration of physical and virtual realms reveals the sector to emerging cybersecurity risks. The shift towards cyber digitization, along with the absence of well-defined information and security standards, has generated opportunities for cybercriminals to take advantage (Homaei et al., 2024). To address these threats, strong cybersecurity measures are crucial. In the chemical industry, it is essential for digital twin systems to focus on secure data transmission, strict access control, robust encryption and sophisticated threat detection capabilities (Gupta et al., 2023). The integration of artificial intelligence within digital twins demonstrates potential in bolstering cybersecurity through advancements in threat detection and response strategies (Homaei et al., 2024). Additionally, the proposal of Security Digital Twins (SDTs) has emerged as a strategy to execute cybersecurity operations during both the design and runtime phases, thereby guaranteeing the precision of data feeds for security monitoring objectives (Mohsin et al., 2023).

5.3 Skill Gap and Training

Chemical manufacturing is experiencing a significant transformation with the implementation of digital twins, which are improving productivity and driving innovation, particularly in tackling workforce skill gaps and training requirements. This technology generates a virtual representation of physical environments, providing a safe and cost-effective approach for training new personnel in complex and hazardous chemical manufacturing sites (Shin & Son, 2024). This method connects theoretical understanding with practical industry application, allowing trainees to acquire practical skills while minimizing the risks often linked to conventional on-site training. The integration of digital twins with extended reality (XR) and the Internet of Things (IoT) is paving the way for innovative advancements in the chemical sector (Kolekar et al., 2023). These technologies enable tailored training simulations, optimizing processes and refining decision-making skills. Nonetheless, the implementation of digital twins encounters challenges, particularly the need for ongoing investigation and innovation to completely harness their capabilities (Kolekar et al., 2023; Luo & Ball, 2023).

5.4 Initial Investment and ROI

The chemical industry has undergone significant transformation due to the implementation of digital twins, leading to enhanced efficiency and fostering innovation. The virtual models of physical systems facilitate real-time monitoring, predictive maintenance and operational optimization, leading to significant improvements in productivity and cost-effectiveness (Alfred et al., 2024; Dayneko et al., 2024). The integration of artificial intelligence and advanced analytics significantly enhances the capabilities of digital twins, facilitating thorough testing and analysis before the onset of physical production (Alfred et al., 2024). Nonetheless, the adoption of digital twin technology in the chemical industry encounters challenges, especially in terms of upfront investment and the assessment of return on investment (ROI). The significant initial costs linked to the implementation of digital twins can pose a considerable challenge, particularly for smaller enterprises (Ogundare et al., 2024). Furthermore, the integration of digital twins with current legacy systems poses technical challenges that could demand considerable resources to resolve (Nalioglu et al., 2023; Ogundare et al., 2024).

Evaluating the return on investment for digital twin technology involves a nuanced and comprehensive methodology. Organizations need to set clear Key Performance Indicators (KPIs) that are specific, measurable, achievable, relevant and time-bound (SMART) to accurately assess the success of their digital investments (Zhang, 2024). These KPIs should include both financial impacts, such as cost reductions and revenue growth, as well as non-financial benefits, like improved operational efficiency and safety (Dayneko et al., 2024; Zhang, 2024). Evaluating digital twin implementations requires a critical comparison of performance against industry benchmarks or historical data, as this provides essential context (Zhang, 2024). Nonetheless, challenges in measuring ROI continue to exist, encompassing issues related to defining appropriate metrics, concerns regarding data quality and the intricacies involved in assessing intangible assets, like enhanced customer experience or heightened employee productivity (Zhang, 2024).

In light of these challenges, digital twins present considerable advantages for the chemical industry. Their contributions to sustainability initiatives involve minimizing resource waste and mitigating environmental impact throughout manufacturing processes (Abu-Hassan et al., 2024; Alfred et al., 2024). Furthermore, digital twins foster an environment that encourages innovation and ongoing enhancement, supporting technological progress and flexibility within business and industrial settings (Alfred et al., 2024). With the ongoing evolution of the chemical sector, it is crucial for companies to invest in digital twin technology to maintain competitiveness and foster positive transformations in a complex global environment (Alfred et al., 2024; Dayneko et al., 2024) (Table 3).

