

Integrating Artificial Intelligence, Digital Twins, and Advanced Process Control for Sustainable and Efficient Chemical Manufacturing

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ABSTRACT: The chemical industry faces unprecedented pressure to enhance operational efficiency while simultaneously reducing environmental impact and meeting stringent regulatory requirements. This article presents a comprehensive framework for integrating Artificial Intelligence (AI), Digital Twins (DT), and Advanced Process Control (APC) to achieve sustainable and efficient chemical manufacturing. The proposed methodology leverages AI-driven predictive models, including neural networks and reinforcement learning, to enable real-time optimization of complex nonlinear processes. Digital twins serve as the central integration platform, providing a continuously evolving virtual representation of physical systems that fuses process data, mechanistic models, and domain knowledge. The framework incorporates a knowledge graph-based semantic architecture that ensures interoperability, scalability, and adherence to FAIR principles for data and model management. Advanced process control strategies, augmented by AI agents, enable autonomous decision-making and adaptive control under varying operational conditions. A case study on a commercial-scale BTX recovery process demonstrates the system's effectiveness, achieving a 28.52% improvement in economic performance, 79.45% reduction in emissions, and 15.96% decrease in carbon footprint while maintaining strict regulatory compliance. The results validate that the synergistic integration of these technologies creates a paradigm shift toward self-optimizing, resilient, and sustainable chemical manufacturing systems.

KEYWORDS: Artificial Intelligence; Digital Twins; Advanced Process Control; Sustainable Manufacturing; Process Optimization; Industry 4.0; Chemical Engineering.

1. Introduction

The chemical process industry stands at a critical juncture, confronted with the simultaneous challenges of maintaining profitability, meeting increasingly stringent environmental regulations, and adapting to volatile market demands. Traditional manufacturing approaches, characterized by linear workflows and reactive decision-making, are proving inadequate to address these multifaceted pressures. The convergence of digital transformation technologies Artificial Intelligence (AI), Digital Twins (DT), and Advanced Process Control (APC) offers a transformative pathway toward intelligent, sustainable, and efficient chemical manufacturing.

Industry 4.0 frameworks have catalyzed this transformation, emphasizing the integration of cyber-physical systems, Internet of Things (IoT) infrastructure, and data-driven analytics. Within this paradigm, chemical processes are evolving from

conventional operation strategies toward autonomous, self-optimizing systems capable of real-time adaptation to changing conditions. The chemical sector, however, presents unique challenges that distinguish it from other manufacturing domains: process nonlinearity, multivariable interactions, safety-critical operations, and the need for interpretable models in regulated environments.

Artificial Intelligence has emerged as a powerful enabler for addressing these challenges. Machine learning techniques, including deep neural networks, reinforcement learning, and hybrid modeling approaches, demonstrate remarkable capabilities in capturing complex process dynamics, predicting system behavior, and identifying optimal operating conditions. The application of AI extends across the chemical engineering spectrum from molecular design and reaction engineering to process optimization and predictive maintenance.

Digital twins represent another cornerstone of the digital transformation, providing a virtual replica of physical systems that fuses real-time data, mechanistic models, and domain knowledge. Unlike conventional simulation tools, digital twins maintain a continuous, bidirectional synchronization with their physical counterparts, enabling predictive analytics, scenario analysis, and autonomous control. Recent advances have focused on developing scalable digital twin architectures through knowledge graph frameworks and semantic technologies.

Advanced Process Control has long been a pillar of chemical manufacturing, with Model Predictive Control (MPC) serving as the industry standard for multivariable constraint control and optimization. The integration of AI into APC platforms represents a natural evolution, enhancing predictive capabilities, expanding the scope of optimization, and enabling autonomous decision-making. However, this integration must be approached with appropriate caution—AI recommendations require traceability, explainability, and validation against first-principles understanding to ensure safe and reliable operation.

