AI-Enhanced Multi-Scale Smart Systems for Decarbonization in the Chemical Industry: A Pathway to Sustainable and Efficient Production

Xuequn Chong[1], Lanyu Li[1,*], Chuan Zhang[2], Yingru Zhao[3], Markus Kraft[4,5], Xiaonan Wang[1,*]

[1] Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

[2] Institute of Energy, Peking University, Beijing 100871, China

[3] College of Energy, Xiamen University, Xiamen, 361100, China

[4] CARES, Cambridge Centre for Advanced Research and Education in Singapore, 138602, Singapore

[5] Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, CB3 0AS, United Kingdom

*Corresponding author； Lanyu Li, lilanyu@mail.tsinghua.edu.cn; Xiaonan Wang, wangxiaonan@tsinghua.edu.cn

Abstract

In the quest for sustainability, decarbonizing the energy-intensive chemical industry emerges as a pivotal challenge in recent years. This article investigates decarbonization imperatives within the chemical sector, employing a multi-scale smart systems engineering approach. It highlights the dual role of the chemical industry as a significant energy consumer and carbon dioxide emitter, underlining the urgent need for a shift towards green and smart chemistry and processes driven by both environmental and economic benefits. By examining innovations across various scale — from micro-level materials discovery to meso-level process optimization, and up to macro-level chemical industrial park design/redesign — this paper illuminates how intelligence approach can revolutionize efficiency, sustainability, and carbon neutrality. Overall, this paper presents a cohesive overview of interconnected strategies for the chemical industry's pivotal transition towards sustainability. It also highlights the transformative power of intelligent technologies in redefining current methodologies to meet ambitious future sustainability targets. The critical role of innovation in ensuring the sustainable development of the chemical industry by bridging the gap between current practices and future sustainable development goals was also reaffirmed.

Keywords

Chemical industry; multi-scale process system engineering; decarbonization; artificial intelligence; digital twins; sustainable production

1 Introduction

The pursuit of sustainable and efficient production in the chemical industry is at the forefront of global

efforts to combat climate change and advance sustainable development goals (SDGs). Recent meteorological statistics reveal that in 2023, global temperatures has soared to 1.31°C above the pre-industrial average [1, 2]. Climate-related disasters resulted in 2 million deaths and inflicted $4.3 trillion in economic damage [3]. The climate-related issues has catalyzed the formulation of international frameworks designed to limit global temperature escalation and diminish fossil fuel dependency, including but not limited to controlling the global temperature increase to less than 1.5 to 2.0 °C by 2050 [4], and reducing the reliance on fossil fuels to 8% and achieving a cumulative reduction of 300 Gt in carbon dioxide emissions, thereby mitigating the climate impact of greenhouse gases [5, 6].

The chemical industry, as the largest industrial energy consumer and a major emitter of CO2, is integral to these efforts [7–11]. Its interconnection with various sectors (e.g. energy, transportation, pharmaceuticals, construction, mining, agriculture, etc.) underscores the pervasive influence of chemicals on both the economy and the environment. In particular, the global chemical demand has consistently increased, with total production barely contracting by 0.4% in 2020 despite the pandemic, followed by 7.7% surge during the economic rebound [12, 13]. However, this growth comes with environmental implications, a research show that the process of converting fossil fuels into platform chemicals emitting 151.6 Gt CO2 indirectly and 286.8 Gt CO2 directly [14].

Embarking on the decarbonization journey within the chemical industry unveils a landscape riddled with multifaceted challenges. Chemical industry, segmented into petrochemicals, coal chemicals, bio-chemicals, and fine chemicals, showcases a vast diversity in terms of production processes and product types. Such differentiation not only underlines the multi-layered essence of the sector but also introduces a broad spectrum of process scales, economic considerations, and technological hurdles. Additionally, this compound complexity is further intensified by the protracted nature of R&D cycles and the extended payback periods for infrastructural investments, often exceeding a decade, thus imposing substantial economic and technological strains on the sector's forward momentum. This inherent diversity necessitates a triple-faceted approach towards transformation: one that is tailored and precise at the micro level, focusing on customized research and development (R&D), further modular design at the meso-scale aims to improve process efficiency through design and operational optimization, and another that is strategic and overarching at the macro level, aimed at devising targeted systemic solutions.

Moreover, the industry's transformation is intricately linked to internal dynamics and external demand, including inter-factory coordination, raw material sourcing, and adaptation to fluctuating market demands, as well as external pressures stemming from international and national regulatory frameworks and policy directives. Green transformation is contingent upon the execution of multi-dimensional decision-making processes and the cultivation of robust multi-stakeholder cooperation, aimed at aligning the deployment of green technological innovations with the diverse needs and

expectations of various interest groups. This intricate web of challenges underscores the pressing urgency and the intricate complexity inherent in the chemical industry's quest for decarbonization.

The decarbonization of the chemical industry is a complex challenge with the goal of meeting emission reduction targets within strict timelines, guaranteeing the practical application and continuous improvement of technologies, and confirming their viability both industrially and economically. Further, as the chemical industry operates across multiple levels: at the microscopic scale (research and development for product/material discovery), the mesoscopic scale (covering equipment, and processes), and the macroscopic scale (including factories, parks, supply chains, and broader regional and environmental impacts), the innovation requires holistic approaches that span various scales of chemical processes to minimize energy consumption, optimize material use, reduce pollutant emissions, and maximize profitability.

The adoption of cutting-edge technologies, including Artificial Intelligence (AI), digital twins, and big data analytics, signifies a transformative stride towards environmental stewardship in the chemical sector. This movement is underpinned by the critical role such technologies play in elucidating complex molecular interactions and overseeing the dynamics of expansive industrial ecosystems. By offering a strategic pivot away from conventional trial-and-error methodologies, these smart technologies catalyze technological innovation, thus enhancing efficiency at multiple scales.

This review embarks on an in-depth examination of the green transformation journey, a journey characterized by its complexity, spanning various temporal and spatial dimensions, each presenting unique challenges (Figure 1). The forthcoming discussion is dedicated to the exploration of the synergistic integration of smart technologies within the chemical industry. It aims to illuminate the critical role these technologies play in facilitating a cohesive strategy for decarbonization efforts across different operational scales, highlighting the essential contribution of intelligent solutions to the industry's sustainable transformation. In the second section, we delve into the multifaceted roles assumed by the chemical industry at multiple levels and investigate the deployment of intelligent technologies within each layer. The discourse then progresses to unravel the complexities involved in interlinking these varied levels of industrial parks, drawing on research insights to provide a comprehensive understanding. The concluding segment of this paper will shed light on both the challenges and the potential applications of intelligent technologies within the multifarious layers of chemical industry, offering a critical analysis that bridges theoretical perspectives with practical implications in the realm of sustainable industrial advancement.