Table 3. *Challenges and Solutions in Implementing Digital Twins*

Challenge	Description	Proposed Solution
High Initial Investment	Costly infrastructure and setup	Modular implementation, phased rollout
Data Integration Issues	Legacy systems and heterogeneous data	Use of middleware, IoT gateways
Lack of Skilled Workforce	Need for expertise in multiple domains	Training programs, skill development
Cybersecurity Concerns	Risks of data breaches	Advanced encryption, secure networks

6. FUTURE TRENDS AND OPPORTUNITIES: IMPLEMENTATION OF DIGITAL TWINS

6.1 AI and Machine Learning Integration

The manufacturing sector has undergone significant transformation due to the implementation of digital twins, leading to enhanced efficiency and fostering innovation. The integration of virtual models of physical assets and processes with advanced technologies such as IoT, AI and ML is aimed at optimizing operations and refining decision-making (Kolekar et al., 2023; Rathore et al., 2021). In the chemical sector, digital twins are utilized to improve production processes, forecast maintenance needs and reduce downtime (Kolekar et al., 2023). These advancements facilitate extensive data analysis and the integration of artificial intelligence and machine learning, opening up new pathways for optimizing processes and developing predictive models (Rathore et al., 2021). Implementing digital twins in this industry, however, poses challenges including cybersecurity threats, data privacy concerns and the need for specialized software and infrastructure (Dayneko et al., 2024; Sarker et al., 2024). The future prospects for digital twins within the chemical sector appear promising. Continuous progress in artificial intelligence and machine learning is expected to enhance digital twin functionalities, enabling more accurate simulations and predictive analytics (Rathore et al., 2021). The incorporation of technologies like blockchain, augmented reality and cloud computing is anticipated to lead to the development of more sophisticated applications (Dayneko et al., 2024). With the ongoing digital transformation in the industry, digital twins are set to play a crucial role in advancing sustainable development and ensuring a competitive advantage in a more intricate global marketplace (Dayneko et al., 2024; Vetrivel et al., 2024).

6.2 Extended Reality (XR) Applications

The Industrial sectors is poised for a significant transformation, as digital twins and extended reality (XR) applications are expected to enhance efficiency and foster innovation. The integration of digital twins with XR technologies presents exceptional opportunities for enhancing processes, refining decision-making and reducing waste in chemical production (Kolekar et al., 2023). XR technologies, which include virtual reality (VR), augmented reality (AR) and mixed reality (MR), provide advanced user experiences that can be seamlessly integrated into digital twin simulations. This integration facilitates the development of dynamic and interactive settings that enhance real-time monitoring, control and optimization of chemical processes (Oh & Shon, 2024). For instance, tools that utilize augmented reality can aid operators in the setup and maintenance of equipment by providing enhanced visualization and digital information, which may lead to increased productivity and reduced processing times (Mahmood et al., 2024). It is essential to acknowledge that the increasing adoption of XR devices in industrial control systems (ICS) and digital twin environments brings with it significant cybersecurity risks. Given that these devices are connected to networks, the control and production data they manage are at risk of cyberattacks. Therefore, establishing strong security measures and performing digital forensic analyses are crucial for guaranteeing the secure and reliable functioning of XR-enhanced digital twins within the chemical industry (Oh & Shon, 2024). In light of these challenges, the integration of digital twins and XR technologies in the chemical sector presents significant opportunities for improving efficiency, driving innovation and advancing sustainability in the context of Industry 5.0 (Kolekar et al., 2023; Tu et al., 2023).

6.3 Blockchain for Data Integrity

The manufacturing sector stands at the threshold of a significant transformation, driven by the integration of digital twins and blockchain technology, which heralds improvements in efficiency, innovation and data integrity. This technological integration presents significant opportunities for enhancing processes, ensuring quality and optimizing supply chains (Yang, 2024). The decentralized, transparent and unalterable features of blockchain greatly enhance the reliability, authenticity and safety of digital twins in chemical manufacturing (Chougule et al., 2024). Utilizing the distributed ledger capabilities of blockchain, chemical companies can ensure the integrity and traceability of data across the entire product life cycle, from the sourcing of raw materials to the delivery of the final product (Yang et al., 2024; Ijaz et al., 2024). One significant advantage of integrating digital twins with blockchain in chemical manufacturing is the capacity to oversee and manage production processes in real-time. This integration facilitates more accurate predictive maintenance, reduces downtime and improves overall equipment efficiency (Huang & Liu, 2024). Moreover, blockchain technology has the potential to enhance the security and confidentiality of sensitive information pertaining to chemical formulations and manufacturing techniques, which is crucial in this intensely competitive industry (Yulianjani et al., 2024). However, the widespread adoption of these technologies in the chemical sector encounters hurdles including technical constraints, regulatory difficulties and concerns regarding data privacy (Yang, 2024). Overcoming these challenges requires joint effort among industry stakeholders, technology suppliers and regulatory bodies.

