Applied Chemical Engineering (2026) Volume 9 Issue 2 ISSN: 2578-2010 (O)
doi: 10.59429/ace.v9i2.5949

RESEARCH ARTICLE

Artificial Intelligence in Chemical Process Optimization: Techniques, Applications, Challenges, and Future Directions

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ABSTRACT

Chemical processes are often complex nonlinear reactions, with large numbers of operating variables, and high energy consumption; therefore, optimization is not an easy task. With the industrial data from sensors and monitoring systems becoming more widely available, artificial intelligence (AI) is being deployed to enable process efficiency as well as better decision making. Further, unlike the more traditional optimization methods used, especially for complex and high dimensional systems as in molecular design, AI techniques can do so much more efficiently than exploring the whole computational landscape thanks to their powerful predictive capabilities. This review provides an overview of recent developments in machine learning, deep learning (DL), reinforcement learning, and evolutionary algorithms for chemical process optimization across four key industrial applications: reactor design; distillation; energy management; and predictive maintenance. Results suggest that AI-driven solutions enhance process performance, energy savings and promote sustainable industrialization in the context of SDGs 7, 9, 12 and 13.

Keywords: Artificial Intelligence, Chemical Process Optimization, Deep Learning, Digital Twins, Machine Learning, Reinforcement Learning.

ARTICLE INFO

Received: 19 March 2026
Accepted: 1 June 2026
Available online: 18 June 2026

1. Introduction

As chemical industries are usually complex processes (reaction kinetics, heat and mass transfer), optimization in the process is necessary for better productivity, energy savings and improved operational safety [1,2]. On the one hand, traditional approaches based on first-principles models can be very informative but have difficulties capturing strong nonlinear responses [1]. Machine learning and reinforcement learning are some of the most powerful methods

introduced in 2020 and later for such aspects as complex process optimization, autonomous decision-making, renewable energy integration using artificial intelligence techniques [3,4]. To this end, various approaches have been proposed; the hybrid methods that combine physical and data-driven models have proven to be more accurate in prediction results and better in process control performance [5,6]. For example, Physical knowledge incorporation into AI models increases also improves the reliability and safety of AI systems [7–10] as well as certain computations efficiency.

Artificial Intelligence (AI) is Found in the eld of Predictive Modeling, Process Monitoring, Fault Detection and Control, Supply-chain Optimization in Chemical Plants [11]. Its integration with process systems engineering allows for better product design, process synthesis, and safety management [12]. Nevertheless, reliance on high-quality data remains limited, stringent safety demands persist and practical AI-legacy industrial infrastructure integration in regulated environments faces difficulties [1,13,14].

Machine learning-based model predictive control (MPC) has significant potential for chemical process optimization, although its adoption is constrained by high computational requirements and the lack of standardized sensor data systems [15]. Reinforcement learning is increasingly integrated with MPC to improve process stability through adaptive parameter adjustment and reward-based control strategies [16]. The development of open-access databases and standardized frameworks is essential for reducing data silos and improving model interoperability [17,18]. At the same time, generative AI, large language models, transformer architectures, and generative adversarial networks are advancing process synthesis, fault diagnosis, molecular design, and synthetic data generation, helping to address data limitations [19–21].

The widespread availability of real-time industrial data from sensors, control systems, and process historians has accelerated the application of AI in chemical engineering [11]. Deep reinforcement learning has demonstrated strong capabilities in solving complex multi-timescale optimization problems, particularly in refinery operations and process control [22]. Reinforcement learning and evolutionary algorithms also support sustainable plant design and operation by generating optimized process configurations with reduced human intervention, contributing to circular economy objectives and renewable feedstock utilization [23]. In addition, machine learning enables real-time optimization by learning operational patterns and improving decision-making accuracy in dynamic industrial environments. Table 1 explains the key findings of AI in Chemical Process.

Table 1. Key findings of Artificial Intelligence in Chemical Process Optimization.

