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RESEARCH ARTICLE

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ARTIFICIAL INTELLIGENCE IN CHEMICAL PROCESS OPTIMIZATION:
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ABSTRACT

This review focuses on the use of these data-driven approaches in optimizing complex chemical processes using artificial intelligence. Non-linear reactions, multivariable control parameters and high energy demand require advanced optimization techniques in industrial chemical systems. With the increased availability of process data coming from sensors, control systems, and monitoring platforms there is a new opportunity for enhancing operational efficiency using intelligent analysis. While conventional methods principally based on first-principles modeling and mathematical programming are indispensable, they often make simplifying assumptions that hinder performance on high-dimensional, nonlinear systems, sometimes requiring prohibitive computational resources. It covers the main paradigms of AI, such as machine learning, deep learning, reinforcement learning and evolutionary algorithms and describes their application in the context of process simulation and digital twin technologies. A comprehensive review of recent applications in reactor optimization, separation through distillation, energy management and predictive maintenance is presented. Based on these findings, it can be concluded that AI-based models have the potential to analyze big operational data and help in achieving optimal operating conditions while also enhancing process stability and reducing energy consumption. These advancements enable industrial development to realize sustainability by improving energy efficiency, resource utilization and reducing pollution from chemical manufacturing process.



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I. INTRODUCTION

Reaction kinetics, mass and heat transfer are examples of highly complex and interrelated processes typical of chemical industries. The optimization of chemical and industrial processes is critical for productivity enhancement, energy savings, and safety [1] [2]. Mathematical and first-principles models typically provide much insight but give a reduced view of behavior in some complex systems [1]. Artificial intelligence methods, especially reinforcement learning and data-driven techniques, are frequently utilized for autonomous decision-making and improved efficiency to tackle high-dimensional and non-linear problems [3]. Such methods also enable decarbonization and the integration of renewable energy systems into chemical processes [4]. Recent approaches based on hybrid models that synergize physical laws with data-driven strategies have achieved better predictive performance for complex dynamics in a variety of settings [5] [6]. However, the growing black box nature of deep learning models is coupled with the need to impose physical constraints to promote safety and robustness [7]. Incorporating physical knowledge into learning paradigms enhances robustness and facilitates realistic control policies, bridging theoretical insight with computational efficiency [8–10]. Social and political issues associated with the chemical reactions that are being monitored have resulted in tighter regulation of our output, which runs the risk of hamstringing supply chain efficiency but at least creates opportunities for improvement thanks to recent developments in artificial intelligence. AI algorithms can capture complex relationships directly from process data and can manage nonlinear, multivariable systems much better than conventional methods. Modern chemical plants utilize machine learning extensively for predictive modeling, process monitoring, fault detection and control. These strategies are implemented at a range of scales, including molecular design and reaction analysis to whole plant optimization and supply chain management [11]. The application of AI with conventional process systems engineering can lead to enhanced solutions in product design, process synthesis and safety management [12]. However, limitations still exist owing to a lack of adequate high-quality experimental data and stringent safety requirements during in situ implementation [13] [14]. Challenges for seamless integration are also posed by legacy infrastructure, which requires careful data preprocessing, and synchronization to maintain compliance in regulated environments [1].

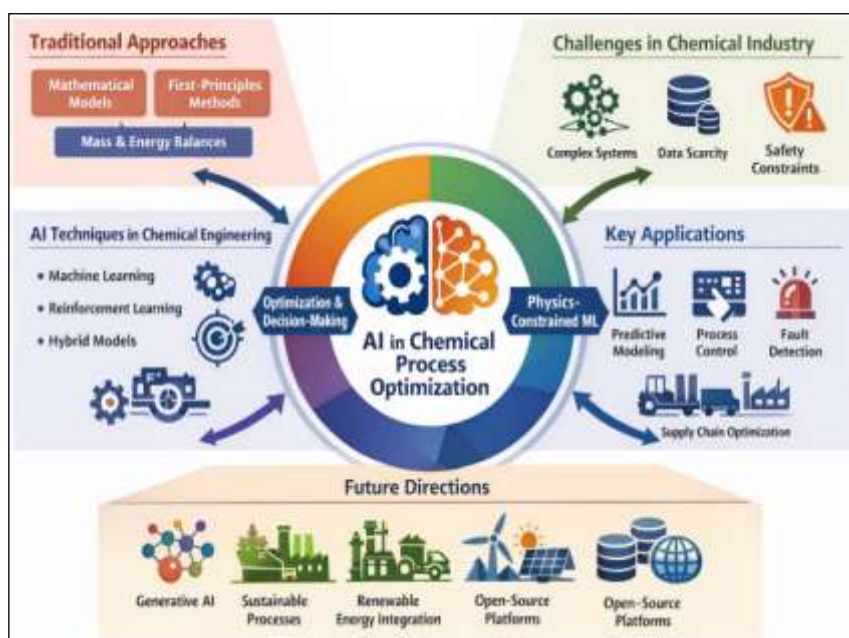


Figure 1: AI-Driven Framework for Chemical Process Optimization.
Source: Authors (2026).

