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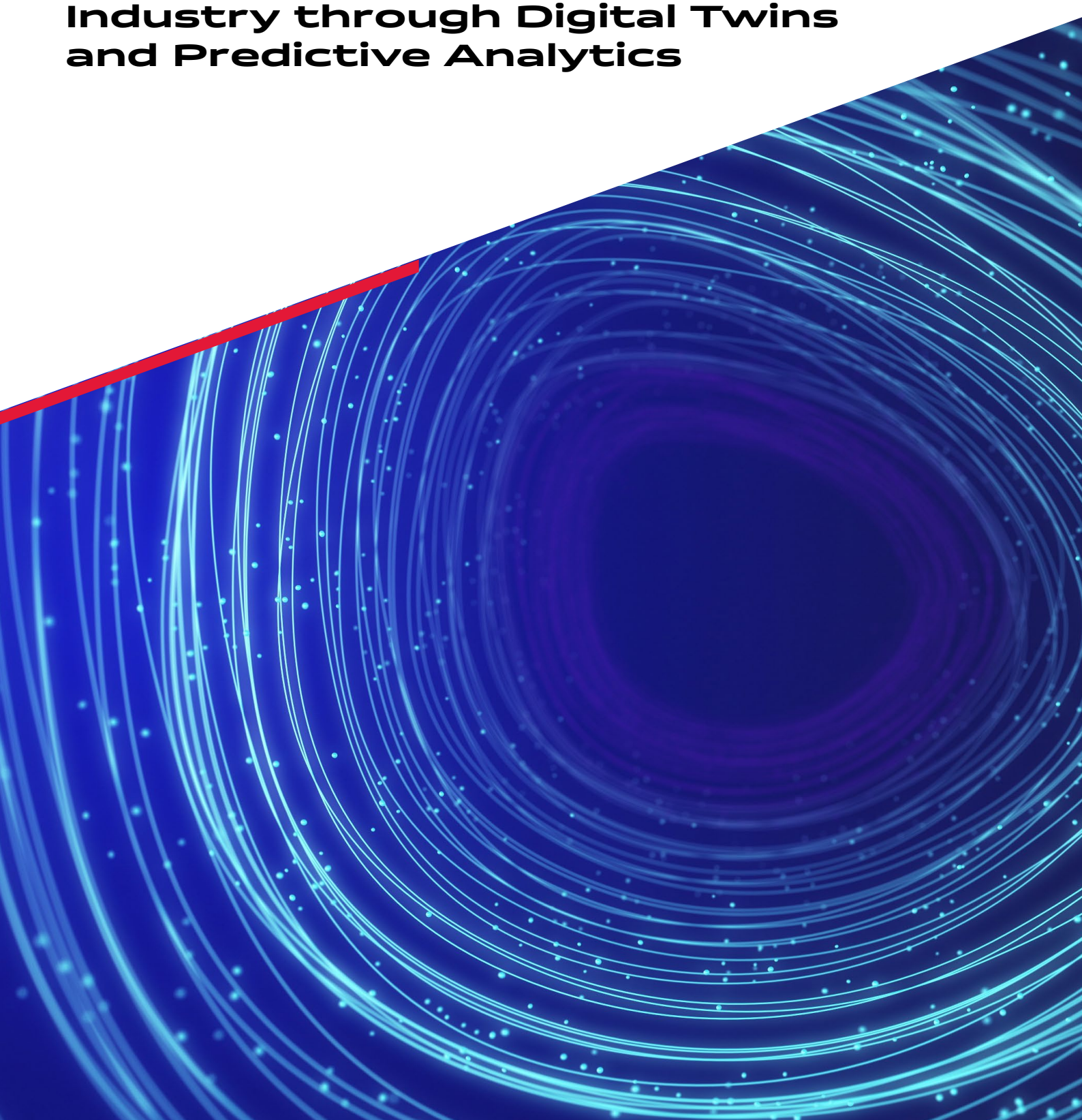
WHITEPAPER

Unlocking Operational Excellence in the Chemical Industry through Digital Twins and Predictive Analytics



Summary

Digital Twins and Predictive Analytics are revolutionizing the chemical, pharmaceutical, and energy sectors by **enabling real-time monitoring, intelligent forecasting, and data-driven decision-making.** These technologies help industries optimize operations, enhance safety, improve product quality, and support sustainability. Real-world applications demonstrate their impact: Tech Mahindra's AI-powered digital twin improved vaccine production consistency; predictive models in oil & gas boosted asset reliability and ESG compliance; and chemical industry twins enhanced planning and environmental performance. Despite their potential, challenges like data integration, model fidelity, cybersecurity, ROI justification, and standardization must be addressed. Overcoming these barriers is key to building agile, future-ready ecosystems. **Looking ahead, the convergence of Digital Twins, Predictive Analytics, and Industry 4.0 technologies is driving autonomous, intelligent, and sustainable industrial operations.** These innovations are not just technological upgrades—they are strategic imperatives for industries aiming to thrive in a rapidly evolving global landscape.