6.4 Cross-Industry Collaboration

The chemical company stands at the threshold of a significant transformation, propelled by cross-sector collaboration and the innovative use of digital twins. The virtual representations of physical assets and processes facilitate real-time monitoring, simulation and optimization, which enhance decision-making and reduces waste in global operations (Kolekar et al., 2023). The integration of digital twins with extended reality (XR) and Internet of Things (IoT) technologies presents remarkable opportunities for innovation across multiple industries, such as chemicals (Kolekar et al., 2023). Nonetheless, in spite of their significant benefits, the

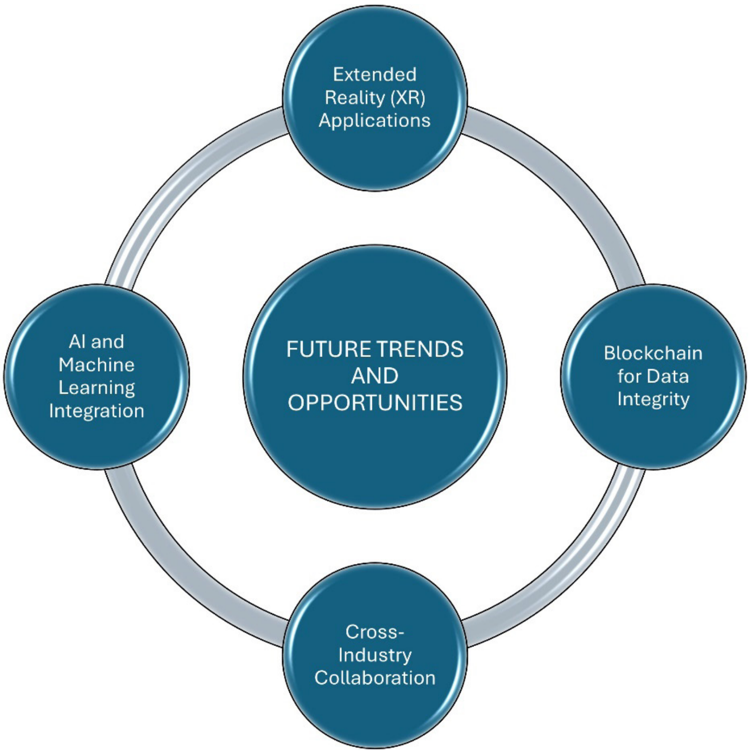

Figure 3. *Future Trends and Opportunities: Implementation of Digital Twins*

implementation of digital twins encounters challenges including data transfer delays, model accuracy and user interface design (Liu et al., 2024). Furthermore, as technology connects physical and virtual realms, cybersecurity emerges as a vital issue, necessitating strong strategies for secure data transmission, access management, encryption and threat identification (Gupta et al., 2023) (Table 4) (Figure 3).

7. CONCLUSION: EMBRACING THE DIGITAL FUTURE

The chemical industry has seen the rise of digital twins as a groundbreaking technology, presenting significant opportunities for enhancing efficiency and promoting innovation. The virtual representations of tangible assets and processes facilitate real-time monitoring, simulation and enhancement of chemical production activities. In the chemical sector, digital twins can be employed to improve process management, predict equipment failures, optimize resource utilization and enhance overall operational efficiency. For instance, these methods can be utilized to simulate and improve chemical reactions, monitor equipment efficiency and predict maintenance needs, leading to reduced downtime and increased productivity. The integration of digital twins with artificial intelligence and machine learning algorithms enhances their functionalities, allowing for more accurate predictions and data-driven decision-making. While there are many benefits to adopting digital twin technology in the chemical sector, obstacles remain. These encompass challenges associated with data protection, integration with existing systems and the necessity for standardization. As technology continues to advance and develop, it is anticipated that these challenges will be addressed, leading to wider acceptance and more sophisticated applications within the chemical sector. The integration of digital twins within the chemical sector represents a vital advancement towards enhanced efficiency, innovation and sustainability, in accordance with the goals of Industry 5.0 and future developments.

Table 4. *Emerging Trends and Innovations*

Trend	Description	Expected Impact
AI-Driven Digital Twins	Use of AI for advanced analytics	Higher accuracy in predictions
Cloud Integration	Hosting digital twins on cloud platforms	Scalability, cost efficiency
AR/VR Integration	Enhanced visualization for training	Improved operator understanding
Blockchain for Security	Securing data transactions	Robust cybersecurity

CONFLICT OF INTEREST DECLARATION

The author declare that they have no affiliations with or involvement in any organization or entity with any financial interest in the subject matter or materials discussed in this manuscript.

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