Figure 1 illustrates the integration of traditional modeling approaches with artificial intelligence techniques to optimize complex chemical processes. It highlights key challenges, applications, and future directions, emphasizing the role of physics-constrained and data-driven methods in enhancing efficiency, safety, and sustainability. While Machine learning based model predictive control (MPC) methods are still being developed, the higher real-time computational costs and lack of standardized sensor data capture have limited their adoption outside of large facilities: in small-scale laboratory settings [15]. Reinforcement learning is increasingly combined with MPC to automatically adjust parameters and constraints for stable system operation driven by rewards [16]. There is also a need to support the development of open-access databases and standardized modeling frameworks to reduce data silos [17] [18]. Simultaneously, generative AI and large language models accelerate capabilities in advanced decision-making, e.g., process synthesis and automated fault diagnosis [19] [20]. The application of techniques including transformer architectures and generative adversarial networks enables novel new molecular designs and synthetic defect scenarios, thereby addressing data scarcity [19–21]. Moreover, access to massive amounts of industrial data from real-time sensors, control systems or process historians is propelling the recent integration of AI in chemical engineering [11]. Data that can be used to predict and make decisions regarding the best way for their processes. Deep reinforcement learning approaches have shown great promise for multi-timescale decision problems in areas such as improving the stability and flexibility of refinery operations [22]. Moreover, reinforcement learning and evolutionary algorithms offer effective solutions for optimizing complex process models that enable sustainable design and operation of chemical plants. Such strategies enable the generation of optimized process layouts with reduced human involvement and play a part in advancing goals along lines of the circular economy and renewable feedstock usage [23].

Machine learning is also used more in operations where the timeliness of a solution matters, enabling adaptive models to learn operational patterns and improve the accuracy of real-time optimization. Table 1 summarizes important AI approaches for chemical process development categorized with three roles including modeling, monitoring, and advanced methods with the corresponding contribution to efficiency, safety, and sustainability followed by recent trends and future research directions.

Table 1: Key Themes and Applications of Artificial Intelligence in Chemical Process Optimization.

Key Theme	Description	AI / Computational Techniques	Industrial Significance
Complexity of Chemical Processes	Chemical industries involve interconnected phenomena such as reaction kinetics, heat transfer, and mass transfer, which require efficient optimization for productivity and energy management.	Mathematical programming, first-principles models	Supports process understanding but often relies on simplifying assumptions.
Role of Artificial Intelligence	AI methods enable exploration of nonlinear and high-dimensional process spaces that are difficult to solve using conventional deterministic techniques.	Machine learning, reinforcement learning	Enhances decision making and improves operational efficiency in chemical plants.
Hybrid Modeling Approaches	Integration of physical laws with data-driven models improves prediction accuracy for complex chemical processes.	Physics-informed machine learning, hybrid models	Provides better representation of industrial systems while maintaining interpretability.
Challenges in AI Adoption	Implementation of AI faces barriers such as limited high-quality datasets, legacy infrastructure, and safety constraints in industrial environments.	Data preprocessing, sensor integration, model validation	Ensures reliable and safe deployment of intelligent optimization systems.
Process Monitoring and Control	AI models are applied for predictive analysis, fault detection, and real-time control of chemical processes across multiple operational scales.	Model predictive control, deep learning	Improves plant reliability, process safety, and production stability.
Advanced AI Innovations	Emerging techniques such as generative AI and large language models assist in molecular design, process synthesis, and automated fault diagnosis.	Generative adversarial networks, transformer models	Enables innovative chemical product development and process automation.
Future Research Directions	AI integration with process systems engineering and reinforcement learning frameworks supports sustainable and autonomous chemical process optimization.	Deep reinforcement learning, evolutionary algorithms	Contributes to energy efficiency, renewable integration, and sustainable industrial operation.

Source: Authors (2026).

II. FUNDAMENTALS OF CHEMICAL PROCESS OPTIMIZATION

The chemical process optimization is concerned with finding optimal operating conditions that enhance performance subject to safety and technical constraints. Research in these areas aims to improve product yield and selectivity, energy efficiency, and cost. Control systems, plant historians and similar tools are providing valuable data for predictive decision-making that also includes optimization in modern industries [24]. Now, let's go for what comes after Traditional methods are based on first-principles models and mathematical programming approaches, which can be trusted but turn out to be complex, computationally demanding, and less applicable for large dimensional systems [25] [26]. Artificial intelligence (AI) has come to the rescue, specifically allowing for data-driven and derivative-free optimization. Such approaches can model complicated, non-linear interactions (component systems) without designing the details; thus they are suitable for black-box and large-scale issues. Thus, approaches based on AI increase the efficiency and speed of locating optimal operating conditions in data-rich industrial environments [27–30].