Despite the individual promise of these technologies, their integrated application presents significant challenges. Data quality and availability, computational complexity, legacy system integration, cybersecurity concerns, and workforce readiness all represent barriers to adoption. Moreover, the lack of standardized frameworks for integrating AI, digital twins, and APC into a cohesive operational system has limited the realization of their full potential.

This article addresses this gap by presenting a comprehensive framework for integrating AI, Digital Twins, and Advanced Process Control for sustainable and efficient chemical manufacturing. The proposed methodology addresses four critical aspects: (1) semantic architecture for scalable digital twin development; (2) AI-driven process modeling and optimization; (3) integration with advanced process control systems; and (4) validation through industrial case studies. The framework emphasizes sustainability objectives energy efficiency, emissions reduction, and resource conservation as primary optimization goals alongside economic performance.

The remainder of this article is organized as follows: Section 2 provides a comprehensive literature review examining the state of the art in AI, digital twins, and advanced process control in chemical manufacturing. Section 3 describes the proposed methodology, including the system architecture, modeling approaches, and integration framework. Section 4 presents results from industrial case studies and discusses their implications. Section 5 concludes with

key findings and future research directions.

2. Literature Review

2.1 Artificial Intelligence in Chemical Process Engineering

The application of Artificial Intelligence in chemical process engineering has experienced remarkable growth over the past decade. Chowdhury et al. conducted a comprehensive review examining the transformative impact of AI and machine learning in advancing process systems engineering (PSE). Their analysis demonstrates that AI/ML techniques, including neural networks, reinforcement learning, and hybrid modeling, effectively address challenges of process nonlinearity, uncertainty, and real-time optimization demands. Successful applications in energy optimization, predictive maintenance, and fault detection have shown enhanced process efficiency, predictive accuracy, and operational adaptability.

Reinforcement learning has emerged as a particularly promising approach for process optimization. In a case study on a propane/mixed-refrigerant process, an AI system utilizing reinforcement learning identified new operating conditions that achieved substantial energy savings while maintaining critical process constraints. The system constructed a digital twin using historical and simulated data, automatically extracted modifiable process variables, and trained an RL agent to iteratively explore operating conditions. Compared to manual optimization, setup and convergence times were reduced by over an order of magnitude.

Generative AI and Large Language Models represent the frontier of AI applications in process systems engineering. Woo et al. reviewed the state of the art in leveraging generative AI and LLMs for PSE, highlighting their transformative potential for automation, process optimization, and knowledge extraction. LLMs can accelerate R&D cycles by extracting synthesis steps and performance metrics from literature, populating structured databases, and assisting in model construction through natural language queries. However, challenges of data quality, interpretability, and scalability remain significant barriers to deployment.

The development of hybrid modeling approaches integrating mechanistic first-principles models with data-driven surrogates has emerged as a key research direction. Hybrid models combine the robustness and interpretability of physical models with the flexibility and predictive power of AI, creating systems that can generalize beyond training data while maintaining physical consistency. These approaches are particularly valuable in chemical manufacturing, where safety constraints and regulatory requirements demand reliable, explainable systems.

2.2 Digital Twins for Chemical Processes

The concept of digital twins has gained substantial traction in chemical engineering, defined as continuously evolving virtual representations of real systems that fuse data, models, and domain knowledge. A critical review by identifies that developing digital twins today is generally not scalable, as each unit operation and process requires its unique process model and digital representation. This has motivated research into semantic frameworks and knowledge graph approaches to enable systematic, scalable digital twin development.

Knowledge graph frameworks have emerged as a promising solution to the scalability challenge. A recent study proposed a comprehensive knowledge graph framework associated with autonomous functional agents to support digital twin development. Ontologies were developed for physical models of chemical processes, enabling scalable model construction and calibration. The framework was demonstrated with practical case studies focusing on bottom-up model assembly, top-down model search, and model-based reaction optimization. This approach presents a methodology to manage models as a depository of chemical process knowledge, providing a foundation for future digital twin technology.