Theme / Area	Key Findings	AI Techniques / Tools	Industrial Significance
Chemical Process Complexity	Chemical processes involve nonlinear reaction kinetics, heat transfer, and mass transfer requiring efficient optimization.	First-principles models, Mathematical modeling	Improves productivity, safety, and energy efficiency.
Limitations of Conventional Models	Traditional models struggle with highly nonlinear systems.	Mathematical programming, Mechanistic models	Limited applicability to dynamic systems.
AI-Driven Process Optimization	AI handles high-dimensional nonlinear optimization problems.	ML, RL	Enhances autonomous decision-making and efficiency.
Hybrid Modeling Approaches	Combines physical knowledge with data-driven methods.	Physics-informed ML, Hybrid AI	Improves accuracy, reliability, and control.
Industrial Applications of AI	Used for monitoring, fault diagnosis, predictive modeling, and optimization.	ML, DL, Intelligent Control	Improves plant performance and safety.
Challenges in AI Adoption	Limited data quality, safety concerns, and legacy systems.	Data Analytics, Industrial AI	Restricts large-scale deployment.
AI-Based Process Control	ML-based MPC improves process control.	MPC, ML	Enhances operational stability.
Reinforcement Learning for Control	RL enables adaptive parameter tuning.	RL, MPC	Improves dynamic decision-making.

Data Standardization and Accessibility	Open databases reduce data silos.	Data Management Frameworks	Improves interoperability.
Generative AI and Advanced Intelligence	Supports synthesis, molecular design, and fault diagnosis.	Generative AI, LLMs, GANs, Transformers	Accelerates innovation.
Industrial Data Integration	Real-time data accelerates AI adoption.	Industrial IoT, Data Analytics, ML	Supports intelligent operations.
Deep Reinforcement Learning Applications	Addresses multi-timescale optimization problems.	DRL	Enhance flexibility and efficiency.
Sustainable Process Design	Supports sustainable plant configurations.	RL, Evolutionary Algorithms	Promotes circular economy.
Real-Time Optimization	Adaptive models improve operational decisions.	ML, DL	Enables real-time optimization.

1.1. PRISMA flow diagram

A flow diagram representing the procedure of systematically selecting literature for this review according to PRISMA guidelines is shown in Figure 1. A total of 545 records were identified from key scientific databases and other sources. These resulted in 420 records remaining for title/abstract screening, after the removal of 125 duplicate records. After this, 240 records were removed from the review for being not relevant to the objectives of the review. On the other hand, we screened 180 full-text articles for eligibility and excluded 109 because they were either poorly represented its technique applied details (n=40), not directly applying to AI-based chemical process optimization (n=22), having no application on chemical engineering (n=21) or had duplicate findings (n=22). Ultimately, 71 studies met all inclusion criteria and thus were included in the qualitative synthesis, which serves as the foundation of the current review.