III. ARTIFICIAL INTELLIGENCE TECHNIQUES FOR CHEMICAL PROCESS OPTIMIZATION

III.1 MACHINE LEARNING

Machine learning has found extensive applications for predictive modeling and optimizing chemical processes [31]. These approaches take advantage of historical or syntactic data to learn complex non-linear relationships between temperature, pressure, and concentration. For instance, various machine learning techniques such as artificial neural networks, support vector machines, random forests and gradient boosting are employed to predict KPI (key performance indicator) metrics like reaction conversion, product yield and energy consumption [31]. They aid in optimization by determining the best operating conditions and enhancing overall efficiency. They also assist in system identification, as they can build models based on data-driven approaches instead of heavily relying on physical laws [31].

Model development is also expedited by automated model selection and parameter tuning. [32] Aside from predictive modeling, machine learning helps in optimization by studying historical data to expedite the efficiencies of algorithms [4]. This databased approach allows for creation of adaptive systems, which improve over time in their accuracy and decision-making ability [14]. Figure 2 explains the AI techniques for chemical process optimization.

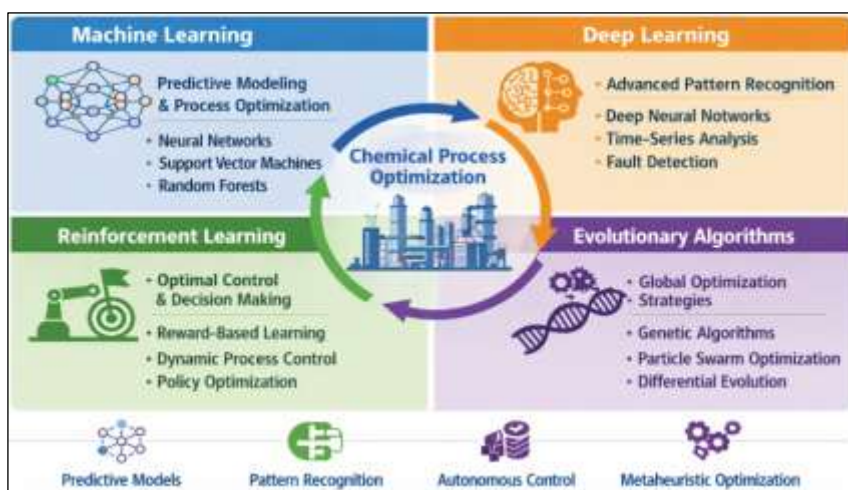


Figure 2: Artificial Intelligence Techniques for Chemical Process Optimization.
Source: Authors (2026).

III.2 DEEP LEARNING

Deep learning is an advanced version of machine learning in which multilayer architectures of neural networks are used to analyze large and complex datasets. Deep learning models can learn hidden patterns and relationships in process data, without the need for manual feature extraction as used in classical machine learning models. In chemical process analysis where time sequence industrial data is generated through sensors and control systems, deep learning techniques can be very useful. Such models have been extensively implemented for time-series prediction of process variables, detection of process failures and prediction of energy consumption patterns at industrial plants. Among different deep learning architectures, Long Short-Term Memory networks are very proficient with sequential data as well as extrapolating future process behavior based on historical patterns. Deep learning models help to enable more effective resource allocation and operational planning in chemical manufacturing systems by accurately predicting process performance and energy demand. Further, the ability of such architectures to automatically learn higher-order features from raw input makes it possible to build highly sophisticated models that predict property values from molecular data [33] that can be transferred downstream (eg., catalyst saturation prediction in fluid catalytic cracking). Moreover, the "deep learning revolution" has introduced a paradigm shift in reinforcement learning methodology allowing agents to rapidly learn about complex, stochastic chemical environments via continuous optimization of control policies based on interaction [2]. These deep architectures, despite operational advantages — whether it is improved efficiency in training via Grads or tapering off additional neurons delivering diminishing returns — also struggle with issues around sensor noise and data at scarce locations (e.g., noise-blind areas); therefore, recent research has explored the addition of interpretable stages [34]. In industry, these architectures were successfully integrated into superstructure approaches for solving complex NLPs, such as biodiesel production or carbon capture systems [35].