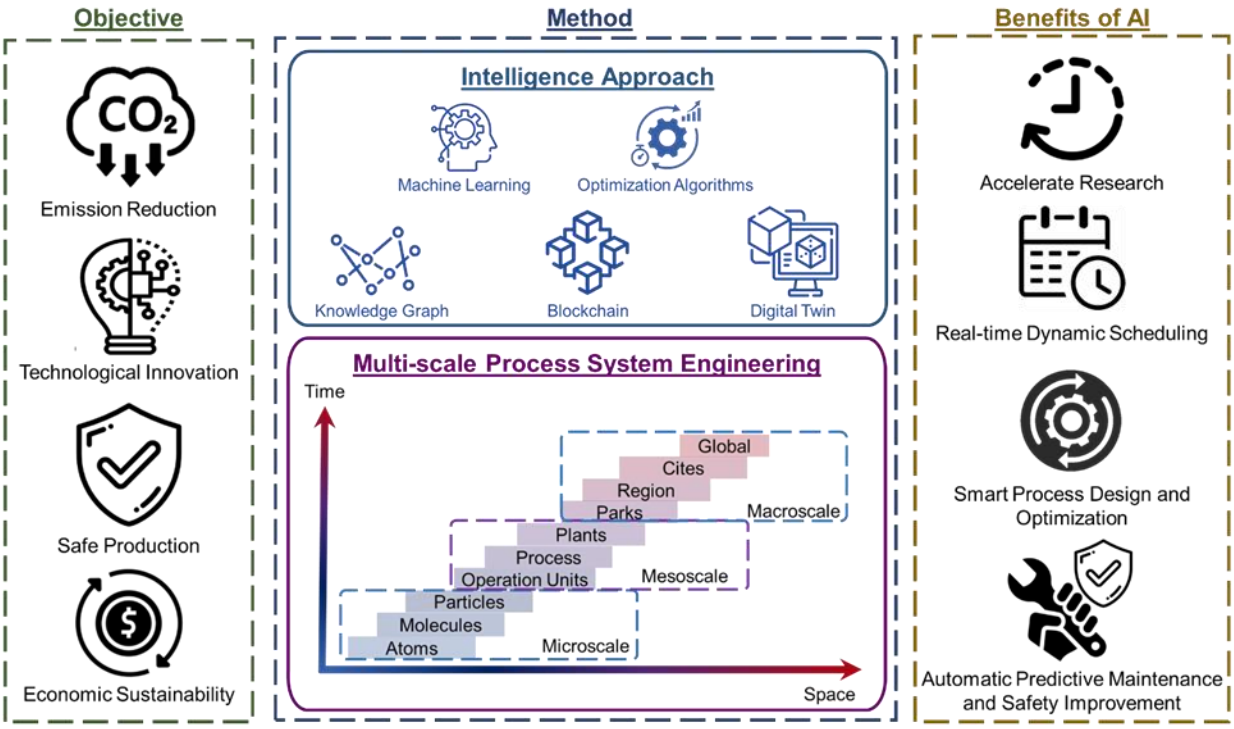

Fig. 1 Empowering sustainable development: AI-enhanced multi-scale smart systems for the decarbonization of chemical industry.

2 Intelligent decarbonization of chemical industry at different scales

In the context of decarbonization, the enhancement of scalability and implementation is markedly augmented by the integration of smart technologies. These technologies offer sophisticated, data-driven approaches, enabling a systematic and thorough deployment of technological interventions. To this end, the nuanced application of decarbonization strategies is facilitated through the harnessing of digital capabilities and the employment of intelligent solutions, thereby broadening the reach and effectiveness of technological deployment within the chemical industry.

Building upon the integration of smart technologies for decarbonization strategies, it is imperative to consider the multifaceted scales at which these technologies can be applied and their respective impacts on the chemical sector. The spectrum of scales ranges from the micro/nanoscale to the macro-scale, each offering unique advantages and challenges in the pursuit of sustainable practices.

At the microscale, nanotechnology and microscale processes play a pivotal role in accelerating material and chemical innovations. These processes enable the manipulation of matter at the atomic and molecular levels, leading to the development of new materials with enhanced properties and the potential for more efficient chemical reactions with reduced environmental impact. The precision afforded by nanotechnology can lead to the creation of catalysts that are more effective and less resource-intensive, thereby contributing to the decarbonization efforts.

Transitioning to the mesoscale, systems intelligence is employed to optimize process efficiency and minimize resource wastage to achieve decarbonization. This intermediate scale focuses on the integration of smart sensors, control systems, and data analytics to monitor and manage industrial processes in real-time. By doing so, it becomes possible to fine-tune operations, reduce energy consumption, and recycle waste streams, all of which are critical for achieving a more sustainable and low-carbon footprint.

Finally, at the macro-scale, adaptive management of industrial operations is crucial for aligning with sustainable, low-carbon, and safety objectives. This involves the strategic planning and execution of operations at a larger scale, considering the broader environmental, economic, and social implications. Macro-scale interventions may include the redesign of supply chains, the adoption of renewable energy sources, and the implementation of policies that promote a circular economy.

This section will discuss the effective deployment of smart technologies at different scales, which is essential for a comprehensive approach to decarbonization.

2.1 Microscale strategies: Accelerating Material Discovery

Material research and development, alongside process implementation, are pivotal in driving the progress of the chemical industry. Currently, most industries predominantly rely on fossil fuels, resulting in substantial carbon emissions during production processes. In addition to process optimization and substance substitution, a critical strategy for carbon reduction involves the direct capture of carbon dioxide from industrial emissions or atmospheric air, along with its subsequent reuse, forming a cornerstone of the chemical industry's approach to carbon management. Central to Carbon Capture and Utilization (CCU) is the development of materials that facilitate the absorption and transformation of carbon dioxide at the microscopic level. Despite numerous advances in this domain, the interplay among the parameters creates an extensive experimental search space complicating the traditional approaches to material research and development. Therefore, the selection of appropriate material systems and processes tailored to specific production requirements presents a significant challenge due to the myriad of available methodologies.

The integration of machine learning techniques offers a solution by significantly narrowing the search scope. Algorithms with high adaptability can be seamlessly applied to analogous systems, guiding the targeted development of materials. Given the extensive body of research already available in the field of carbon capture materials, the application of machine learning techniques to experimental data can diminish reliance on experiential knowledge, thereby expediting material development. The introduction of targeted algorithms enhances the precision and speed of achieving research objectives, while the transferability of models provides a foundational reference for similar or identical system studies. Furthermore, data mining assists in uncovering underlying mechanisms, facilitating the optimization of conditions with a goal-oriented approach. This multifaceted strategy underscores the

potential of machine learning to transform the development and application of carbon capture technologies, aligning with the imperative for innovative solutions in the pursuit of environmental sustainability.

This section delves into the utilization of intelligent technologies in the development of materials for the capture and conversion of carbon dioxide, showcasing their potential to revolutionize material research by facilitating the efficient identification and optimization of novel material systems for CCU applications.

2.1.1 Carbon capture

Carbon capture technology, pivotal in addressing environmental challenges, demands tailored approaches across varying conditions, necessitating specific selections in capture methods, materials and their preparation techniques. Machine learning models, designed with transferability in mind, enable the prediction of material performance and when combined with experimental efforts, significantly refine the experimental scope. The development of these transferable models, alongside the integration of automated platforms, substantially accelerates the iterative process. This advancement not only guides the synthesis and enhancement of carbon capture materials but also underpins more strategic research decisions. By leveraging such intelligent systems, the field can advance more rapidly towards effective and efficient carbon capture solutions, tailored to diverse environmental scenarios.

Intelligent technology offers substantial benefits in processing large datasets and incorporating a broad spectrum of factors in the development of carbon capture materials. By utilizing experimental and structural data, it facilitates performance predictions, thereby expediting the initial exploration phase. This approach leverages the capacity of machine learning and artificial intelligence to sift through complex data patterns, identify correlations, and predict material behavior with high accuracy. Consequently, it significantly reduces the time and resources required for material development.

For instance, Song et al. [15] utilizing Artificial Neural Networks (ANN) and Support Vector Machines (SVM) developed group contribution models based on a dataset of 10,116 carbon dioxide solubility data points. These models correlate CO2 solubility with the ionic structure, temperature, and pressure to predict the solubility of CO2 in different ionic liquids accurately, achieving prediction results with a Mean Absolute Error (MAE) of less than 0.024 and an R-squared (R2) value greater than 0.978. Furthermore, material systems with research data record, discovering new or specific applications through existing data requires extensive verification. Machine learning modeling can significantly narrow down this scope. As an example, a study collected 527 data points from the literature to predict the CO2 adsorption capacity of biomass waste-derived porous carbons (BWDPCs), focusing on their structural properties, compositional characteristics, and adsorption properties as training data(Figure 2a) [16]. The objective was to elucidate the relationship between these parameters

and the adsorption performance, thereby guiding the synthesis of porous carbons optimized for targeted CO2 adsorption. Another study involving 6013 MOFs used a random forest algorithm to predict CO2 selectivity and identified 14 MOFs with the best target performance [17]. Similarly, random forest models have been employed to optimize biochar production by predicting yield and carbon content [18]. This approach illustrates how predictive modeling can be employed to direct the development of materials with enhanced functionality for environmental reasons.

Moreover, utilizing performance prediction models, in conjunction with experiment data and existing literature, can significantly enhance the strategic direction of material synthesis, enabling a more focused and informed approach. A study reported the development of a machine learning workflow for the advancement of mixed matrix membranes (MMMs) for CO2 separation [19]. This workflow leverages literature data to guide the preparation of CO2/methane separation membranes. The data collected from separation tests and performance evaluations of these membranes are then fed back into the machine learning model to expand the dataset and guide the generation of new MOFs, thereby improving model accuracy (Figure 2b). The optimal structure of MOFs in mixed matrix membranes was revealed (pore size larger than 1 nm, surface area approximately 800 m^2/g), providing a reference for material preparation. This highlights the efficacy of incorporating artificial intelligence at appropriate stages to avoid extensive condition optimization, thus preventing the time and resource wastage associated with numerous experiments.