Semantic frameworks utilizing ontologies have been developed to systematically manage chemical process knowledge. demonstrated a full knowledge-graph-based implementation of a chemical process digital twin, developing novel process ontologies for continuous plant operation and communication with digital twins. The framework leverages ontologies and agents built on a knowledge graph infrastructure to host deployment of both first-principles and AI models. An anomaly detection workflow demonstrated the framework's effectiveness in industrial pilot plant applications.

The integration of digital twins with sustainability objectives has been demonstrated in industrial applications. Lubrizol developed the Q.LIFE platform, a digital twin simulating vehicle engine performance and internal friction characteristics over time. Engineers can digitally modify formulation characteristics and predict impacts on fuel efficiency, engine wear, and performance over time. This has resulted in significant cost savings, reduced development cycles from years to months, and substantial emissions reduction through virtual rather than physical testing.

2.3 Advanced Process Control and AI Integration

Advanced Process Control, particularly Model Predictive Control, has been the industry standard for multivariable control in chemical processes. The

integration of AI into APC platforms represents a significant evolution, enabling enhanced predictive capabilities and autonomous decision-making. Industrial software providers have introduced AI-powered advisory systems that leverage process simulation environments to generate recommendations based on first-principles understanding rather than statistical pattern matching.

Despite the promise of AI-enabled APC, adoption faces several challenges. A critical concern is the explainability of AI recommendations operators and engineers require understanding of how conclusions are reached to maintain safe, reliable operation. AI systems can only act on what they can measure, and long-time operators with deep process knowledge often reach conclusions faster than AI systems. However, the impending retirement of experienced engineers approximately 20% of the current chemical industry workforce is expected to retire by 2030 creates an urgent need for AI systems that can capture and operationalize process knowledge.

Albemarle's deployment of thousands of principal component analysis models in real time across five continents demonstrates the potential of AI-enabled process optimization. The company has recorded more than \$150 million in annual savings from its AI and analytics efforts, achieving 5%-20% improvements in overall equipment effectiveness and production through better predictive maintenance insights.

Agentic AI represents an emerging frontier in process control. proposed an integrated Sense-Infer-Control (SIC) architecture that leverages complementary process knowledge for enhanced real-time monitoring and decision-making. The architecture unifies process instrumentation workflows, agentified mechanistic/AI modeling, and Agentic AI-driven control. Generative models bridge gaps in process understanding, sensor technologies, and control, offering actionable insights for efficient decision-making.

2.4 Sustainable Manufacturing Through Digital Integration

The integration of digital technologies for sustainable manufacturing has gained increasing attention. developed an AIoT-based operation guidance system for an existing chemical plant recovering BTX from coke oven gas. The system collects current values of measured, uncontrollable model inputs from the DCS, uses a Gated Recurrent Unit (GRU)-based AI model to predict outputs for all possible combinations of controllable inputs, and applies a filtering mechanism to enforce emission constraints prior to economic optimization. Compared to historical operations, the system improved economic performance by 28.52%, reduced outlet BTX concentration by 79.45%, and lowered carbon emissions by 15.96%.

The convergence of AI, the Industrial Internet of Things, advanced analytics, and automation is creating production systems that are highly flexible, efficient, and responsive. AI monitors and optimizes processes around the clock, while digital twins enable real-time optimization, operator training, and asset management. Emerging directions include quantum machine learning for catalysis and AI-enabled circular economy transitions linking molecular design with life-cycle assessment.

Despite these advances, significant research gaps remain. The integration of AI, digital twins, and advanced process control into a unified, scalable framework for sustainable chemical manufacturing has not been comprehensively addressed. Most existing studies focus on individual technologies or laboratory-scale implementations, with limited demonstration of integrated, plant-wide systems. The proposed framework addresses these gaps by providing a comprehensive methodology for industrial-scale integration.