III.3 REINFORCEMENT LEARNING

Reinforcement learning Reinforcement learning is designed for decision making which interacts with the environment. Here, an agent learns to determine its optimal actions by exploring various schemes and learning or being retrained from responses (rewards) or mistakes (penalizations). Reinforcement Learning for Chemical Process Optimization goal of chemical process optimization is to determine optimal control policies for dynamic and continuous systems, situations where the behavior of the system varies over time or precise mathematical models are hard to have. It is applied in optimal control of chemical reactors [4], dynamic tuning of process variable, and automation of complex industrial tasks. In large-scale plants, state-of-the-art approaches have been employed to co-develop feasible flowsheet designs and operational tactics, enhancing flexibility and productivity. These methods are adequate for the context of multi-step decision problems such as automated flow chemistry, in which strategies iteratively improve [36]. The foundational model is often modeled around Markov Decision Processes with an agent optimizing its actions by maximizing cumulative rewards, which are typically expressed through equations such as the Bellman equation [37]. Reinforcement learning is well-suited for stochastic and uncertain process conditions, enabling effective management of complex industrial environments [38]. In addition to real-time control, its application in automating the design of continuous process systems has also been reported recently, proving its ability to learn complicated decision-making through interaction [39], [23].

III.4 EVOLUTIONARY ALGORITHMS

Evolutionary algorithms are optimization techniques based on the process of natural selection wherein possible solutions to a problem evolve across generations to arrive at an optimal solution. Population approaches are particularly well-suited for chemical process optimizations, since they can accurately capture nonlinear relationships, the performance of multiple objectives and large decision spaces.

Common methods include genetic algorithms, particle swarm optimization and differential evolution. Such methods are often used in combination with machine learning models to create hybrid frameworks which can efficiently explore complex parameter spaces. Such techniques are used in a variety of areas, including optimizing reactor configurations, operating conditions and control strategies to increase efficiencies while minimizing costs within the chemical industries among others. They perform very well on the type of problems that prove challenging for classical gradient based methods, those with discontinuities or poorly defined constraints [40]. Evolutionary algorithms are population-based search strategies that avoid being trapped in local optimum and thus provide a coupled approach to non-convex optimization problems common in chemical systems. Other types of metaheuristic techniques (e.g., harmony search and particle swarm optimization) also allow for the exploration of discrete design spaces and can therefore facilitate better configurations in a process [41]. These methods are scalable to high-dimensional problems and use nature-inspired operators that seek stable solutions without strict mathematical convergence needed, which is often hard for complex industrial systems [42–44]. Table 2 summarizes the major artificial intelligence techniques applied in chemical process optimization, including machine learning, deep learning, reinforcement learning, and evolutionary algorithms. It outlines their underlying principles, common models, industrial applications, advantages, and limitations relevant to improving efficiency and decision making in chemical processing systems.

Table 2: Artificial Intelligence Techniques and Their Applications in Chemical Process Optimization.

AI Technique	Principle / Concept	Common Algorithms / Models	Chemical Process Applications	Advantages	Limitations
Machine Learning	Learns relationships between input process variables and outputs using historical or simulation data.	ANN, SVM, Random Forest, Gradient Boosting	Reaction yield prediction, energy consumption estimation, process modeling	Handles nonlinear multivariable systems	Requires large, high-quality datasets
Deep Learning	Uses multilayer neural networks to automatically learn hidden patterns from large datasets.	CNN, LSTM, Deep Neural Networks	Fault detection, sensor data analysis, time-series prediction	High accuracy for complex datasets	High computational cost and limited interpretability
Reinforcement Learning	Agent learns optimal decisions through interaction with environment using reward signals.	Q-learning, Deep Reinforcement Learning, Policy Gradient	Reactor control, adaptive process control, automated operations	Effective for dynamic decision problems	Training requires extensive simulations
Evolutionary Algorithms	Population-based optimization inspired by biological evolution processes.	Genetic Algorithm, Particle Swarm Optimization, Differential Evolution	Reactor design optimization, parameter tuning	Suitable for nonlinear multi-objective problems	Slow convergence for large search spaces
Hybrid AI Models	Combines data-driven learning with optimization or physics-based models.	ANN-GA, ANN-PSO, Physics-informed ML	Process design optimization, catalyst performance prediction	Improves prediction and optimization accuracy	Increased model complexity
Time-Series Prediction Models	Analyzes sequential industrial sensor data to forecast future process behavior.	LSTM, Recurrent Neural Networks	Energy demand forecasting, equipment monitoring	Effective for dynamic process systems	Sensitive to noisy sensor data
Data-Driven Optimization	Uses data-derived surrogate models to support process optimization and decision-making.	Random Forest, Gradient Boosting, Surrogate modeling	Quality prediction, operational planning	Reduces reliance on physical models	Dependent on training data quality
Metaheuristic Optimization Methods	Population-based search techniques exploring large design spaces.	Harmony Search, Ant Colony Optimization, PSO	Process flowsheet synthesis, plant layout optimization	Effective for high-dimensional problems	No guarantee of global optimum

Source: Authors (2026).