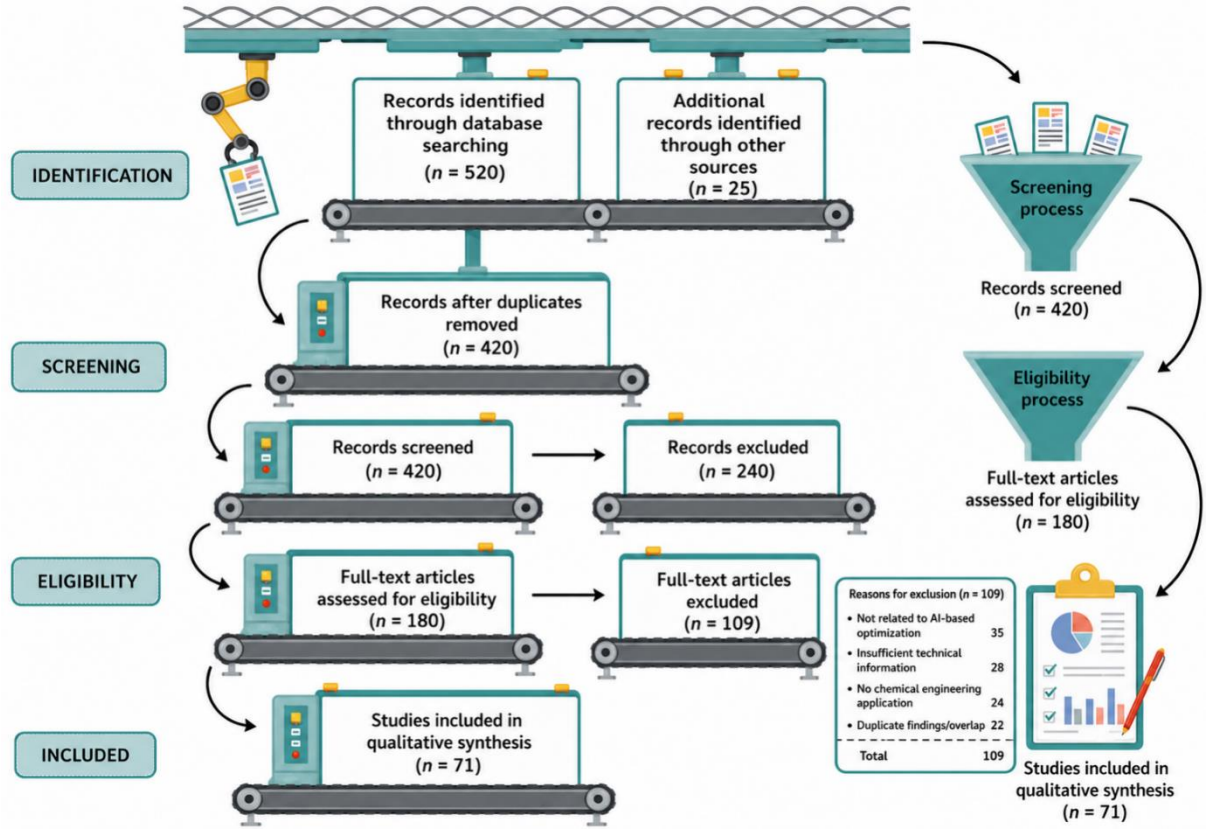

Figure 1. PRISMA flow diagram.

This review offers a thorough overview of state-of-the-art AI methods for the optimization of chemical processes, including machine learning (ML), deep learning (DL), reinforcement learning (RL), evolutionary algorithms, digital twins and hybrid physics-informed models. This is the only study to merge the latest

developments in AI into their application for reactor design, separations processes, energy management and predictive maintenance while focusing on sustainability and practical industrial challenges. The goal is a critical assessment of the status of AI-enabled optimization in chemical engineering, an identification of research gaps, and future directions towards developing intelligent, reliable & sustainable process industries.

2. Artificial Intelligence Techniques for Chemical Process Optimization

2.1. Machine Learning

Machine learning is commonly applied on predictive modelling and optimization of chemical processes from historical data by understanding complex correlations between process variables [24]. Methods like NN, SVM, RF and GBM were used to predict KPIs such as reaction conversion, product yield and energy consumption loss [25–28]. Such models assist in finding ideal operating conditions, enhance process efficiency, and leverage data-driven system identification instead of depending on physical modeling alone [29–31]. The model development is also accelerated through automated model selection and further, parameter tuning [32]. Using supervised machine learning, historical data is analyzed to produce adaptive systems capable of learning the patterns of the dataset and as such continuously improving prediction accuracy and decision-making performance over time [4,14].