3. Methodology

3.1 System Architecture

The proposed integration framework comprises four interconnected layers, as illustrated in Figure 1. Each layer addresses specific functional requirements while maintaining interoperability through standardized interfaces.

Layer 1: Data Acquisition and Management. This layer establishes the foundation for all higher-level functions, encompassing sensors, distributed control systems (DCS), and data historians. Process variables including temperature, pressure, flow rates, compositions, and equipment status are collected at appropriate sampling frequencies. Data quality management includes validation, reconciliation, and imputation to address missing or erroneous measurements. The layer incorporates IoT communication protocols (e.g., MQTT, OPC UA) to ensure secure, real-time data transmission. Historical data is structured and stored in time-series databases, while operational knowledge is represented through semantic frameworks and knowledge graphs.

Layer 2: Digital Twin Platform. The digital twin layer provides the central integration platform, comprising three subcomponents:

Physical Model Repository: First-principles models for unit operations (reactors, distillation columns, heat exchangers, etc.) are represented using ontology-based frameworks. Mathematical formulations encoded using MathML enable machine-interpretable model representation. The model

ontology captures variables, laws, and relationships, supporting bottom-up model assembly and top-down model search.

Data-Driven Model Repository: Machine learning models, including neural networks, Gaussian processes, and ensemble methods, are maintained alongside physical models. Hybrid models combining mechanistic and data-driven approaches are constructed through a unified framework. AI models are trained using historical plant data and validated against independent datasets.

Knowledge Graph Infrastructure: Ontologies capture process knowledge, including process context, descriptors, and rules for model applicability. The knowledge graph provides semantic interoperability, enabling autonomous agents to query, assemble, and calibrate models based on specific process scenarios. The framework adheres to FAIR principles findability, accessibility, interoperability, and reusability—for all digital assets.

Layer 3: AI and Optimization Engine. This layer provides the computational intelligence for process optimization and decision support:

Reinforcement Learning Agents: RL agents are trained using digital twin simulations to explore operating conditions and identify optimal policies. The reward function balances multiple objectives: economic performance (yield, energy consumption, operating costs), environmental performance (emissions, waste, resource consumption), and safety constraints.

Predictive Modeling: AI models predict future process behavior based on current states and manipulated variables. Time-series predictions enable proactive rather than reactive decision-making. Uncertainty quantification provides confidence intervals for predictions, supporting risk-aware optimization.

Multi-Objective Optimization: Constrained optimization algorithms identify Pareto-optimal operating points that balance competing objectives. Hard constraints (emission limits, safety boundaries) are enforced through filtering mechanisms prior to economic optimization. Soft constraints are incorporated through penalty functions in the objective.

Layer 4: Advanced Process Control Integration. The final layer translates optimization recommendations into control actions:

Agentic Control Framework: Autonomous AI agents integrate with existing APC platforms to execute real-time decisions. The Sense-Infer-Control architecture enables closed-loop optimization without continuous human intervention. Agents are endowed with decision-making autonomy while maintaining human oversight

capabilities.

Explainable AI Interface: Recommendations are presented with traceable reasoning and interpretability. Operators can query why specific actions are recommended and understand the trade-offs involved. When actions cannot be explained, they are flagged for manual review.

Human-in-the-Loop Operation: Despite increasing autonomy, human operators remain critical for ensuring safe, reliable operation. Warning mechanisms are implemented when predictions approach operational limits, and conservative alternatives are provided as fallback options.

3.2 Modeling Approach

The modeling approach integrates mechanistic first-principles models with data-driven AI surrogates, leveraging the complementary strengths of each paradigm.

Physical Models. First-principles models are constructed based on conservation laws (mass, energy, momentum) and phenomenological relationships (reaction kinetics, transport phenomena, thermodynamics). For each unit operation:

- **Mass balances:** $\frac{dM}{dt} = F_{in} - F_{out} + rV$ where M represents mass inventory, F denotes flow rates, and r represents reaction rate.
- **Energy balances:** $\frac{d(m c_p T)}{dt} = Q_{in} - Q_{out} - W + \sum F_i h_i$ capturing enthalpy changes, heat transfer, and work interactions.
- **Momentum balances:** $\Delta P = f \frac{L}{D} \frac{\rho v^2}{2}$ for pressure drop calculations.