Automated platforms combined with machine learning in chemical synthesis reduce human error, allowing high-throughput and accurate operations. Advanced predictive models and task planning translate natural language into machine commands, enhancing usability of automated platforms for non-experts, and expediting molecular discovery and synthesis[20, 21] (Figure 2c). ChemTS, combining Monte Carlo tree search with a recurrent neural network, offers a molecular generation platform for tailoring MOFs for greenhouse gas separation, this approach simplifies early-stage exploration by designing MOFs based on target performance, metal nodes, and topological network information[22, 23].

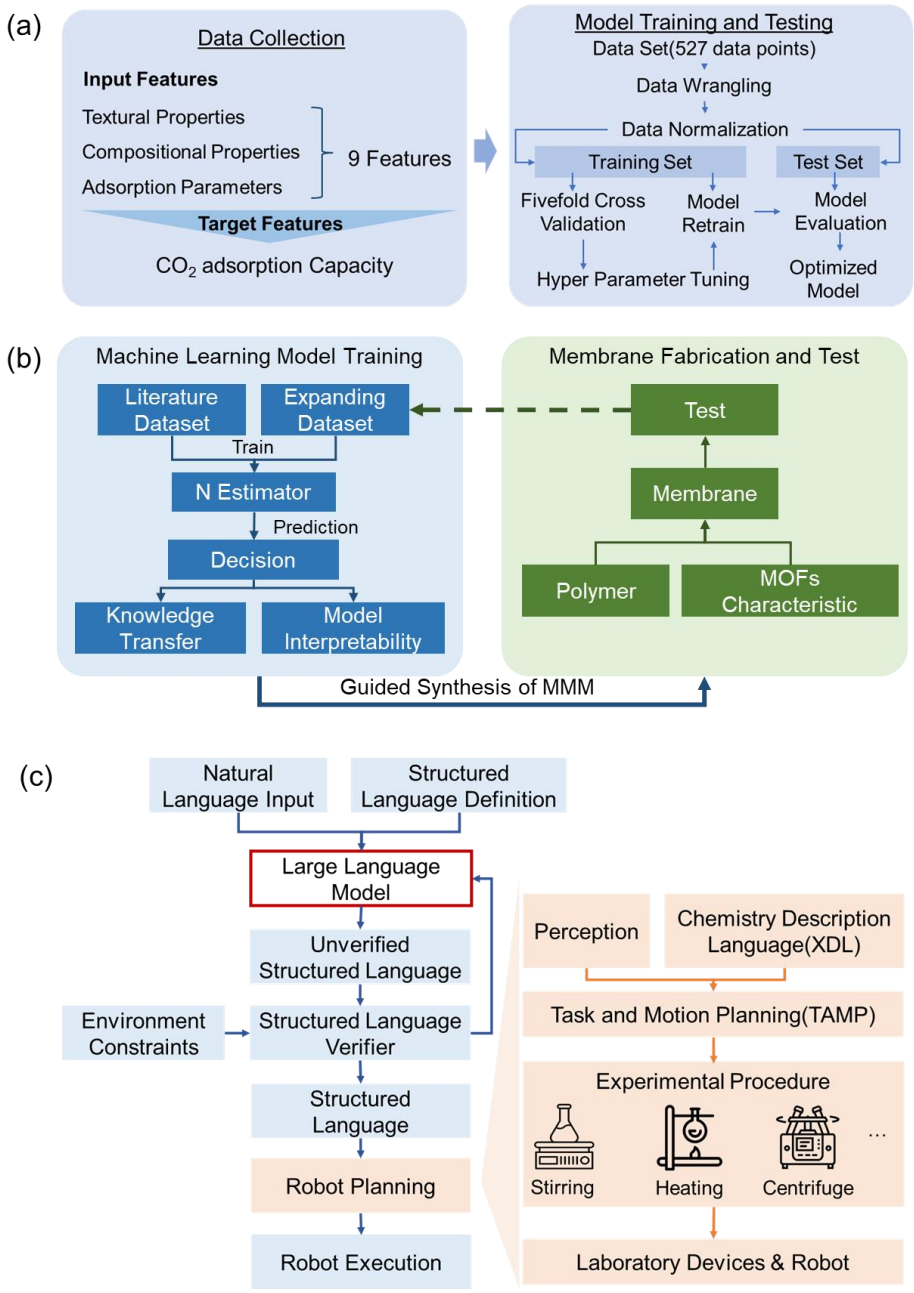

Fig. 2 Harnessing Machine Learning for Breakthroughs in Carbon Capture Materials. (**a**) Materials performance prediction (Redrawn by [16]); (**b**) Narrowing research area: Enhanced model accuracy with machine learning and experimental data integration (Redrawn by [19]); (**c**) Construction of automated platforms in chemical synthesis(Redrawn by [21])

2.1.2 Carbon conversion

In the realm of carbon conversion, the vast amount of literature and diverse methods from different teams present a challenge for manual analysis, often leading to oversights and a heavy reliance on trial-and-error experimentation. Full data-driven machine learning frameworks used for predicting

performance can guide experiments and optimization in systems with extensive experimental backgrounds.

For instance, Suvarna et al. [24] developed a machine learning framework using 1425 data points from literature to predict the space-time yield of methanol production from carbon dioxide hydrogenation and found that the prediction error was only 0.11 g MeOH h-1 gcat-1. They identified key experimental conditions impacting the system, providing a basis for further research. Additionally, researchers used algorithms like extreme gradient boosting regression, gradient boosting regression, and random forest regression, optimized with genetic algorithms, to predict optimal process parameters for electrodes used in CO2 reduction to various products [25]. Moreover, for systems challenging to simulate traditionally, Pablo-García et al. [26] developed a graph neural network, GAME-Net, which quickly screens catalytic materials with an average absolute error of only 0.18eV, significantly faster than DFT methods. The integration of AI in materials science narrows the experimental scope and accelerates predictions.

On the other hand, machine learning models' transferability substantially improves efficiency in similar exploratory work. The complexity and diversity in chemical structure-property relationships make identifying and designing specific function catalysts challenging. Combining first-principle methods with AI, Mazheika et al. [27] identified materials properties optimal for CO2 activation. This approach is not limited to CO2 conversion catalysts but extends to accurately identifying and designing catalysts with specific functions, guiding other activation indicators. Full data-driven machine learning models can be deployed across different catalytic processes, facilitating experimental condition selection and accelerating technological innovation.

In conclusion to this section, the integration of intelligent approaches with experimental data and mechanistic insights significantly enhances the pace of catalyst discovery and deepens the understanding of their mechanisms. This approach is particularly beneficial in the context of carbon dioxide capture and conversion, positively impacting the development of novel capture materials and catalysts. Nonetheless, the application of intelligent methods in the realm of microscopic material discovery encounters several challenges: (1) the critical influence of data quality on the precision of machine learning models; (2) the feasibility of synthesizing materials as predicted by these models; and (3) comprehending the operational mechanisms of materials for further optimization. Therefore, addressing the interpretability of machine learning methods emerges as a crucial direction to advance and expedite the development of materials at the microscopic level, ensuring that these innovative approaches yield practical and actionable insights for the chemical industry.

2.2 Mesoscale Strategies: Unit Operation, Process and Plant

The concept of scale is pivotal in the chemical industry, delineating the macroscale as dimensions above millimeters, and the microscale as those below[28]. In the chemical industry, dimensions

ranging from millimeters to kilometers are typically classified as the mesoscale. The mesoscale is crucial for understanding phenomena that are not apparent at the macro level yet are too large to be considered at the molecular or atomic level, playing a pivotal role in the development and optimization of chemical processes and materials. At the heart of material conversion lies the unit operation, which, when orchestrated into a cohesive sequence, forms a process. In turn, a collection of these processes constitutes a factory. The incremental complexity from unit operations to plant level underscores the multifaceted nature of chemical production, where material characteristics, operational parameters, and environmental conditions all play crucial roles.