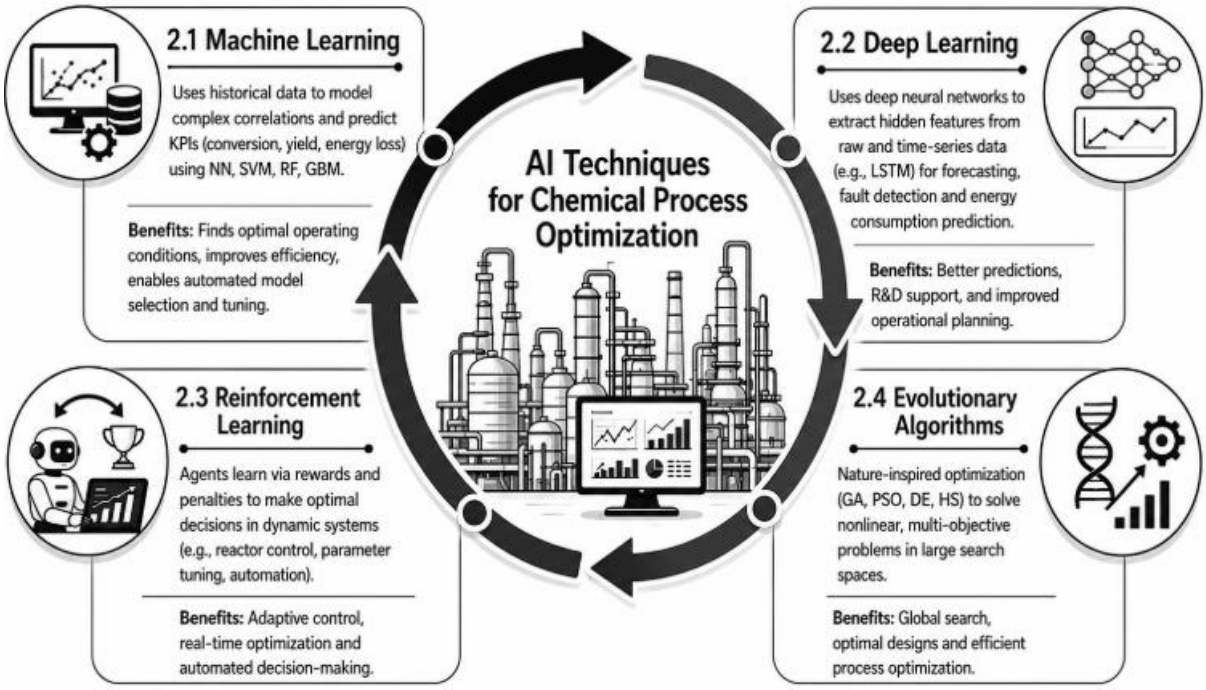

Figure 2. Artificial Intelligence Techniques for Chemical Process Optimization.

Figure 2 explains the major AI techniques in chemical process optimization, with abbreviations such as Machine Learning (ML), Deep Learning (DL), Reinforcement Learning (RL), and Evolutionary Algorithm (EA). They facilitate the application of process modeling, prediction, control, parameter optimization and decision-making which consequently improves efficiency, productivity and operational performance in chemical industries.

2.2. Deep Learning

Deep learning is a machine learning sub-type that uses multilayer neural networks to automatically extract hidden features from raw process data while working with large and complicated datasets. Especially suitable for time series data of sensors and control systems in chemical process applications, such as process forecasting, fault detection and energy consumption prediction. This kind of data has many applications in modeling

sequential industrial data, forecasting future process behavior using architecture like Long Short-Term Memory (LSTM) networks. Deep learning has given R&D researchers new medication leads and improved operational planning, resource allocation, predicting the performance of processes [33]. It has also improved reinforcement learning by enabling intelligent agents to improve control strategies for large chemical decision processes in which they operate [2]. Despite these advantages, deep learning does face several challenges including sensor noise and data sparsity, as well as the debate between model interpretability and performance from a black box approach in a more transparent and explainable framework [34]. They have also been successfully utilized for complex industrial optimization problems, such as biodiesel production and carbon capture systems [35].

2.3. Reinforcement Learning

Reinforcement learning (RL) is an artificial intelligence (AI) approach that allows the agent to learn to make the best decision based on feedback from its environment in response of rewards and penalties. In the case of chemical process optimization, RL is applicable to dynamic and continuously varying systems for which accurate mathematical models are generally not available, making it a suitable choice for this application domain. Its application includes the automatic control of reactors, tuning of process parameters and automation of several complex industrial operations which have enhanced the flexibility and productivity for large scale plants [4,36]. RL is concerned with maximizing cumulative rewards, and according to a Markov Decision Process framework RL engages in continual learning and adaptation [37]. Its performance under uncertainty and stochastic assumptions qualifies it for application in the industrial complexity [38]. It was also shown to address the challenge of real-time process control and automated design of continuous systems [23,39].