IV. APPLICATIONS OF ARTIFICIAL INTELLIGENCE IN CHEMICAL PROCESS OPTIMIZATION

IV.1 REACTOR DESIGN AND OPTIMIZATION

Cascading chemical reactors define reaction efficiency, product yield, and ultimately productivity — they are at the heart of chemical manufacturing. Optimization of operating parameters such as temperature, pressure, catalyst concentration and residence time is necessary to achieve high conversion and selectivity. Traditional methods depend on kinetic modeling and numerical simulations, which are computationally expensive for large systems. AI shields it with process data to derive an ideal state of operation. Many of the AI-powered frameworks perform integration between the machine learning models and simulation tools that mimic reactor behavior under different scenarios. Different hybrid approaches, such as using machine learning with reinforcement learning or genetic algorithms have demonstrated better reactor performance and faster convergence toward an optimal solution. This results in a more comprehensive search of the design and operating parameters, improving efficiency and lowering operational costs. Neural network-based approaches facilitate constructs involving complex reaction kinetics representation that can reliably predict under transient thereof conditions [45]. Such frameworks also enable systematic exploration of reaction spaces, rather than relying solely on trial-and-error methods [10]. Moreover, they enhance detection robustness over parameter uncertainties and maintain stable results in changing environments. Further developments are the use of computational fluid dynamics combined with deep learning and genetic algorithms, enabling tremendously faster optimization [46]. These approaches, when combined with experimentally proven microkinetic models, allow for exactly tuning catalyst properties and feed conditions to maximize yield [47]. Machine learning is also used on self-optimizing systems to make recommendations for optimal reaction conditions and relationships between process variables and catalytic performance [48]. Figure 3 shows the main applications of AI in chemical engineering, for example reactor optimization, distillation efficiency, energy management and predictive maintenance. First, it shows how AI-based approaches improve process performance and energy utilization efficiency while allowing the proactive adoption of measures in industrial operations.

IV.2 DISTILLATION AND SEPARATION PROCESSES

Distillation is one of the most employed separation techniques and among the most energy-consuming processes in chemical industries. Thermal management introduced very large heats to maintain the vapor–liquid equilibrium leading to separation of chemical components. AI techniques are increasingly applied to optimize major distillation column operating parameters, including reflux ratio, feed composition, tray design and column pressure. Machine learning models use historical process data to predict the effect of these features on product quality and energy consumption. Coupled with optimization algorithms, these models help in determining the operating conditions that minimize energy footprints while also satisfying required specifications for products. It has been shown that AI-driven strategies can reduce energy consumption without any impact on the separation efficiency or product purity. Furthermore, data-driven approaches also facilitate the scale-up transition from laboratory to industrial applications, where the number of operating variables increase appreciatively and typical mechanistic models are tightly related to computational costs [49]. Such advanced systems are a step in the direction of Process Intensification 4.0, where equipment design and control can be iteratively improved by means of data-driven response surface models to increase sustainability for an entire system [50]. Furthermore, the enabling of autonomous reasoning agents now enables full automation of both distillation simulation and carbon emission accounting, allowing for the design of heat pump-assisted processes that dramatically reduce the cost of industrial separation [51]. In addition to the above-mentioned evolution at system level, artificial intelligence is also crucial in screening environmentally friendly solvents (ionic liquids and deep eutectic solvents) to substitute traditional fossil raw material-based alternatives in demanding separation processes [52]. Moreover, machine learning-based predictive frameworks present the opportunity of real-time energy optimization for distillation processes by applying systematic learning and validation to define optimal operating points from a hyper-parameter standpoint [53]. To illustrate the concerns above, neural network-based strategies are already following second-law thermodynamic principles to improve the exergy efficiency of their performance while maintaining near perfect product quality.

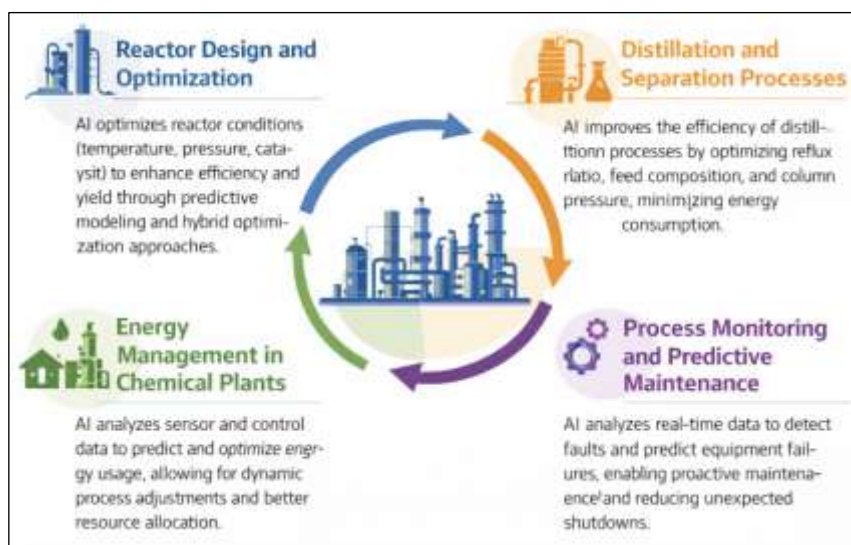


Figure 3: Applications of Artificial Intelligence in Chemical Process Optimization.
Source: Authors (2026).