The challenge of digitalization in the chemical industry is compounded by the complexity of constructing mechanism models and the extensive computational demands they entail. The adoption of intelligent methodologies at the modeling stage offers a promising solution, enabling the creation of simplified, data-driven models that leverage historical data for process prediction and operational adjustments, ensuring consistent performance. Furthermore, these models facilitate the rapid screening of optimal operating conditions tailored to desired outputs, thereby expediting the design and implementation of equipment. This section aims to explore the deployment of intelligent technologies across the three hierarchical levels of unit operation, process, and plants. Through this exploration, we delve into how these technologies can unravel the complexities inherent in each stage, offering insights into achieving efficiency, precision, and innovation in the chemical industry's mesoscale operations and the interaction between three layers will be discuss in section 3 (Figure 3).

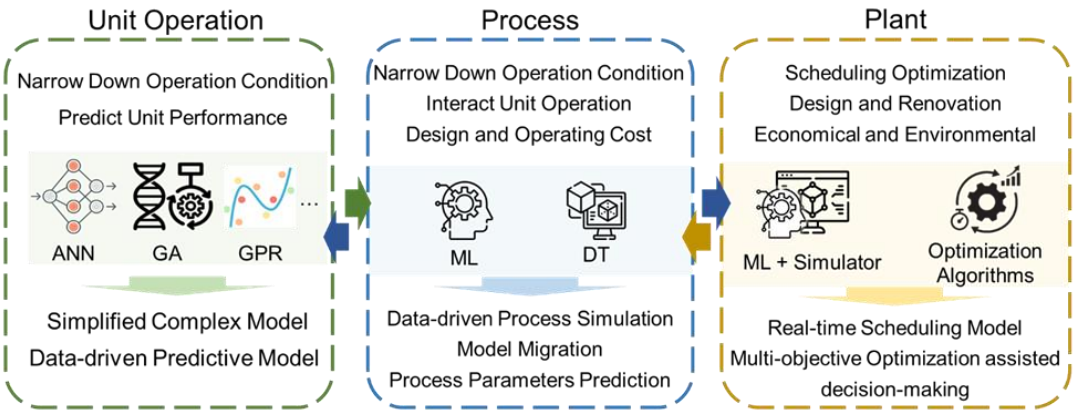

Fig. 3 Mesoscale strategies: Intelligence approach advancing chemical engineering simulations from unit operation through plant.

2.2.1 Unit Operation

Unit operations, pivotal for material transformation within chemical processes, serve to streamline intricate flows and refine conditions for each segment. The challenge of harmonizing a multitude of parameters and performance metrics within these elaborate operations is amplified by the intricacy and computational demand of mechanistic models[29], [30]. The advent of machine learning

algorithms, including Artificial Neural Networks (ANN), Genetic Algorithms (GA), and Gaussian Process Regression (GPR), offers a pathway to simplify these first-principles models while maintaining precision. These technologies enable the modeling of unit operations, particularly those of considerable complexity and computational requirement, culminating in the establishment of data-driven predictive models. Such models are instrumental in forecasting operating conditions and production outputs, thereby expediting the optimization process.

For instance, in the domain of carbon dioxide capture, solution-based post-combustion capture has emerged as a notably mature technology. Research by Shalaby et al. [29] delineates the comparative efficacy of various data-driven models—such as fine trees, Matérn GPR, rational quadratic GPR, squared exponential GPR, and Recurrent Neural Networks (RNN)—in predicting the outputs of post-combustion capture units. Optimization methods, including Sequential Quadratic Programming (SQP) and Genetic Algorithms (GA), have been employed to refine model parameters, achieving prediction accuracies approaching 98%. Furthermore, surrogate models utilizing artificial neural networks and fine trees have demonstrated the capability to supplant complex physical models, thereby diminishing computational load and enhancing optimization efficiency. The employment of an ANN-based surrogate model alongside Partial Least Squares regression for dimensionality reduction mirrors the outcomes of mechanistic models, albeit with markedly less optimization time[30]. These advancements underscore the efficiency in selecting operating conditions and underscore their potential for real-time implementation in industrial contexts.

2.2.2 Process level

Chemical engineering processes, encompassing a broad array of unit operations such as reactions, separations, heat exchanges, and synthesis, are fundamental in transforming raw materials into finished products, all while adhering to defined production goals. Process simulation, an essential preparatory phase within chemical engineering, plays a crucial role in ensuring the feasibility and stability of these operations in real-world scenarios, thereby mitigating potential construction and operational cost overruns. These simulations incorporate a diverse set of variables, including material properties, operating conditions, catalyst specifics, quality of raw materials, design of equipment, and reaction kinetics, alongside considerations for energy and mass balance, economics, environmental impact, and safety standards. The inherent complexity and non-linearity of these processes render optimization a challenging, multi-objective endeavor, significantly complicating the task of making accurate predictions and optimizations in industrial contexts[31].

The advent of machine learning technologies offers a streamlined approach to navigating this multi-objective optimization landscape, enhancing the potential for discovering optimal solutions. Moreover, machine learning facilitates the estimation of otherwise unknown properties within process simulations, thereby enabling more precise calculations and expediting the optimization of intricate

chemical processes. The primary applications of intelligent technology at the process level include data-driven process simulation optimization, model migration, and the prediction of process parameters. The deployment of entirely data-driven or hybrid modeling techniques not only allows for the precise calculation and swift optimization of complex processes but also aids in predicting physical properties essential for model development. This section is dedicated to examining the integration of intelligent technology across these three domains, highlighting its transformative impact on the accuracy and efficiency of process simulation and optimization in chemical engineering.

In chemical engineering, process efficiency, low energy consumption, low emissions, and cost-effectiveness are key goals, adding complexity and non-linearity to process optimization. Black-box models based on numerical methods can simplify complex system simulations, but they lack symbolic expressions and analytical derivatives critical for optimization and can introduce computational noise affecting gradient-based optimization methods[32]. Furthermore, these models often don't provide precise function boundaries for deterministic global optimization[33]. Kriging surrogate models in GAMS nonlinear programming (NLP) have been proposed to optimize black-box simulation issues effectively [32]. Combining physical-dynamic models with machine learning not only provides foundational understanding for black-box models, enhancing interpretability and reducing dataset quality dependence [34] but also avoids the computational slowdown of physical models, speeding up early-stage design predictions and assessments. For optimal process solutions, a hybrid model combining continuous grouped kinetics production and artificial neural networks has been developed. This model integrates optimization using NSGA-II for hydrocracking reaction performance, with a mean squared error of just 0.01 compared to physical models [31].

Optimization models for chemical processes adaptable to various feedstocks and operating conditions can reduce time costs and avoid redundancy. Digital twin models developed for the benzene and propylene liquid-phase alkylation process, optimize petroleum chemical production processes[35]. The complex system involves reactors, mixers, heat exchangers, separators, and distillation columns. The framework first undergoes simulation and data collection, followed by neural network training to predict process outputs, and further achieve automatic optimization. Another study considered key factors affecting the supercritical water gasification process (SCWG), using neural networks to predict syngas composition under different conditions, facilitating faster adjustments in hydrogen production and CO2 emissions[36].

In context to the prediction of process parameters, accurate data on properties such as viscosity, density, and surface tension are vital for process modeling in chemical engineering. Experimental data acquisition can be costly and time-consuming. Machine learning has been employed for precise prediction of ionic solvent physical and thermodynamic properties. For example, Gaussian regression models and support vector machines have been used to predict the solubility, density, and molar heat capacity of 1-butyl-3-methylimidazolium hexafluorophosphate [Bmim][PF6] during CO2 capture,

guiding solvent design improvements [37]. Moreover, even with simplified modeling of complex processes, high-fidelity models require extensive data collection and computation. Intelligent methods improve data collection efficiency and reduce model building time[38].

2.2.3 Plant level

The low-carbon transformation of chemical plants can be summarized in three approaches: (1) Incorporating low-carbon technologies in initial plant design to optimize energy, heat, and material utilization; (2) Optimizing existing plant operations with a focus on economic and sustainable goals, ensuring efficient operation and coupling of multiple processes; (3) Streamlining and modifying processes using new technologies to reduce unnecessary consumption. However, challenges include high initial investment costs and complex mechanical, physical, and chemical structures. New plants may face substantial additional investments, while older plants might see fewer effective transformations. Balancing product performance, environmental standards, and economic indicators is crucial for a green transition in factories.