2.4. Evolutionary Algorithms

Evolutionary algorithms are optimization methods inspired by nature that find optimal solutions through iterative improvement of a population of candidate solutions. These are class of algorithms which can solve any nonlinear objective, but there are complexities when using them for chemical processes as we have multivariate nonlinear relationships such as multiple objectives and very large search spaces. Popular methods include genetic algorithms, particle swarm optimization, and differential evolution which we often see integrated with machine learning models to create hybrid optimization frameworks. In most cases, they are adopted in reactor design, identifying optimal operating conditions and controlling processes for more efficient operation at lower costs [40]. In contrast to most gradient based approaches, evolutionary algorithms work effectively on nonconvex problems with discontinuous functions and intricate constraint sets. Moreover, other metaheuristics techniques like harmony search and particle swarm optimization help to explore large design spaces for optimal process configurations [41]. They scale well and find High-dimensional Industrial Optimization Problems [42–44].

3. Applications of Artificial Intelligence in Chemical Process Optimization

3.1. Reactor Design and Optimization

The role of reactors in chemical industries has a profound impact on critical factors such as reaction efficiency, product yield and productivity. The parameters influencing the conversion and selectivity are temperature, pressure, catalyst concentration and residence; which impact on all the stages of this process. Before implementing AI, this process was enhanced by conventional modeling and simulation methods based on actual ingested data to identify the best conditions for operating [45]. Operationally integrated hybrids, each leveraging fundamental principles and synergistically working together such as advanced machine learning with reinforcement learning algorithms, genetic algorithms, deep learning for knowledge discovery in the chemical space coupled with computational fluid dynamics tools to accelerate reactor design [10,45,46]. These methods enable reliable prediction of complicated reaction behavior, systematic investigation of the

experimental parameters in the reactions, optimization of catalysts, and self-optimization control [47,48]. Some advancements in AI for Chemical Engineering depicted in figure:3 and their roles to improve process efficiency and operational reliability.

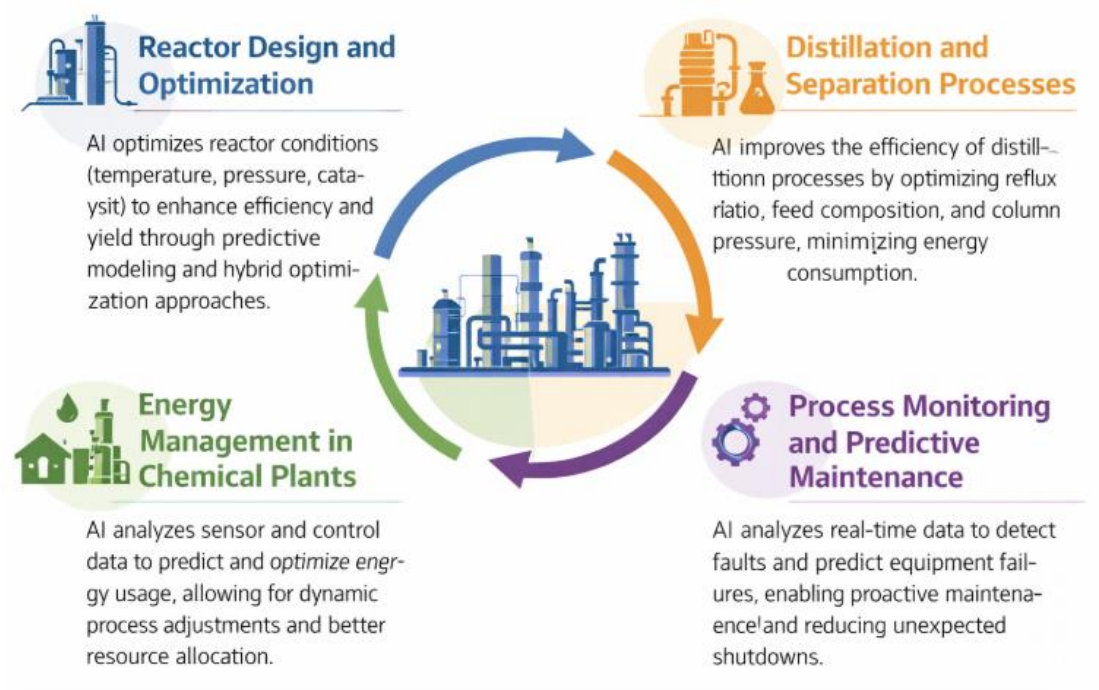

Figure 3. Applications of Artificial Intelligence in Chemical Process Optimization.