IV.3 ENERGY MANAGEMENT IN CHEMICAL PLANTS

Energy management in chemical plants is crucial because energy costs contribute greatly to overall production costs [1]. Moreover, a plethora of environmental regulations compels industries to curtail emissions and enhance energy efficiency. AI models can help analyze the vast amount of operational data generated by sensors, control systems and energy monitoring devices to understand general trends about how a facility uses energy over time. These models allow us to understand how energy demand at nested process units is impacted by operating conditions. Because of the abundance of time-series data in manufacturing processes, deep learning methods are widely used to forecast energy demand through such process data. Precise predictions of energy consumption also allow plant operators to vary process parameters dynamically to allocate resources more efficiently. Thus, AI-based energy management systems enable chemical manufacturing plants to make more data-driven decisions regarding their energy usage to be more efficient and environmentally friendly. While unit-level changes are still the most accessible, multi-scale smart systems engineering is being employed to apply these optimizations at the facility scale where complex interactions between micro-scale materials discovery and macro-scale industrial park layouts must be coordinated. To this, a unified approach ensures the transition to carbon neutrality by matching industrial productivity with sustainable requirements [54]. Digital platforms allow monitoring of environmental emissions in real-time and provide direct implementation of mitigation strategies based on hybrid energy systems [55]. Additionally, the design of advanced integrated energy systems is imperative for balancing economic profitability and decarbonization goals in industrial landscapes [56].

IV.4 PROCESS MONITORING AND PREDICTIVE MAINTENANCE

In the chemical industries, process monitoring and predictive maintenance are largely based on artificial intelligence. Novel plants produce massive amounts of real-time data from sensors, control systems, Excel sheets to monitoring platforms which can be employed with Machine Learning models for anomaly detection, faults identification and predictions of equipment failures beforehand. Examples of such applications are early fault detection in reactors, pipelines, pumps, and heat exchangers as well as long-term process stability. In predictive maintenance systems, AI algorithms predict the remaining useful life of mission-critical equipment and help plan timely maintenance to reduce unexpected shutdowns, operational risks and costs. This transforms approaches making plants more reliable and enabling safe and efficient operation with proactive decisions. Moreover, intelligent control architecture also allows for modularization of processing units, providing flexibility and scalability in manufacturing systems [57]. ENCORE utilizes multi-agent systems that promote coordinated decision-making by interconnecting diagnostic and automation tools between process units [58]. Nevertheless, more studies are needed to assess economic viability and related hazards at large-scale implementation [59]. Some machine learning models, for instance random forest models, have been shown to improve predicted catalyst deactivation based on real-time data and thereby allowing a change in maintenance regimes. Likewise, deep learning applications in carbon capture systems allow for optimizing operational conditions such as temperature and pressure to improve CO₂ sequestration performance [60]. Transitioning to condition-based maintenance incorporates continuous diagnostics as early warning metrics that improve the long-term durability of critical assets [61]. The incorporation of diverse datasets like pressure, flow rates and operational signals has aided in minimizing downtime of equipment while enhancing the lifespan of equipment, leading to enhanced operational performance of chemical plants [62] [63]. The major current and potential applications of artificial intelligence to chemical process optimization are summarized in Table 3, which include OLED design, distillation systems, energy management, process monitoring and predictive maintenance.

Table 3: Major Applications of Artificial Intelligence in Chemical Process Optimization.

Application Area	Key Process Variables	AI Techniques Used	Optimization Objective	Industrial Benefits	Challenges / Limitations
Reactor Design and Optimization	Temperature, pressure, catalyst concentration, residence time	Machine Learning, Neural Networks, Genetic Algorithms	Improve reaction conversion and product yield	Higher reactor efficiency and reduced operational cost	Complex reaction kinetics and limited experimental data
Distillation Column Optimization	Reflux ratio, feed composition, column pressure, tray configuration	Machine Learning, ANN, Optimization Algorithms	Reduce energy consumption while maintaining product purity	Improved separation efficiency and lower energy use	High system complexity and sensitivity to operating conditions
Separation Process Design	Solvent properties, vapor–liquid equilibrium, operating pressure	Deep Learning, Predictive Modeling	Enhance separation efficiency and sustainability	Improved solvent selection and reduced environmental impact	Data availability and process variability
Energy Management in Chemical Plants	Energy consumption patterns, operating load, process parameters	Deep Learning, Time-Series Models	Predict energy demand and optimize energy usage	Lower operational energy cost and emissions	Dependence on accurate sensor data

Process Monitoring	Temperature, pressure, flow rate, concentration	Machine Learning, Pattern Recognition	Detect abnormal conditions and maintain stability	Improved safety and operational reliability	Noise in sensor data
Predictive Maintenance	Equipment vibration, temperature, historical maintenance data	Random Forest, Deep Learning	Predict equipment failure and remaining life	Reduced downtime and maintenance cost	Requires long-term operational data
Integrated Plant Optimization	Multiple plant-wide operating variables	Hybrid AI Models, Reinforcement Learning	Optimize overall plant performance	Improved productivity and sustainability	Complex model integration

Source: Authors (2026).