Industrial energy consumption, accounting for 35% of total energy use, sees a significant portion wasted as heat. Efficient utilization of waste heat is crucial to minimizing industrial energy waste[39], [40], [41].In complex chemical processes, optimizing waste heat reuse involves adjusting multiple parameters, impacting energy savings, costs, environment, production efficiency, and system design[42], [43], [44]. Real-time data acquisition and adjustments can cause delays. Machine learning-based predictive models can leverage limited historical data for real-time process monitoring and adjustments, ensuring the stable and efficient utilization of energy and materials in cyclic operations. For example, to facilitate waste heat utilization in carbon fiber production, an energy balance model of carbon fiber manufacturing was developed. The team analyzed the flow and consumption of energy throughout the production process and used neural network models and nonlinear regression to predict indicators such as energy consumption and efficiency based on the analysis data[45]. The results indicated that integrating a heat exchange system could recover 64% of the total energy consumption, enhancing the overall energy efficiency to 86%.

Furthermore, optimizing factory inputs, energy, and processing capacities within set targets can be a cost-effective way to reduce emissions, especially in older processes with large optimization potential. Techniques like Bayesian optimization and digital twin models address technical optimization conflicts, feedback delays, and decision-making within plants[46]. Surrogate models enhance production process understanding, aiding multi-factor decision-making through mechanistic model simplification. For instance, surrogate models created using random forests, support vector regression, and neural networks based on Aspen HYSYS data, assess technical-economic aspects of production processes, aiding in operational decision-making [47].

2.3 Macroscale Strategies: Navigating the Chemical Industry's Interactions Beyond Production

The chemical industry's operations are significantly influenced by a myriad of factors at the macro scale, including policies, societal attitudes, environmental shifts, and market demands[48], [49]. The adoption of carbon dioxide capture and utilization (CCU) technology epitomizes a strategic response to these factors, enabling the transformation of captured CO2 into a valuable resource—whether as a carbon sink, a means for enhancing oil field recovery, or as a feedstock to produce chemicals and fuels. Artificial Intelligence (AI) methodologies present a powerful tool for navigating the uncertainty of these external influences, offering the capability to distill complex models into actionable insights through the analysis of historical data. Such insights are pivotal for the iterative optimization of chemical processes, facilitating the development and adjustment of dynamic systems that are adept at aligning with production objectives and schedules (Figure 4).

This discourse will focus on the deployment of intelligent technologies within two key domains: the fostering of industrial symbiosis at the chemical park level and the optimization of interactions between the park and its broader environmental context. By leveraging intelligence approach, the chemical industry can anticipate and adapt to external pressures, streamline operations, and enhance sustainability and efficiency. The application of these technologies enables the construction of systems that are not only reactive but also predictive, capable of adjusting to changes in real-time to optimize both environmental and economic outcomes.

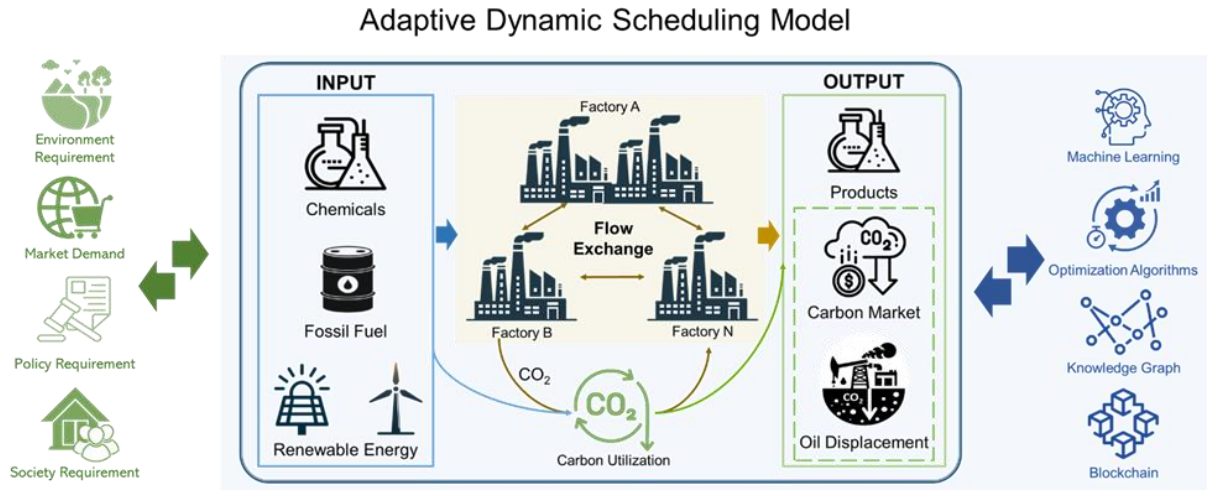

Fig. 4 The carbon management application landscape of intelligent technology at a macroscale.

2.3.1 Industrial Symbiosis in Chemical Industry Parks

The establishment of Chemical Industry Parks (CIPs) represents a deliberate strategy to consolidate chemical production in specialized zones, enhancing industrial symbiosis, resource efficiency, and environmental sustainability. Anchored in a robust regulatory framework, this initiative promotes the industry's migration to these parks, aiming to develop a standardized, operationally excellent, and

competitive ecosystem[50]. By 2020, China had inaugurated 616 chemical industry parks, playing a pivotal role in the sector's structural transformation and highlighting their contribution to high-quality development through optimal resource utilization[51]. These parks facilitate industrial symbiosis by fostering interconnectedness among raw materials, products, and systems, which enhances cross-sectoral collaboration, resource management, technological innovation, and socio-economic and environmental sustainability.

Central to these parks' operational ethos is the shared infrastructure designed to optimize utilities, waste management, and energy distribution, thus boosting efficiency, minimizing pollution, and reducing operational costs. Centralized management within these parks aids in the efficient exchange of materials and energy, lowering carbon footprints and advancing sustainable and innovative practices. Examples from Denmark, the Netherlands, Canada, and the UK demonstrate how specific regulatory frameworks can drive technological progress and the circular economy's expansion[52]. The strategic management of material, product, and by-product circulation within the parks aims to achieve regional industrial symbiosis, enhancing both economic and environmental benefits.

The integration of optimization algorithms and knowledge graph in managing CIPs significantly curtails operational costs, starkly contrasting with the solitary management of individual factories. The design and operation of these parks necessitate a focus on collaborative efficiency among diverse entities, aiming for mutual benefits and profit maximization through optimization of park modeling and prediction based on historical environmental data. Carbon neutrality initiatives within these parks have propelled the development of value chains that transform waste gases from high-emission processes into inputs for high-value products, thereby forging vital pathways towards industrial decarbonization. Traditional optimization algorithms like genetic and particle swarm optimization can address the non-linear, multi-objective complexities of park management.

For instance, integrating renewable energy, low-carbon steel plants, CO2 capture, and methanol production in the steel industry has shown promising results using heuristic algorithms like particle swarm optimization for efficient gas, thermal energy, electricity, and carbon interaction coordination under varying weather and load conditions[48]. The DigiCirc uses resources or material flows as nodes to link processes and technologies, allowing users to understand transformation pathway information by retrieving material flow information in the park[53]. Trokanas et al.[54]designed an algorithm based on the similarity of material flow properties and geographical distance to discover material exchange opportunities within and across the park to assist industrial symbiosis decision-making.

2.3.2 The interlink between chemical industry with societal and environmental factors

The interplay between industrial energy consumption and socioeconomic development is a vital area of study. Data analysis integrating physics, ecology, and economics reveals a positive correlation

between per capita energy use and GDP, illustrating the crucial link between societal progress and energy utilization[55]. Industries, as major energy consumers, show a direct relationship between energy use and manufacturing value-addition[56]. This underscores that energy-saving technologies do not inhibit industrial growth but instead enhance energy efficiency and production efficacy[57]. Regional economic environments influence factory and industrial park scheduling, necessitating the integration of ecological, technological, financial, and market parameters into the interaction models between plants/parks and the external world. This includes strategies for supply-demand choices, pricing, facility management, and incentive compensation mechanisms[58].