Introduction

In 2024, the chemical industry saw steady growth, surpassing 2023 production levels. This momentum is expected to continue into 2025, driven by easing destocking and rising demand. The American Chemistry Council forecasts global chemical production **growth of 3.4% in 2024 and 3.5% in 2025**. After a strong post-pandemic rebound, the industry faced challenges in 2022-2023, including supply chain normalization and declining margins, prompting cost-cutting measures that improved performance by early 2024.

Despite recovery, the sector faces ongoing pressures from economic shifts, regulatory changes, and evolving customer needs. Companies are responding with investments in decarbonization, innovation, and strategic transformation to build a resilient, low-carbon future. **Operational excellence, process redesign, and asset upgrades have been key focus areas, with 18% of firms prioritizing efficiency and 26% replacing aging infrastructure.** Yet, challenges persist—batch variability, energy inefficiencies, and reliance on paper-based tracking hinder optimization. Skilled labour shortages further complicate operations.

Digital innovation is reshaping the landscape. Technologies like Digital Twins and Predictive Analytics are helping manufacturers reduce costs, improve agility, and enhance product quality—ushering in a smarter, more adaptive era for chemical manufacturing.

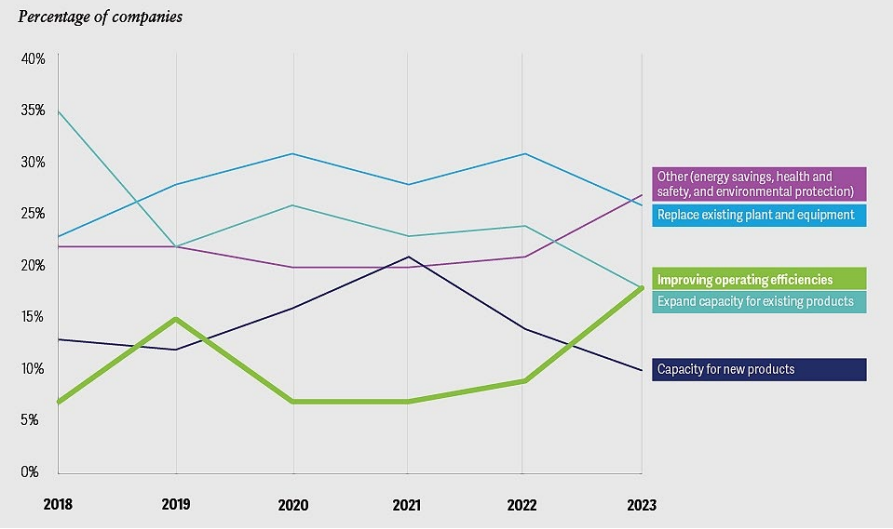


Figure 1: The Percentage of companies surveyed that identified 'improving operating efficiencies' as a key motivation for capital investment doubled between 2022 and 2023

The Power of Digital Twins

A digital twin in the chemical industry is a virtual representation of a physical chemical process, system, or product, mirroring its characteristics and behaviour throughout its lifecycle. Digital twins can be implemented in both offline and online modes. Offline digital twins are used for simulation, analysis, and long-term planning, while online digital twins are used for real-time monitoring, control, and decision-making, providing a dynamic, two-way connection between the physical and digital worlds using real-time data from sensors, control systems (SCADA, DCS), and historical records. Unlike static models, digital twins evolve dynamically, enabling industries to optimize operations, reduce costs, and make smarter decisions .