V. INTEGRATION OF ARTIFICIAL INTELLIGENCE WITH PROCESS SIMULATION AND DIGITAL TWINS

This type of artificial intelligence can be combined with process simulation and data analytics tools to enhance the decision-making in chemical industries. Digital Twin is a key concept in this domain and refers to the representation of the physical system (plant or process, etc.) mirrored to the virtual world — dynamically updated by incoming real-time data captured from sensor devices and control units. This model reflects real plant behavior and allows the engineers to monitor, simulate, and analyze performance at different operating conditions without disturbing the actual operations. Applying AI into digital twin frameworks expands its potential for processing large amounts of data and uncovering intricate connections between processes. By integrating design parameters, communication protocols and operational variables, these systems allow for simulation realization with high levels of accuracy [64-68], which can improve predictive maintenance as well as lifecycle assessment. Hybrid approaches such as these are found to be particularly beneficial in carbon capture, utilization and storage systems as they aid in optimizing the use of energy while reducing operational costs [69-73]. Digital twins also employ machine learning models that can be used to optimize capture processes based in solvents type, achieving cost reductions of 10–20% for large-scale applications [67]. Moreover, the real-time analytics and hybrid modeling proposed in these platforms are valuable for managing complex industrial data when integrating with legacy systems and cybersecurity issues [74]. In general, AI-powered digital twins can be used for real-time decision-making and life cycle management, which can assist with the development of adaptive and autonomous systems [75]. This led to systems that aid the engineers know how alterations in parameters like temperature, pressure, flow rate and feedback affect process performance. Moreover, these systems drive real-time optimization by continuously evaluating the incoming process data and suggesting optimal operating conditions. The other major advantage is implementing predictive maintenance models that are data-driven and predicting potential equipment failures by detecting deviations from normal patterns in which the equipment works.

Furthermore, digital twin environments enable engineers to verify new process strategies and control algorithms as well as design modifications in a virtual space prior to partaking them within the physical plant. Hybrid modeling (HM) approaches that merge artificial intelligence models with first-principles equations based on mass, energy, and momentum balances are increasingly acknowledged as some of the most powerful tools for chemical process optimization, due to their ability to combine the predictive power of data-driven methods with the physical insight provided by traditional chemical engineering models. However, while fundamental models are more accurate than their black-box counterparts, they can also be computationally expensive to evaluate and create a high barrier to entry for real-time iterative optimization. This is where data-driven surrogate models effectively alleviate this limitation at sub-second execution speeds [76-83]. Further, these surrogate models also facilitate real-time optimization strategies and maximize an objective function in the context of non-linear constraints and frequent disturbances to the process. This further enables hybrid semi-parametric modeling to provide more parsimonious yet useful representations of the system at hand by combining mechanistic insights with data-driven precision, thus ensuring that the generated models are both physically meaningful and computationally efficient [84]. In addition to performance improvements, the deployment of such frameworks also helps to enable autonomous operational decision-making through continuous learning which refines predictive insights [85-90].

VI. CHALLENGES IN AI-BASED CHEMICAL PROCESS OPTIMIZATION

While artificial intelligence offers tremendous advantages in the optimization of chemical processes, several issues inhibit its widespread adoption in industrial chemical facilities. These challenges are primarily related to data availability, model transparency, system integration and operational safety. Four major challenges (data quality, model interpretability, integration with first-principles models and cybersecurity) stand in the way of its successful industrial introduction for chemical processes as illustrated by Fig. 4.



Figure 4: Challenges in AI-Based Chemical Process Optimization.
Source: Authors (2026).

VI.1 DATA QUALITY AND AVAILABILITY

Access to high-quality and well-structured datasets has been a major bottleneck in applying AI methods in the chemical processes. Often the industrial plants run based on incomplete, noisy or inconsistent data due to limitations in sensor systems, issues of data collection and/or disturbances to the process. Machine learning models rely on a vast amount of accurate up-to-date data for them to learn well and predict accurately. The performance of AI models may deteriorate if the quality & accuracy of training data is poor. Moreover, due to the nature of these processes and low-frequency breakdowns, they are characterized by a lack of quality labeled data which makes it especially difficult to train robust diagnostic agents [91]. Additionally, the black-box nature of many deep learning architectures limits their utility due to at least two reasons; [92] high levels of resource consumption for developing such algorithms and the difficulty in interpreted reasoning behind "black box" prescription that can be cumbersome for some operations [93]. To address this, there is a growing emphasis among researchers for explainable AI frameworks with traceable rationales behind optimization decisions, building the trust needed for human-in-the-loop oversight in safety-critical settings [94].