3.2. Distillation and Separation Processes

Distillation is one of the most common but energetically demanding separation techniques in the chemical industry. Artificial Intelligence (AI) has been increasingly used focus on optimizing key operating parameters from aspects such as reflux ratio, feed composition, tray configuration and pressure at the column [16]. Machine learning models recognize the historical process data to predict product quality and energy consumption, while optimization algorithms search operating conditions to minimize energy use without reducing separation efficiency or product purity [49] Similarly, AI-driven approaches also aid process scale-up, process intensification and design of automated distillation equipment, as well as carbon emissions evaluation [50,51], systems into energy-efficient heat pump-assisted systems. Moreover, AI facilitates the screening of green solvents and in situ energy optimization with the help of predictive modeling and thermodynamic-based control strategies to enhance sustainability and exergy efficiency [52,53].

3.3. Energy Management in Chemical Plants

Energy management is an important part of chemical plant operation as the energy expenses constitute a large piece in production costs and, moreover, industries are facing higher pressures to lower emissions [1]. AI makes sense of a big data set and operates on the operational data and sensor data to study the energy consumption patterns as well as predict how much energy would be needed going ahead, given corner cases for many operating conditions. Prediction with deep learning is a state-of-the-art approach for accurate energy forecasting that provides flexibility of process parameters optimization and effective allocation of resources over time. Data-driven decision-making in AI-based energy management systems enables development of smart buildings using their data to improve energy efficiency and environmental performance [54]. These also enable facility-wide optimization, real-time emission monitoring, remediation strategies and the design of integrated energy systems that facilitate trade-offs between economic performance and decarbonization [55,56].

3.4. Process Monitoring and Predictive Maintenance

Artificial intelligence (AI) is an essential method for process monitoring and predictive maintenance in a chemical industry. Real-time data obtained through sensors and also control systems are analyzed by machine learning models to detect anomalies, identify faults or predict equipment failure before it occurs. These applications provide early fault detection capabilities on reactors, pipelines, pumps and heat exchangers to enhance process stability and reliability. Predictive maintenance systems diagnose the time remaining before critical equipment stops functioning, which optimizes maintenance schedules and reduces downtime, operational risks, and costs [57]. The use of AI control architectures and multi-agent systems continues to play an essential role in achieving coordination, flexibility, scalability in manufacturing [58]. In addition, advanced machine learning and deep learning models have been applied to predict catalyst deactivation, optimize carbon capture operations [60], and implement condition-based maintenance strategies for better equipment longevity[61]. With the incorporation of operational data like pressure, flow rates and process signals, AI reduces equipment downtimes and enhances overall plant performance [62]. Table 2 explains the AI Applications in Chemical Process Optimization.

Table 2. AI Applications in Chemical Process Optimization.

Application Area	AI Techniques	Main Applications	Key Benefits
Reactor Design and Optimization	ML, RL, GA, DL	Reaction prediction, catalyst optimization, process control	Higher yield, improved efficiency
Distillation and Separation Processes	ML, Optimization Algorithms	Product quality prediction, energy optimization, solvent selection	Reduced energy use, improved purity
Energy Management	ML, DL, Predictive Analytics	Energy forecasting, resource allocation, emission monitoring	Lower costs, better energy efficiency
Process Monitoring and Predictive Maintenance	ML, DL, Predictive Models	Fault detection, equipment monitoring, maintenance planning	Reduced downtime, improved reliability
Carbon Capture and Sustainability	ML, DL	Carbon capture optimization, emission reduction	Enhanced sustainability, lower emissions
Automated Plant Operations	AI Control Systems, RL	Autonomous control, process coordination	Greater flexibility and productivity

4. Integration of Artificial Intelligence with Process Simulation and Digital Twins

AWIP provides integrated AI solutions for simulating chemical processes, analyzing big data in real time to substantially enhance decision making on the shop floor. The digital twin is a special application, and it is a virtual substitute for the actual plant or process which continually refreshes using real-time metadata from sensors and control. Digital twins allow the engineers to observe, simulate and optimize process performance in a non-intrusive manner. AI-enabled digital twins provide predictive maintenance, lifecycle assessment, energy optimization, and cost reduction for carbon capture and storage systems [63]. The platforms also provide an environment to perform real-time analytics, optimize processes and test new control strategies in a virtual setting prior to execution. Moreover, hybrid modeling methods of integrating the AI techniques to first-principles engineering models not only yield fast and reliable solutions for optimization, real-time decision-makings and autonomous plant operations via continuous learning and adaption [64].