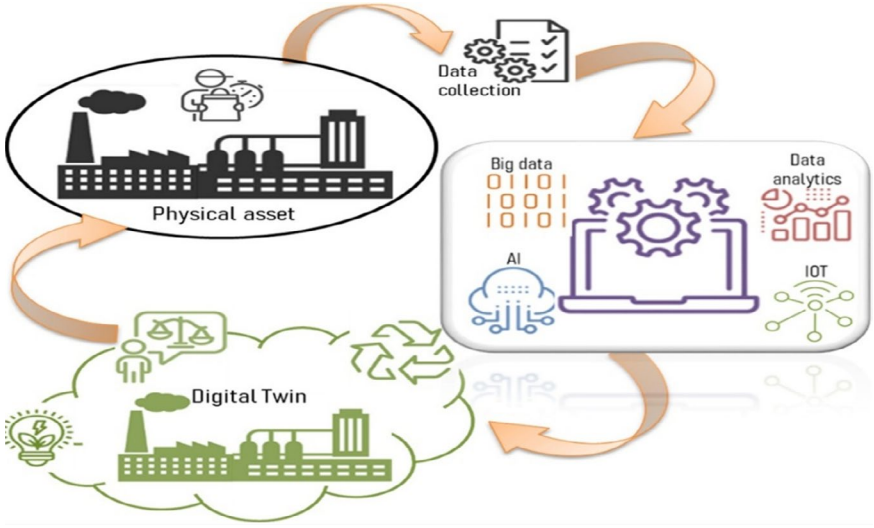
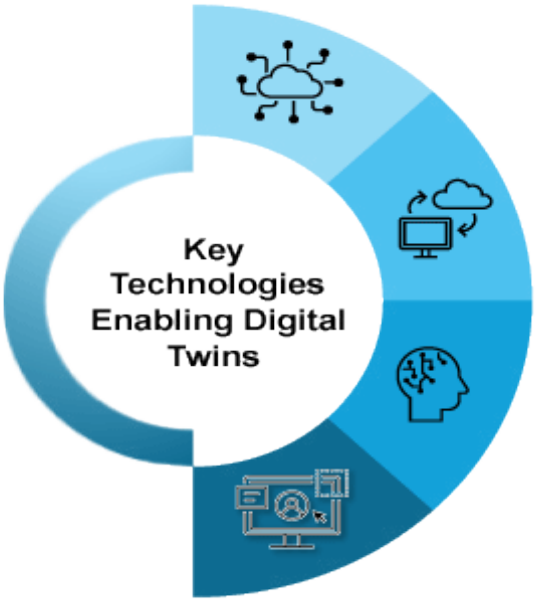


Figure 2:Schematic of digital twin in the chemical industry



INTERNET OF THINGS (IOT)

lot forms the sensory and nervous system of digital twins. It connects devices-from sensors to machinery that collect and transmit real-time data, making digital twins responsive and data-driven.

CLOUD COMPUTING

Cloud platforms provide the scalable infrastructure and computational power needed to store, process, and analyse the vast data streams from digital twins. This enables real-time simulations, analytics, and accessibility

AI ML

Al and ML empower digital twins to analyse data, predict outcomes, and optimize performance. They detect anomalies, forecast failures, and support scenario planning, transforming digital twins into intelligent, adaptive systems.

SIMULATION SOFTWARE

This software underpins digital twins by modelling and visualizing physical systems. When integrated with real-time data, it enables continuous monitoring, predictive analytics, and performance optimization, turning static models into dynamic, intelligentreplicas.

Together, these technologies create a robust framework that enhances operational efficiency and asset understanding.

Benefits of Digital Twins in the Chemical Industry

Training and Simulation:

Digital twins replicate entire chemical plants, offering immersive, risk-free training environments. Operators can practice startup, shutdown, and emergency procedures, simulate malfunctions, and receive real-time feedback. This builds confidence, improves decision-making, and ensures compliance through continuous learning and certification tracking.

Enhanced Safety:

Digital twins continuously monitor operations to detect anomalies and simulate hazardous scenarios. They forecast risks like pressure spikes or equipment fatigue, enabling preventive actions. They also support emergency planning by modelling failure impacts and guiding mitigation strategies, fostering a safer work environment.

Process Optimization:

Digital twins provide real-time insights into process parameters, enabling early detection of inefficiencies. Engineers can simulate "what-if" scenarios—like changes in feedstock or temperature—without disrupting operations. This helps optimize reaction kinetics, heat exchange, and separation processes, improving resource efficiency and reducing waste.

Predictive Maintenance:

By simulating equipment behaviour and integrating sensor data with ML, digital twins predict component failures before they occur. This allows proactive maintenance, reducing unplanned downtime and extending asset life. Companies like BASF and Dow have cut downtime by up to 50% using this approach.

Improved Product Quality:

Digital twins help manufacturers test formulations and detect quality deviations early. This reduces trial-and-error, accelerates troubleshooting, and enables faster scaling from lab to production—ensuring consistent, high-quality output.