VI.2 MODEL INTERPRETABILITY

A related problem is the interpretability of AI models. More sophisticated techniques such as deep learning work as complex computational systems with internal thresholds that are often hard to interpret. These models are often referred to as "black box" systems. Engineers working in the chemical industry tend to favor interpretable models that explain how process variables affect outputs. Interpretability also has value in that limited interpretability can undermine confidence in AI-based decision systems. The black-box nature decreases regulatory compliance and risk management while enforcement of multidimensional regulations requires an advancement in explainable AI methods that build stakeholder trust in algorithmic decision-making activity [95]. Additionally, current research is biased towards a focus on the properties of algorithms and their theoretical performance over simulated benchmarks rather than producing lightweight and operable solutions more in line with industry requirements [96]. To overcome this void, future work should reconsider the established machine learning life cycle toward one whose primary focus is the real-life application rather than theoretical performance at a single point in time that ensures robustness to multivocal real-life operations [97].

VI.3 INTEGRATION WITH FIRST-PRINCIPLES MODELS

Traditional chemical engineering analysis uses first-principles models based on mass and energy balances as well as reaction kinetics that describe the physical laws that govern processes. On the other hand, artificial intelligence models are data driven and usually do not explicitly consider physical constraints. Designing hybrid frameworks that combine these two approaches still proves challenging. One major constraint of cutting-edge AI methods, specifically deep learning, is their lack of transparency and inability to leverage known physical, chemical, and biological principles. This can lead to predictions that are not perfectly consistent with actual system behavior [49]. Consequently, future data-driven approaches should incorporate some insight from the domain to increase the reliability of models and keep predictions near thermodynamic and kinetic limits [98-103]. Beyond modeling challenges, applying machine learning to process control brings challenges of robustness, stability and safety [104]. Therefore, adaptive control strategies are needed that can accommodate dynamic data and guarantee reliable performance in large-scale industrial applications such as electrolysis and carbon capture systems [105].

VI.4 CYBERSECURITY AND RELIABILITY

Since chemical plants operate with stringent safety and reliability guidelines, any AI systems integrated into the industrial control platforms must be comprehensively validated prior to deployment. The rising proliferation of connected sensors, digital infrastructure and cloud-based systems creates cybersecurity challenges as well. As a result, secure data transmission and reliable system performance along with safe AI algorithm integration are essential for effective implementation.

Process data can be sensitive or proprietary in nature, requiring advanced measures for data privacy to mitigate the risk of loss of intellectual property [106], malicious interference, and similar risks. Tackling these challenges must involve collaboration across AI specialists, chemical engineers and policymakers for unified protocols to secure data and validate models [107] [108]. The success of such adoption is also dependent on the ongoing investment towards building a multidisciplinary workforce capable of understanding and managing AI-driven systems by plant operators [109]. Moreover, to take advantage of the full potential that AI offers to chemical industries, a transition into interdisciplinary studies is required in which both machine learning practitioners and domain experts (chemical engineers) collaborate [110]. This is necessary to enable digital transformation, minimize inertia towards change and ensure that the safety and reliability required in modern chemical production systems is met on an on-going basis [111].

VII. CONCLUSION

AI has become a gamechanger in the field of chemical process optimization, enabling sophisticated modeling, prediction, and intelligent decision-making in complex industrial processes. Using machine learning techniques, deep learning, reinforcement learning and evolutionary algorithms, etc., modern chemical industries can recover nonlinear (nonlinear), multivariable processes that are not currently developed using common methods. Such AI-powered methods also boost the efficiency of research and product strains, lower energy consumption, and enable sustainable manufacturing practices. Combine this with capabilities of process simulation tools and digital twin technologies, which have taken real-time optimization and predictive maintenance to the next level by enabling much more adaptive and autonomous plant operations. However, it is imperative to diligently consider data quality, model interpretability, system integration as well as cybersecurity challenges to allow for the safe and reliable industrial deployment of such approaches. In terms of the future, developments in hybrid modeling, explainable AI and autonomous systems will further drive the adoption of intelligent optimization frameworks. It will be important to continue conducting research in this area, by combining both fundamental and applied approaches together with research teams from other disciplines to effectively utilize the advance of artificial intelligence to develop smarter, more efficient, and sustainable chemical process industries that align themselves with environmental/economic goals worldwide.

VIII. AUTHOR'S CONTRIBUTION

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