5. Challenges in AI-Based Chemical Process Optimization

Although artificial intelligence (AI) has great potential for chemical-process optimization, certain challenges impede its widespread implementation in industrial chemical plants. The most important challenges that they face are data availability, model transparency, system integration and operational safety. As shown

in Fig. 4, Four key challenges (i.e., data quality, model interpretability and generalizability, integration with first-principles models and cybersecurity) obstruct its successful industrial deployment for chemical processes.

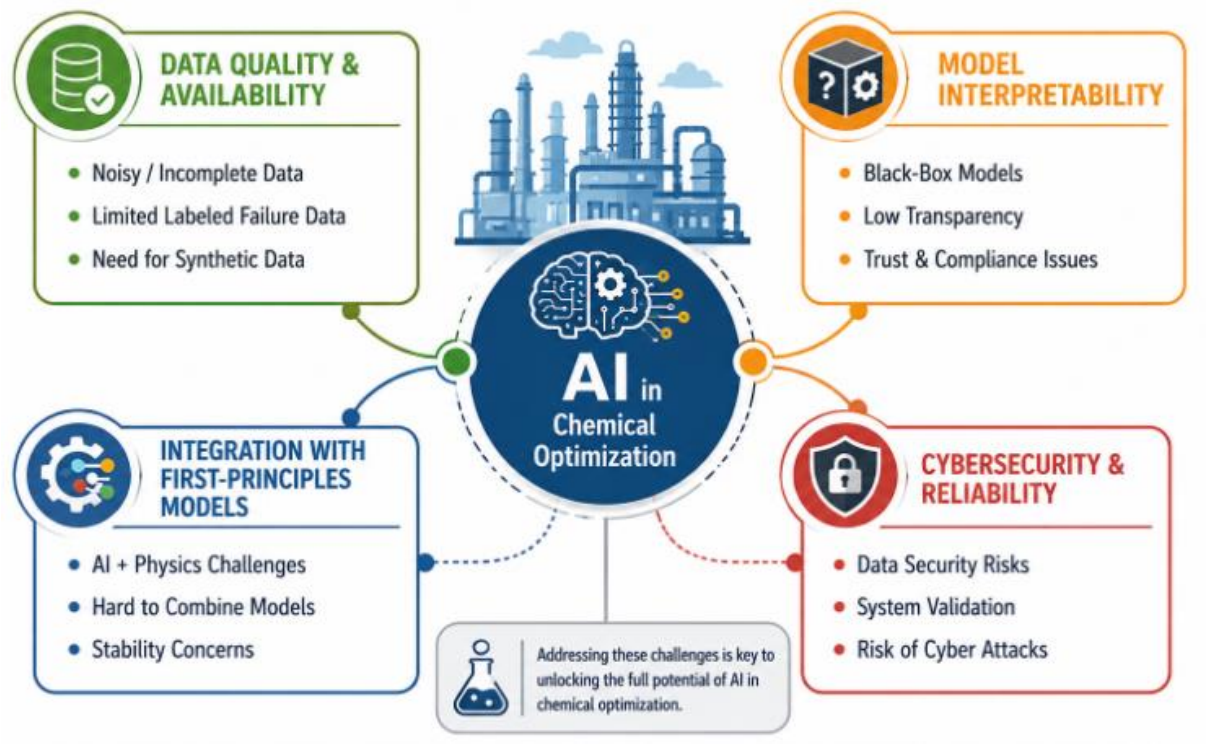

Figure 4. Challenges in AI-Based Chemical Process Optimization.