This section initially examines the green transformation of the chemical industry from a macro perspective, focusing on the dynamics between external power markets and industrial parks. It then delves into establishing a sustainable development assessment framework for the chemical industry, guided by policy initiatives. Furthermore, the discussion extends to the pivotal role of adopting intelligent technology in pollution prevention and control within the chemical sector, highlighting the extensive application of such technologies at the macro level. This comprehensive approach not only underscores the importance of integrating sustainable practices but also emphasizes the potential of intelligent technology in enhancing environmental stewardship across the industry.

The electricity market, pivotal across industries, emphasizes the importance of green electricity usage and distribution in emission reduction. Managing diverse user demands in the context of distributed energy sources is key to ensuring uninterrupted power supply while minimizing emissions. Studies focus on ensuring energy security across sectors while maximizing renewable energy use[49], [59], [60]. Specifically, Li et al.[61] designed a hierarchical management architecture for energy systems, managing the electricity demands of residential, commercial, and industrial sectors through peer-to-peer information exchange. The interactions among these sectors were handled using non-cooperative game theory, and blockchain technology was employed to implement smart contracts and decentralized identifiers, enhancing the reliability, security, and flexibility of energy system interactions. This research highlights the importance of real-time market data exchange and blockchain technology in optimizing demand-side energy management, ultimately improving system operational efficiency, reducing electricity grid procurement costs, and achieving carbon reduction from industrial zones to individuals.

Assessing the implementation and progress of the Sustainable Development Goals (SDGs) serves as a vital metric for gauging the green development trajectory of various industries. A tailored evaluation framework offers benchmarks for industrial construction and management, adapting assessment criteria to fit distinct industrial contexts. For example, the assessment of water environment carrying capacity employs a five-dimensional model enhanced by a quantum genetic algorithm to optimize the projection pursuit model for a comprehensive evaluation[62]. Moreover, achieving equilibrium in wind power utilization to mitigate post-construction curtailment necessitates a multi-indicator

evaluation system that accounts for wind resource attributes, equipment variations, and management approaches[63]. On a broader scale, global evaluation systems are instrumental in measuring the environmental footprint of products, technologies, and human activities, providing a holistic view of their sustainability impact[64]. Looking ahead, the integration of large language models with optimization algorithms heralds a significant advancement in this field, promising to expedite policy cost analysis, facilitate multifactorial classification, and enable tailored evaluations specific to regional, industrial, and corporate attributes. This convergence of technologies is poised to enhance decision-making processes, offering nuanced insights and fostering a more efficient, personalized approach to policy assessment and sustainable development strategies.

On the other hand, artificial intelligence is also utilized to predict the domain of pollution forecasting within chemical industrial parks, where it has received extensive cover age. The wealth of environmental data within parks, through the mining, analysis, and summarization of collected data, utilizing digital and intelligent technologies for predictions, can provide data support for the safety of industrial operations and health management of employees. By integrating learning methods that combine decision trees, multivariate linear regression, Lasso regression, support vector machines, and other machine learning approaches, air pollution in chemical industrial parks can be predicted[65]. For the comprehensive pollution prevention and control of volatile organic compounds (VOCs) in chemical parks, machine learning methods are employed to establish quantitative models linking workshop-level production process parameters with the time series data of VOCs emissions, analyzing the pollution prevention and control effectiveness in fine chemical parks from multiple perspectives[66]. Moreover, computer vision is used to monitor air quality, water quality, and production safety indicators in the surrounding environment of chemical parks, ensuring that the impact of production activities on the environment is effectively controlled. Using characteristics of noise data in chemical parks, wind speed, and surrounding traffic flow information, the data is divided into two parts, which are then trained using LSTM and Prophet models respectively before being integrated to predict the noise model[67]. Similarly, the applications mentioned above can also be transferred to the prediction of carbon emissions in chemical industrial parks, thereby providing guidance for park management methods and scheduling.

Central to the green transformation of the chemical industry are the concepts of park integration and industrial symbiosis, emphasizing the efficient exchange of materials and energy among enterprises to foster low-carbon and energy-efficient production practices. The employment of intelligent technologies is primarily aimed at enhancing the operational scheduling within parks, enabling the anticipation of uncertainties, and supporting managerial decision-making processes. The discourse extends to examining the chemical industry's interactions with external entities, including environmental considerations, market dynamics, policy frameworks, and societal aspects, with a particular focus on managing relationships with other industries and entities. Additionally, efforts are

directed towards developing a comprehensive sustainability assessment framework, aiming to establish refined relationships between parks/enterprises and the environmental and social fabric. This approach underscores the pivotal role of intelligent systems in streamlining operations, predicting future trends, and crafting sustainable development strategies within the chemical industry ecosystem.

3 Integrating Decarbonization Technologies Across Scales

In the context of achieving carbon neutrality, the introduction of new technologies in the chemical industry aims not just at economic benefits, but more importantly, at achieving net emission reductions in production processes. Given the high-cost nature of the chemical industry, simulations should extend beyond showcasing the emission reduction potential at various levels, focusing instead on the net emission reduction across the entire production process to mitigate potential negative impacts post-commissioning. As discussed earlier, different operational levels have varying modes of operation and optimization objectives, necessitating the use of distinct intelligent technologies. The scale of chemical technologies ranges from lab research to application, spanning twelve orders of magnitude. Multi-level models must consider reaction kinetics from picometers to nanometers, catalyst transfer from nanometers to micrometers, fluid dynamics from micrometers to millimeters, and larger-scale complex logistics[68]. Post-construction, the processes in a park are influenced by inputs, techniques, market, and environmental factors, affecting emissions and energy consumption.

As depicted in Figure 5, the analysis of industrial systems encompasses multiple scales: At the microscale, attention is given to the dynamic behaviors at the molecular level, highlighting the foundational interactions that drive material transformations. The mesoscale addresses the flow of materials and energy, alongside pertinent engineering challenges, effectively bridging the microscale's detailed insights with the broader perspectives required at the macroscale. This intermediate scale plays a critical role in translating molecular dynamics into practical engineering applications, such as the transport phenomena of catalysts within reactors, which significantly influence reactor and process design. Transitioning to the macroscale, the focus expands to encompass environmental and ecological considerations, integrating comprehensive system and process analyses to ensure alignment with broader sustainability goals. This scale emphasizes the need for engineering solutions to resonate with ecological and societal expectations, underscoring the systemic nature of industrial activities.

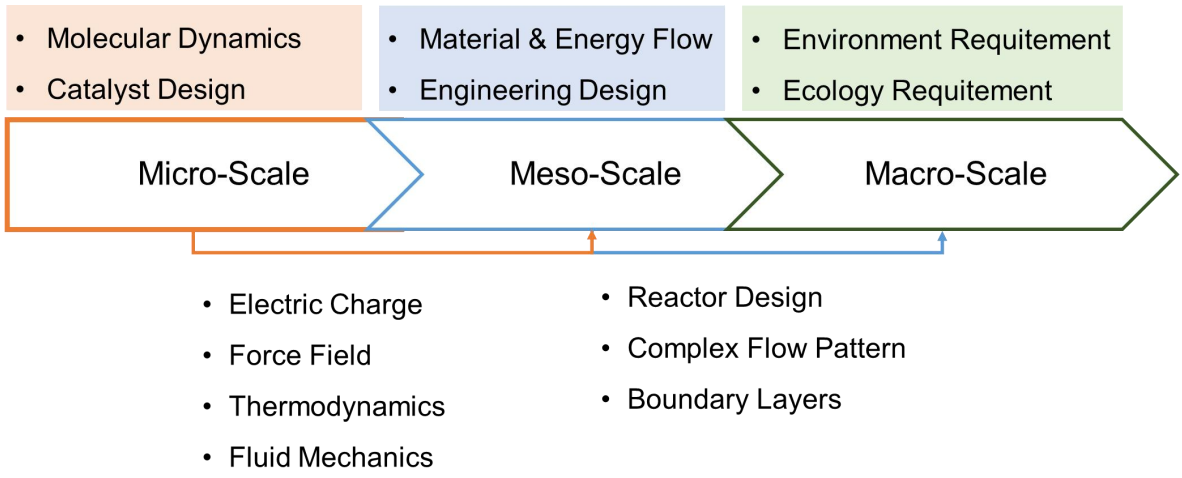

Fig. 5 From Microscale to Macroscale: An Integrative Multiscale Framework for Chemical Engineering Research

The principle underlying multi-level system engineering is the pursuit of harmony and collaboration across these diverse scales, aiming for a holistic optimization that supports sustainable development. However, cross-level optimization introduces increased complexity into the modeling process, underscoring the necessity for innovative approaches to manage this complexity. In this context, artificial intelligence offers a promising avenue for enhancing the efficiency and efficacy of such optimizations. By leveraging AI, it is possible to navigate the intricate landscape of multi-scale system engineering more effectively, streamlining the process of identifying and implementing optimal solutions across different scales.