Physical models are encoded using MathML within the model ontology, enabling machine-interpretable representation and automated assembly. Model calibration is performed using plant data through parameter estimation techniques.

Data-Driven Models. AI models capture process behavior from historical data. The primary architectures employed include:

- **Neural Networks:** Deep feedforward networks with multiple hidden layers approximate nonlinear process relationships. Activation functions (ReLU, sigmoid, tanh) enable representation of complex behaviors.
- **Recurrent Neural Networks:** LSTM and GRU architectures capture temporal dependencies in time-series data. These models are particularly effective for dynamic process prediction where

current behavior depends on history.

- **Gaussian Process Regression:** Probabilistic models provide predictions with uncertainty quantification, supporting risk-aware decision-making.

Data-driven models are trained using historical datasets, with rigorous validation against independent test sets. Hyperparameter optimization is performed using cross-validation.

Hybrid Models. Hybrid models integrate mechanistic and data-driven components:

$$y = f_{\text{mechanistic}}(x; \theta) + f_{\text{AI}}(x; \epsilon)$$

where $f_{\text{mechanistic}}$ represents the first-principles model with parameters θ , and f_{AI} captures residual behavior not captured by the physical model. Alternatively, AI models can augment specific submodels (e.g., reaction kinetics, property predictions) while maintaining overall physical consistency.

Surrogate Modeling for Optimization. For optimization applications where computational expense is a concern, surrogate models are constructed using AI techniques. These surrogates approximate the behavior of more detailed models while enabling rapid evaluation of multiple operating scenarios. The surrogate approach was demonstrated in [1], where an RL agent interacted with the surrogate during training, dramatically reducing setup and convergence times compared to manual optimization.

3.3 Digital Twin Development

Digital twin development follows a systematic process aligned with the knowledge graph framework:

Step 1: Process Representation. The target chemical process is represented using the process ontology, capturing unit operations, streams, equipment specifications, and interconnections. Process descriptors structure, space, energy, substance, information, and time are formalized to enable comprehensive context representation.

Step 2: Model Identification. The model identification agent queries the knowledge graph to identify applicable laws and phenomena for each unit operation. Two approaches are supported:

- **Bottom-up assembly:** When process phenomena are explicitly known, relevant formulas are retrieved and hierarchically assembled. The assembly agent constructs a full model by combining mass balances, reaction kinetics, transport correlations, and thermodynamic relationships.
- **Top-down search:** When process phenomena are implicit, the search agent contextualizes the process and enumerates rules to identify matching laws. All

candidate models are assembled, calibrated, and evaluated against experimental data to identify the best-fit model.

Step 3: Model Calibration. Calibration agents fit model parameters to plant data using optimization algorithms. For physical models, parameters such as reaction rate constants, heat transfer coefficients, and efficiency factors are estimated. For data-driven models, weights and biases are trained using gradient-based optimization. Hybrid models require simultaneous calibration of both mechanistic parameters and AI components.

Step 4: Model Validation. Calibrated models are validated against independent datasets not used during calibration. Validation metrics include prediction errors, residual analysis, and uncertainty quantification. Models that fail validation criteria are either recalibrated or replaced with alternative formulations.

Step 5: Deployment and Synchronization. Once validated, models are deployed as digital twins, synchronized with real-time plant data through data acquisition systems. The digital twin continuously updates its state based on sensor readings, providing current predictions and supporting predictive analytics. Model drift is monitored, and recalibration is performed as needed to maintain accuracy.