5.1. Data Quality and Availability

One of the bottlenecks in using AI for chemical processes is that high-quality organized and labeled datasets are sparse. Industrial data are characterized by incompleteness, noise and inconsistency due to sensor limitations, data collection challenges and process disturbances which reduce the accuracy and reliability of machine learning models [9]. The lack of data associated with failures also makes it difficult to build strong diagnostic systems. Moreover, while many of the deep learning models running out there are "black boxes" that require far too much computational time and cost to use, their decisions often lack interpretability [37,65]. To address these challenges, researchers are witnessing a surge of interest in explainable AI approaches providing insight into solutions through interpretable and verifiable decision-making for human oversight in safety-critical applications [12].

5.2. Model Interpretability

Model interpretability is another significant challenge. In contrast, deep learning algorithms are complex systems that often act like a black-box and do not provide insight on how input variables affect predictions. Conventional chemical engineers tend to prefer transparent models that clearly describe how process features relate to system outputs. Restrictions in interpretability can erode trust in AI-based decision-making—complicating compliance with regulations and risk management. Additionally, a large part of current research focuses on ranking the performance of different algorithms upon simulated datasets rather than producing practical lightweight solutions suitable for the industry [66]. Directing future efforts towards explainable and robust AI, with practical viability for businesses is necessary, whilst retaining transparency and trust from stakeholders based on reliable performance under realistic operating conditions [67].

5.3. Integration with First-Principles Models

Combining conventional first-principles models with data-driven AI methods continues to represent a fundamental challenge in chemical engineering. Conventional models are based on physical laws, reaction kinetics and mass & energy balances, while AI models can function with little or zero explicit consideration of these constraints. Consequently, even deep learning which is very advanced AI model would provide predictions which do not adhere to the physical behavior [49]. Future AI/ML frameworks will need to integrate domain knowledge and physical constraints, allowing predictions based on learned patterns only within thermodynamic and kinetic boundaries to enhance reliability. Moreover, using machine learning for process control needs to resolve the robustness, stability and operational safety issues. Hence, adaptive control strategies that are robust against changing process conditions as they would be encountered in real industrial systems such as large-scale electrolysis and carbon capture processes are indispensable for reliable deployment.

5.4. Cybersecurity and Reliability

AI in chemical industries necessitates verification under stringent safety and reliability standards. An increase in connected sensors, digital infrastructure (e.g., cloud), and extensive reliance on data sharing introduced new cybersecurity and data privacy challenges; hereby, secure transmission of data and reliable operation of the system becomes a necessity. The protection of sensitive process data against unintended access and deliberate meddling is vital for preserving intellectual property and operational security. Ensuring effective data security and model validation frameworks demands collaboration between AI experts, chemical engineers, and policymakers [68-70]. Moreover, ongoing investments in workforce training and cross-disciplinary research are required to effectively catalyze digital transformation, strengthen AI uptake, and execute the safe operation of resilient AI-empowered chemical manufacturing systems [71].

6. Conclusion

AI has become a disruptive technology for chemical process optimization, as it provides better solutions to such inherent issues with modern industrial operations that are complex, nonlinear, and dynamic. AI approaches applicable to the life sciences that have been shown to be of great value in reactor design, distillation processes, energy management, process monitoring and predictive maintenance includes machine learning, deep learning, reinforcement learning and evolutionary algorithms. AI uses huge amounts of industrial data for prediction, control and real-time optimization by enabling autonomous decision-making that yields higher productivity and increases quality whilst reducing operational costs ensuring optimum safety and reduced environmental impact. When paired with process simulation tools and enhanced by digital twin technology, AI reinforces process efficiency — allowing for experimentation in a virtual context, for predictive analysis, and as a driver of continuous performance improvement. These technologies can help enhance sustainable manufacturing efforts by limiting energy usage, reducing emissions and encouraging resource efficiency. However, barriers including data quality, model interpretability, integrations with first-principles models, cybersecurity and regulatory compliance inhibit industrial deployment. Future works should aim to design explainable/safe/trustworthy AI systems, hybrid physics informed models and develop interventions for better standardization of data (especially for digital twins), as well as stronger cybersecurity frameworks. AI, digital twins and IIoT combined with autonomous control systems are forecasted to take the industry one step closer to intelligent and self-optimizing chem-plants. With the development of these technologies, AI will be critical in enabling sustainable, resilient and economically competitive chemical manufacturing for global energy efficiency, industry innovation and infrastructure as well as responsible consumption and production to achieve environmental sustainability.

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