3.1 Digital twin: The Key to Integrating Intelligent Applications with the Physical World

Digital twins represent an interconnected network system that facilitates the analysis, control, simulation, and diagnosis of a physical entity's entire lifecycle through optimization, management, and expert knowledge[69]. Initially developed for aerospace research, digital twins are now applied across a broad spectrum of fields, including satellite operations, energy systems, transportation systems, healthcare, activity monitoring, domestic living, scientific research, and safety management[69], [70], [71]. This technology enables the integration of complex issues into a singular model, linking different units through parameter coupling for synergistic optimization under ideal conditions. In non-ideal states, digital twins rely on their virtual counterparts to provide feedback optimization to the physical layer and achieve overall optimization through parameter coupling integrated into the entire process, making it suitable for multi-level coupled optimization in the chemical industry.

In chemical industrial parks, baseline requirements for production and safety necessitate efficient data acquisition and management, as well as model construction and optimization. The key to successfully implementing digital twins across different levels of a chemical park lies in the integration of physical

and virtual data. Digital and intelligent technologies provide real-time monitoring and predictive analytics, enabling interventions that optimize system performance and facilitate overall park optimization. Digital twins apply intelligent predictions and analyses to actual operations, incorporating automated feedback and self-learning for iterative improvements. Industrial digitalization stores and analyzes various information types, predicting events and system statuses, thereby advancing automation and unmanned operations [35].

In chemical process modeling, ensuring stable operation across cyclical and complex flows is crucial. Digital twins, incorporating uncertainty, enable digital modeling and online iteration of complex systems, enhancing understanding and optimization. For instance, a deep neural network model was used to simulate a Pressure Swing Adsorption system (PSA), integrating online learning and Bayesian inference for a comprehensive digital twin approach. This allowed for dynamic adaptation to changing conditions, improving the system's accuracy and adaptability [72]. Machine learning accelerates the determination of process conditions, and building digital twin models at this scale enables iterative improvements using experimental data, thereby guiding real-world production adjustments more effectively [73]. Digital twins have also been applied in large industrial settings, like heating network optimization in a Finnish city, achieving significant cost savings [74], and in petrochemical process safety and control [75].

Intelligent and digital methods effectively simplify complex models across various levels in the chemical industry, enabling seamless integration of different level models. The essence of digital twin technology is to apply model predictions through a feedback system to physical experimental platforms or factories, iterating on operational outcomes to interact between models and the real world. Adjusting models based on actual data speeds up the process simulation, achieving overall optimization and addressing the lag in chemical process simulation.

3.2 Cross-scale model of chemical industry

Intelligent technologies in chemical engineering accelerate material discovery, optimize plant/park scheduling, hasten process simulations, aid process modifications, and refine experimental/production conditions. Linking these facets to achieve a fully integrated, low-carbon production process is a key research focus. Chemical processes, complex in both chemical reactions and operational procedures, traditionally rely on First Principle Models (FPMs) for detailed process descriptions. However, FPMs can be computationally expensive and inefficient. Surrogate models offer a viable alternative, simplifying complex computations while maintaining accuracy. They are particularly useful in simulating complex chemical processes and speeding up parameter estimation [76].

Material research and development encompasses a multi-scale approach, ranging from atomic and molecular levels to macroscopic system applications. A review systematically presents the principles and methodologies behind data-driven hybrid models that seamlessly integrate material design with

process engineering, illustrating the broad spectrum of applications from material selection to the intricacies of computational chemical engineering processes[77]. Interaction between scales diverges from traditional single-level modeling by necessitating a nuanced understanding of the connections across different hierarchical levels, ensuring the models' relevance to practical scenarios. For instance, in the context of electrode material innovation, optimizing the structure of masonry diffusion electrodes within electrolyzes—a process pivotal to the electrochemical reduction of CO2—demands an intricate cross-scale consideration from the nanometer to millimeter range. Researchers have employed comprehensive imaging across these scales to develop a multi-scale electrode model, utilizing Focused Ion Beam/Scanning Electron Microscopy (FIB/SEM) for detailed analysis of the catalyst and microporous layers. By integrating microcomputed tomography (μCT) to digitally reconstruct the entire electrode structure, this methodological fusion bridges physical modeling with precise parametric inputs, thereby construct a modular, adaptable, and scalable model to enhance the understanding of how structural attributes influence transport dynamics[78] (Figure 6).

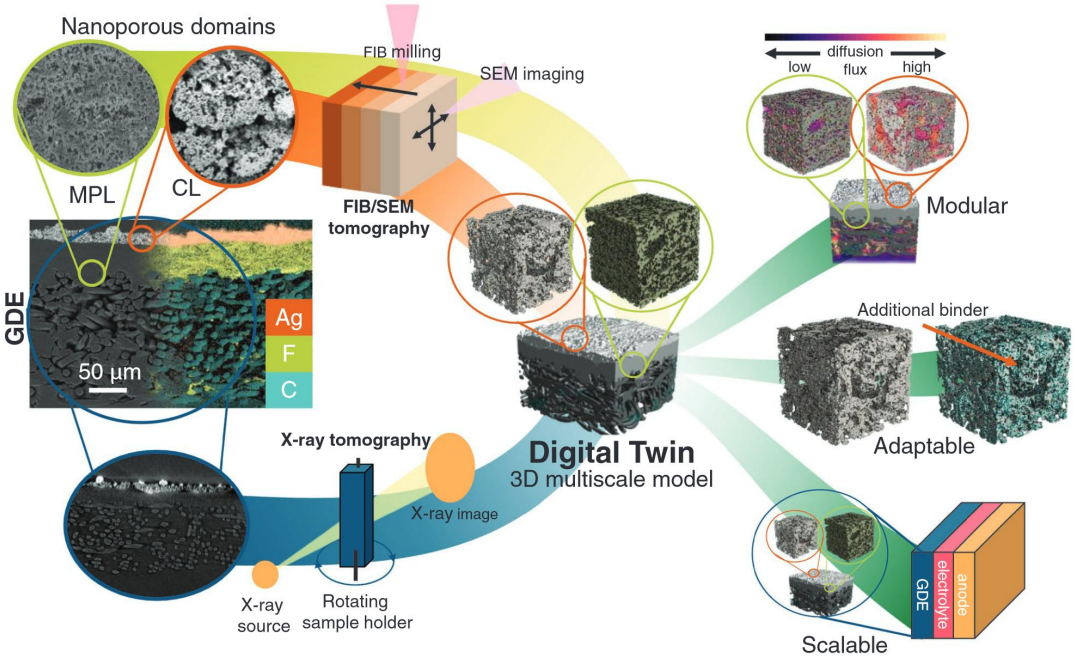

Fig. 6 Multi-Scale Digital Modeling of Material Structures via Imaging Technology [78]

Moreover, the reciprocal influence of catalysts and reactors in chemical processing—encompassing reaction mechanisms, kinetics, and mass transfer—cannot be underestimated. A study[68] explored a multiscale modeling strategy for a dual-modified structured catalyst reactor that processes carbon dioxide and methane. This model, which integrates insights into reaction mechanics, kinetics, catalyst transport phenomena, flow dynamics, and reactor architecture, was designed to facilitate efficient conversion at low pressures while preventing catalyst deactivation due to coking.