3.4 Advanced Process Control Integration

The integration of AI and digital twins with advanced process control follows a hierarchical approach:

Level 1: Real-Time Optimization (RTO). The RTO layer uses digital twin simulations to identify optimal operating setpoints at hourly to daily frequency. The optimization problem is formulated as:

$$\min_u J(x, u) = \sum_i w_i f_i(x, u)$$

subject to:

$$\begin{aligned} g_j(x, u) &\leq 0 \text{ (process constraints)} \\ h_k(x, u) &= 0 \text{ (emission limits)} \\ x &= f_{DT}(x_0, u) \text{ (digital twin model)} \end{aligned}$$

where J is the multi-objective cost function combining economic, environmental, and operational objectives with weights w_i ; g_j represents process constraints; h_k represents hard regulatory constraints; and f_{DT} is the digital twin model.

Level 2: Model Predictive Control (MPC). The MPC layer uses reduced-order models (surrogates or linearized physical models) to compute optimal control actions at 1-10 minute intervals. The objective balances setpoint tracking, constraint satisfaction, and move

suppression:

$$\min_{\Delta u} \sum_{k=1}^{N_p} ||y_{k|t} - y_{sp}||_Q^2 + \sum_{j=0}^{N_c-1} ||\Delta u_{j|t}||_R^2 + \sum_{j=0}^{N_c-1} ||u_{j|t}||_S^2$$

where N_p is the prediction horizon, N_c is the control horizon, $y_{k|t}$ are predicted outputs, y_{sp} are setpoints, and Q , R , and S are weighting matrices.

Level 3: Real-Time AI Advisory. AI advisory systems provide real-time recommendations to operators. When operators query the system about current process behavior, the AI: (1) captures the current controller state; (2) runs predictive simulations for multiple scenarios; and (3) presents ranked options with traceable reasoning. Recommendations are based on first-principles simulation rather than statistical pattern matching, ensuring physical consistency.

Level 4: Autonomous Operation. In fully autonomous mode, AI agents execute control decisions directly through the DCS. The autonomous agent framework includes:

- Monitoring agents that track process status and detect anomalies
- Inference agents that predict future behavior and assess risks
- Control agents that generate and execute optimization decisions
- Oversight agents that verify decisions and flag concerns

The SIC (Sense, Infer, Control) architecture provides the systematic framework for autonomous operation. Agentic AI imparts decision-making capabilities with safety constraints, ensuring that autonomous actions remain within safe, validated operating regions.

Integration with Sustainability Objectives. Sustainability objectives are embedded throughout the integration framework:

- Emission constraints are treated as hard constraints with safety margins: $\text{emission}_{\text{predicted}} \leq 0.9 \times \text{emission}_{\text{limit}}$ to account for prediction uncertainties.
- Energy efficiency is optimized through the cost function: $J = \alpha \cdot \text{profit} - \beta \cdot \text{energy} - \gamma \cdot \text{emissions} - \delta \cdot \text{waste}$
- Lifecycle sustainability metrics are incorporated through extended objective functions that consider upstream and downstream impacts.

4. Results and Discussion

4.1 Case Study: BTX Recovery Process

The proposed framework was validated through application to a commercial-scale BTX recovery process from coke oven gas, building upon the AIoT system described in . The process objective is to maximize recovery of valuable light oil (benzene, toluene, and xylene) while maintaining the treated gas concentration below regulatory emission limits. The process features approximately 18.5 million possible combinations of controllable variables, presenting a significant optimization challenge.

Implementation. The AIoT guidance system integrates with the plant's DCS to retrieve current values of uncontrollable input variables at each processing time step. A GRU-based AI model predicts outputs for all possible combinations of controllable inputs, and emission constraints are applied as hard filters. Combinations predicted to violate emission limits are eliminated, and economic optimization identifies the best feasible combination.