Leveraging Predictive Analytics

Manufacturing is undergoing a digital transformation, moving from manual data collection to IoT-enabled systems that improve accuracy and enable smarter decision-making. This evolution supports a progression from descriptive and diagnostic analytics to predictive and prescriptive analytics, allowing manufacturers to turn raw data into actionable insights. Predictive analytics uses statistical and machine learning techniques to analyse historical and real-time data, helping forecast potential issues and optimize operations

By leveraging sensor data and production system inputs, predictive analytics enables proactive problem-solving, reducing downtime and improving product quality. It also enhances resource allocation, streamlines scheduling, and minimizes waste—making it a key driver of efficiency and profitability in modern manufacturing environments.

Predictive analytics, when integrated with digital twins, further amplifies their capabilities and driving proactive decision-making by:

1 Forecasting Future Trends and Outcomes

Advanced models anticipate changes in production, market demand, and equipment performance. This empowers chemical companies to make proactive decisions, optimize resources, and stay ahead of market shifts—enhancing strategic planning and innovation.

2 Optimizing Operations

Predictive analytics identifies inefficiencies and forecasts equipment behaviour. It recommends optimal conditions (e.g., temperature, pressure), enabling agile adjustments that improve resource use, product consistency, and cost-efficiency.

3 Providing Actionable Insights

Beyond forecasting, it offers prescriptive actions. For instance, if catalyst degradation is predicted, it may suggest feedstock changes or maintenance scheduling—helping maintain performance and reduce risks.

4 Quality Control

Predictive models detect early signs of quality deviations (e.g., viscosity, pH), allowing real-time process adjustments. This minimizes waste, ensures compliance, and boosts customer satisfaction.

5 Energy Efficiency

It identifies energy usage patterns and inefficiencies, recommending operational tweaks or equipment upgrades to reduce consumption—like adjusting distillation pressure to save steam.

6 Sustainability

Digital twins combined with predictive analytics help minimize waste and environmental impact, supporting sustainability goals.

7 Supply Chain Optimization

By analysing historical data and external factors, predictive models forecast demand and guide inventory planning—reducing costs and improving responsiveness.

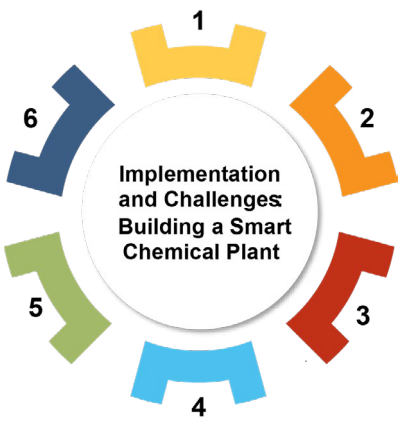
Implementation and Challenges: Building a Smart Chemical Plant

Successfully implementing digital twins and predictive analytics in the chemical industry requires addressing several key challenges:

Data Quality and Integration
Accurate digital models depend on integrating data from sensors, control systems, and historical records. However, legacy systems often produce fragmented, inconsistent data. Overcoming this requires strong data governance, cleansing tools, and seamlessIT-OT integration to enable real-time insights and reliable analytics

High Fidelity Model
Developing precise models demands deep process knowledge, advanced computing, and specialized platforms like Aspen HYSYS. Success depends on building in-house expertise, fostering trust in digital tools, and refining models through collaboration and iteration.

Cost and ROI
High initial costs and uncertain short-term returns make ROI justification challenging Organizations should start with pilot projects, define measurable KPIs, and use success stories to build a strong business case and secure stakeholder support.



Cybersecurity and Data Management
Digital twins are vulnerable to cyber threats due to constant connectivity. Companies must implement encryption, access controls, and regular audits while complying with standards like IEC 62443. Strong data governance and regulatory compliance are essential to protect sensitive information.

Analytic Deployment, Visualization, and Insights
Deploying AI/ML models requires robust infrastructure and real-time data flow. Visualization tools must be intuitive yet capable of handling complex analytics. Aligning legacy systems and ensuring model accuracy across processes are key to effective implementation

Lack of Standardization
The evolving nature of digital twin technology and absence of standardized frameworks hinder seamless integration and interoperability across platforms.

Figure 4: Implementation and Challenges: Building a Smart Chemical Plant

Case Studies

• Predictive Process Optimization in Pharma: A Tech Mahindra Case Study

In bio-vaccine manufacturing, maintaining consistent batch quality is critical, as even small deviations can lead to costly rejections and delays in delivering essential treatments. To address this, Tech Mahindra introduced AI/ML-powered Digital Twins—virtual replicas of production systems that simulate real-time environments. These twins integrate machine data with advanced analytics to monitor process quality, detect trends, and forecast outcomes. The solution provides real-time insights and visualizations of key parameters like flow properties and particle distribution, enabling proactive interventions and reducing variability.