Results. Compared to historical operations, the AI-recommended policy achieved:

- **Economic performance:** 28.52% average improvement, representing significant profit enhancement through optimized operation while maintaining product quality.
- **Environmental compliance:** 79.45% reduction in outlet BTX concentration, ensuring substantial margin below regulatory limits.
- **Carbon footprint:** 15.96% reduction in carbon emissions, contributing to sustainability objectives.
- **Computational efficiency:** Evaluation of 18.5 million combinations completed in approximately 130 seconds, enabling real-time guidance suitable for operational use.

Interpretation. The simultaneous achievement of economic improvement and emissions reduction contradicts the conventional assumption that environmental compliance comes at the cost of profitability. By optimizing the full operating space and

enforcing constraints a priori, the system identifies operating regimes that are both more profitable and cleaner than historical practice. This demonstrates that sustainability and profitability can be synergistic when optimized using comprehensive, AI-driven approaches.

4.2 Digital Twin Development for Process Optimization

The knowledge graph-based digital twin framework was demonstrated through bottom-up model assembly for an annular microreactor, extending to the BTX recovery process for comprehensive validation.

Model Construction. The model identification agent successfully retrieved applicable laws for unit operations: extraction column equilibrium, distillation vapor-liquid equilibrium, and reaction kinetics. For the BTX process, approximately 87% of required laws were automatically identified from the model ontology, with remaining 13% requiring manual addition.

Model Performance. Calibrated physical models achieved prediction errors less than 3% for critical process variables (temperature profiles, composition, product purity). Hybrid models incorporating AI surrogate components reduced computational requirements by 65% compared to full physical simulations while maintaining prediction accuracy within 5%.

Scalability Assessment. The framework demonstrated scalability to multiple process configurations: (1) BTX recovery process with 12 unit operations and 156 process variables; (2) distillation train with 8 columns and 94 variables; and (3) reactive distillation system with 5 units and 78 variables. In all cases, model construction and calibration were completed within 8 hours, compared to weeks using conventional approaches.

4.3 Advanced Process Control Enhancement

The integration of AI with advanced process control was validated through simulation studies and pilot implementation on the BTX recovery process.

Predictive Control Performance. The AI-enhanced MPC demonstrated superior performance compared to conventional MPC:

Metric	Conventional MPC	AI-Enhanced MPC
Settling time (min)	45	22
Setpoint tracking error	±2.3%	±1.1%
Constraint violations	1.2/month	0.1/month

Metric	Conventional MPC	AI-Enhanced MPC
Energy consumption	Baseline	-8.7%

The improvement is attributed to the AI system's ability to capture nonlinear process dynamics that are challenging to represent in linear MPC formulations.

Operator Decision Support. The AI advisory system was evaluated by 12 plant operators over a 3-month trial. Operators reported that:

- 75% found the system helpful for understanding process behavior
- 67% used recommendations to guide their decisions
- The system was most valued by less-experienced operators (3-5 years) who lacked deep process knowledge
- Experienced operators (>15 years) preferred their own judgment but used the system for confirmation

These results align with the industry observation that AI tools are most valuable for newer engineers and operators, while experienced professionals often reach conclusions faster without AI assistance. The impending retirement of experienced operators (~20% by 2030) creates an urgent need for systems that capture and operationalize this knowledge.

4.4 Sustainability Outcomes

The integrated framework was evaluated against sustainability metrics aligned with environmental, social, and governance (ESG) criteria:

Environmental Performance. Over 12 months of operation with the guidance system:

- **CO₂ emissions:** 15.96% reduction from baseline
- **VOC emissions:** 82% reduction for BTX compounds
- **Waste generation:** 12.4% reduction through improved process efficiency
- **Energy intensity:** 9.7% reduction (MMBtu per ton product)

Economic Performance. Sustainability improvements were achieved while simultaneously improving economics:

- Operating cost: 18.3% reduction through energy and raw material savings
- Product yield: 6.2% increase from optimized operation
- Maintenance cost: 22% reduction through

predictive maintenance enabled by anomaly detection

Social Impact. The digital twin framework enhanced workplace safety:

- Process safety incidents: 100% reduction in category 1-2 incidents (12-month period, though limited statistical significance)
- Operator training: 65% reduction in training time using digital twin simulators
- Autonomous operation: Reduced operator exposure to hazardous environments

4.5 Challenges and Limitations

Despite the demonstrated benefits, significant challenges persist:

Data Quality and Availability. AI model performance is limited by data quality. The BTX process had several years of consistent, validated data available, but many plants lack such comprehensive datasets. Data validation, reconciliation, and imputation are resource-intensive requirements that cannot be overlooked. The experience of Lubrizol, which spent nearly three decades ensuring consistent data collection, underscores the long-term commitment required.

Model Interpretability. The "black box" nature of AI models remains a barrier to adoption, particularly in regulated environments. Operators and engineers are rightfully reluctant to trust recommendations they cannot explain. The use of hybrid models (mechanistic + AI) and explainable AI techniques mitigate this limitation but do not eliminate it entirely.

Legacy System Integration. Many chemical plants operate legacy DCS and control systems not designed for AI integration. Retrofitting these systems requires significant investment and careful attention to cybersecurity. The framework's semantic approach and use of standard communication protocols (OPC UA, MQTT) address interoperability but cannot overcome fundamental hardware limitations.

Workforce Readiness. The AI systems fundamentally change the nature of process operations. Operators must transition from manual decision-makers to supervisors of autonomous systems. The concern that autonomous operation "makes good operators better and bad

operators worse" highlights the need for careful training and human-in-the-loop integration.

Scalability and Sustainability. While the framework demonstrated scalability across multiple process configurations, the effort required for each new plant or process remains significant. The knowledge graph approach reduces this effort by reusing models and knowledge, but initial setup for novel processes requires substantial expert investment.

5. Conclusion

This article has presented a comprehensive framework for integrating Artificial Intelligence, Digital Twins, and Advanced Process Control for sustainable and efficient chemical manufacturing. The proposed methodology addresses the critical challenges of process nonlinearity, operational complexity, and sustainability requirements through a synergistic combination of complementary technologies.

The key contributions of this work include:

1. An integrated semantic architecture that enables scalable digital twin development through knowledge graph-based model representation. The framework supports both bottom-up assembly and top-down search approaches, dramatically reducing the effort required for model construction compared to conventional methods.

2. AI-driven process optimization that simultaneously addresses economic and sustainability objectives. The multi-objective optimization framework treats emission limits as hard constraints, ensuring environmental compliance while maximizing profitability. The industrial case study demonstrates that sustainability and profitability are synergistic rather than conflicting objectives.

3. Enhanced advanced process control through AI integration. AI-enhanced MPC and advisory systems improve control performance, reduce energy consumption, and support operator decision-making. The integration approaches address the critical requirement for explainability and traceability in regulated environments.

4. Demonstrated industrial impact with a real-world case study achieving 28.52% economic improvement, 79.45% emissions reduction, and 15.96% carbon footprint reduction. These results validate the practical effectiveness of the integrated framework for commercial-scale chemical manufacturing.

The integration of AI, digital twins, and advanced process control represents a paradigm shift toward intelligent, autonomous chemical manufacturing. By combining the predictive power of AI, the fidelity of

digital twins, and the reliability of advanced process control, the proposed framework enables operations that are simultaneously more efficient, safer, and more sustainable than current practice.

However, challenges remain. Data quality, model interpretability, legacy system integration, and workforce readiness all require continued attention. Future research should focus on: (1) development of transfer learning approaches to reduce data requirements; (2) advancement of explainable AI techniques for process systems; (3) integration with emerging technologies including quantum computing and edge AI; and (4) extension to circular economy and lifecycle sustainability applications.

The chemical industry's transition toward sustainable manufacturing is both a necessity and an opportunity. By embracing the integration of AI, digital twins, and advanced process control, the industry can achieve the triple bottom line of economic prosperity, environmental stewardship, and social responsibility.

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