The deployment has significantly improved operational efficiency, reduced batch rejection rates and enhanced throughput. Real-time alerts and feedback loops allow for immediate corrective actions, while continuous learning refines the AI/ML models over time. Built on a robust architecture with cloud-based data management and edge-deployed analytics, the system ensures low-latency processing and seamless IT-OT integration. By combining predictive analytics with real-time monitoring, Tech Mahindra's Digital Twin solution empowers manufacturers to achieve greater consistency, reduce waste, and uphold high standards of quality—making it a strategic asset in precision-driven pharmaceutical production.

• Tech Mahindra's AI-Driven Reliability Framework for Aging Oil & Gas Infrastructure

One of the notable implementations by Tech Mahindra in the Oil & Gas sector involved a crude preheater heating section, where advanced predictive models were developed to enhance asset reliability and reduce downtime. Using techniques such as Auto Regressive Integrated Moving Average (ARIMA), the solution forecasted the Overall Heat Transfer Coefficient (OHTC) over time. Additionally, multivariate time series models were employed to predict OHTC as a function of both time and exogenous variables like emulsion percentage, filterable solids, and feed flow rate. To further improve prediction accuracy, ensemble learning methods including Random Forest, Gradient Boosting, and Extreme Gradient Boosting were integrated into the platform. This predictive framework enabled the estimation of Mean Time to Repair (MTTR) failures with 95% accuracy, allowing for timely interventions and minimizing unplanned outages. As a result, asset availability improved by 1%, translating to an additional 3.65 days of EBITDA annually. Maintenance costs were reduced by 10% through optimized scheduling and resource allocation. Moreover, refinery planning and scheduling functions benefited from advanced notice of unit constraints, enhancing Gross Refining Margin (GRM) forecasting and overall operational efficiency.

• Enhancing Operational Visibility and ESG Compliance in Oil & Gas

In the Oil & Gas sector, Tech Mahindra implemented Digital Twins for asset management and operational visibility. By integrating ERP systems with telematics, the solution enabled real-time tracking of trucks and job statuses, improving safety and reducing downtime. Specialized twins like Operation and Maintenance (O&M) Digital Twin provided granular insights into asset health, while the Sustainability Twin tracked emissions and resource usage to support ESG compliance. Engineering & Construction (E&C) Twins simulated plant layouts and workflows, enhancing lifecycle planning and safety. These innovations contributed to a $55M productivity gain and optimized MRO inventory spend by 10–15%.

• Optimizing Planning and Compliance in Chemicals

Tech Mahindra's Digital Twin solutions brought a paradigm shift to the chemical industry. These twins enabled predictive maintenance, regulatory compliance, and data-driven decision-making. The Sustainability Twin monitored emissions, energy, and water usage in real time, supporting proactive environmental management. Predictive analytics helped balance demand and supply, integrating with SAP APO and SNP systems to reduce inventory by 20% and improve planning efficiency by 25%. The solution also enhanced safety and compliance through real-time monitoring of hazardous materials and complex logistics.

Conclusion & Future Outlook of Digital Twin and Predictive Analytics in Chemical Industry

Analytics, and other Industry 4.0 technologies like AI and machine learning is paving the way for a more autonomous, intelligent, and sustainable chemical manufacturing future. As the industry continues to embrace these advancements, it can expect further improvements in operational efficiency, safety, and environmental performance, leading to greater profitability and a more competitive edge. Digital Twins and Predictive Analytics are not just buzzwords—they are strategic tools that can revolutionize chemical manufacturing. By embracing these technologies, companies can achieve operational excellence, drive innovation, and maintain a competitive edge in a rapidly changing landscape.

Author

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Pragati is a Chemical Engineer with over 11 years of experience spanning diverse yet interconnected domains within the industrial sector. Her expertise covers process engineering and consulting across verticals such as Chemicals, Oil & Gas, Nutrition & Health, and Process Manufacturing. At the intersection of technology and operations, she specializes in process simulation, R&D, digital transformation, IoT, and vertical consulting—bringing deep domain knowledge to architect innovative solutions that drive efficiency and value across the process industry landscape.
At Tech Mahindra, Pragati is working as a Process SME. With her deep domain knowledge, she is responsible for architecting new solutions across the Process value chain.

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A recognized thought leader in asset performance management and manufacturing operations, specializing in MES, EAM, QMS, PLM, EH&S, and AI/ML applications. Additionally, he is an active mentor to entrepreneurs, providing guidance and insights to foster innovation and growth.

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