Linking unit operations with overall process optimization is achieved at the mesoscale through surrogate modeling, which reduces complexity and computational demand. For instance, a framework based on Kriging was developed to address operability issues in high-dimensional nonlinear systems, relying on sample data and reducing complexity and computational load compared to first-principles simulation methods [79] (Figure 7a). The team demonstrated the effectiveness of this approach in modeling both a Direct Methane Aromatization Membrane Reactor (DMA-MR) and a Natural Gas Combined Cycle (NGCC) plant, thereby proving its utility in both unit operations and overall processes. This enables the modeling of chemical processes across different levels and the combination of surrogate models for holistic optimization. Furthermore, Partial Least Squares Regression (PLSR) was employed as a stopping criterion to generate surrogate models [80], avoiding the need to create a new surrogate model in each iteration cycle and thus accelerating the modeling process. Jog et al. [81]developed a hybrid model combining data-driven surrogate and mechanistic models, employing Bayesian symbolic regression for construction and global optimization of processes(Figure 7b). To achieve global optimization of unit operations, analytical expressions were used as approximations, which were then linked through process flow diagrams to optimize the entire production process globally. Moreover, the transfer application of these models is a key research direction, with techniques like mixed-integer quadratic programming optimizing alternative models for processes like crude oil refining, demonstrating potential for application transfer to other processes [82].

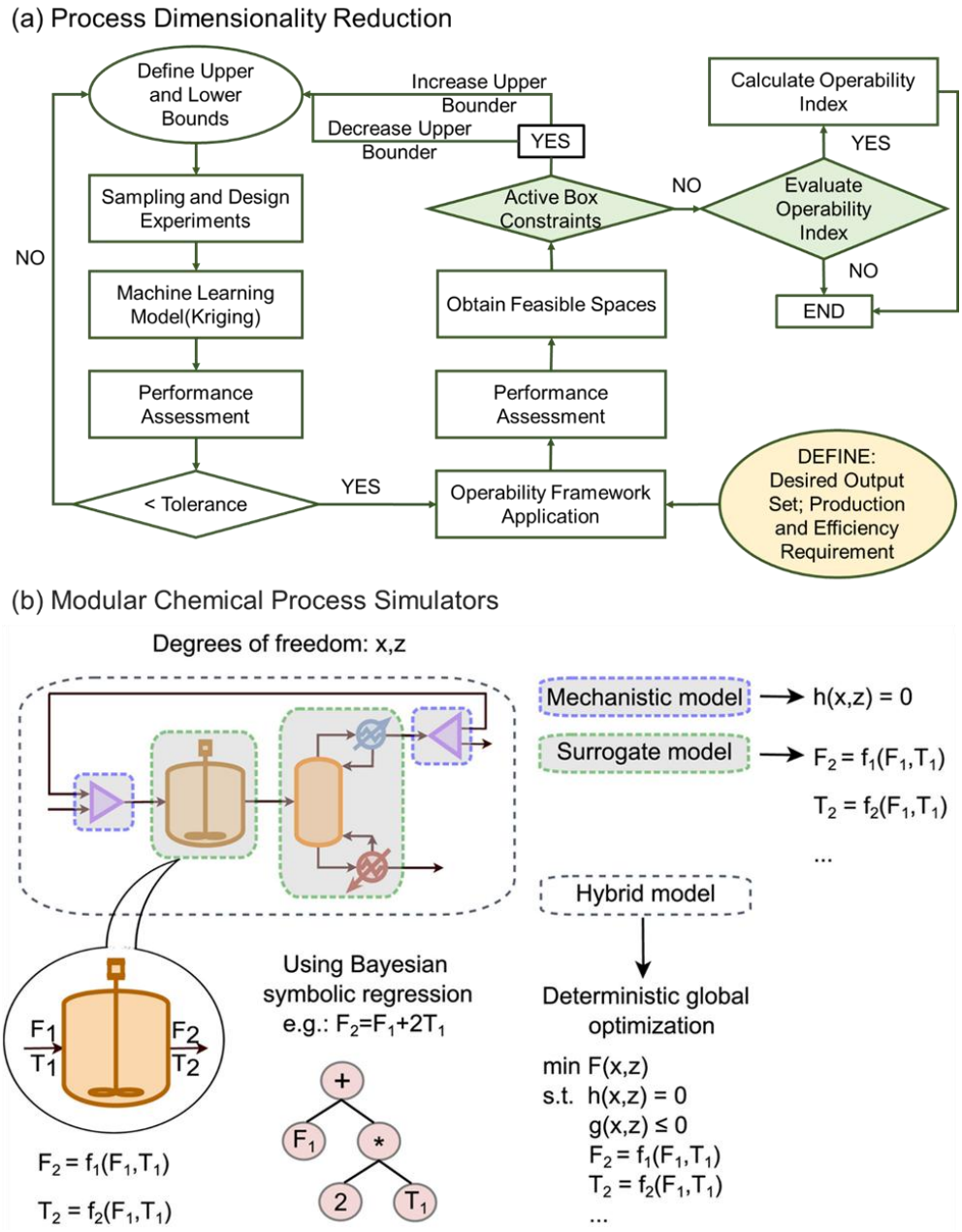

Fig. 7 Cross-scale optimization: linking unit operations to process efficiency (**a**) Kriging-based process dimensionality reduction for simplified first-principles simulation (redrawn by [79]);(**b**)Construction of modular chemical process simulator by hybrid model [81]

In transitioning from process-level to plant-level systems research, the focus shifts from optimizing process conditions to enhancing operational efficiencies of plant. This shift is not merely about optimizing schedules within industrial parks or factories but extends to integrating processes with factory and even park levels to fine-tune operational parameters towards maximizing profitability. The integration of dynamic process simulation with advanced techniques such as recursive neural networks and regression models facilitates this transition. Utilizing two deep learning models to

capture the dynamic behavior of processes and to forecast profits at various time steps enables optimized decision-making across factories or industrial parks [83].

Taking membrane manufacturing and utilization as an example, the evaluation of mass transfer characteristics is described at the nanoscale, while the economic benefits are inherently linked to factory operations. However, bridging the gap between these disparate scales presents a significant challenge due to differences in parameters. A novel approach employed artificial neural networks (ANNs) as surrogate models within a deterministic global optimization framework to address this multiscale gap [84]. The ANNs were trained on data generated from a one-dimensional extended Nernst-Planck ion transport model, facilitating the extrapolation of results to a more accurate two-dimensional distribution of membrane modules. This methodology enabled the synergistic optimization of membrane design and factory layout, optimizing for production objectives, feed concentration, filtration stages, and salt mixtures for the most efficient factory design (Figure 8). Thus, providing computational tools and methodologies for multiscale optimization in membrane science, this strategy effectively facilitates integration between the manufacturing and operational management levels, paving the way for holistic advancements in industrial operations.

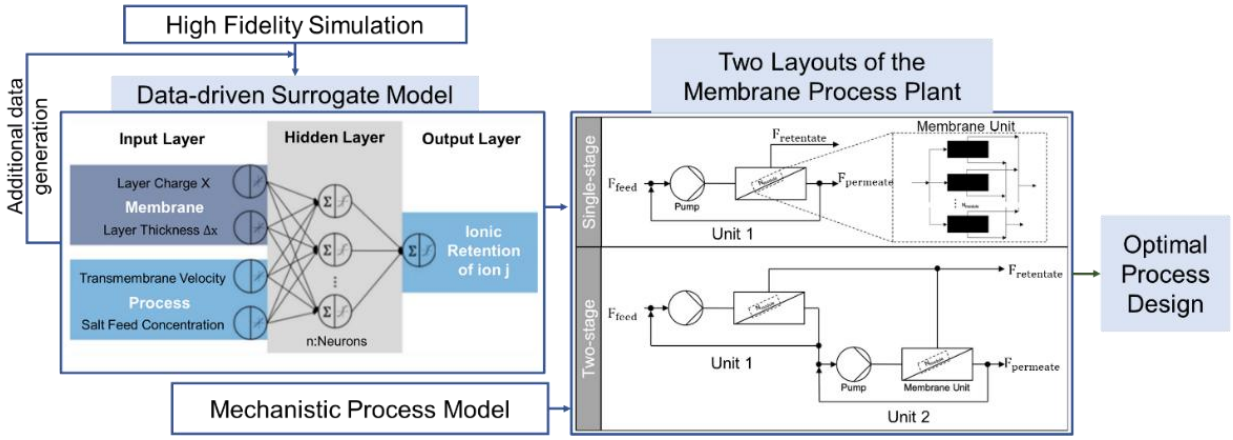

Fig. 8 Processes to plant: protruding multi-scale, multi-objective optimization through machine learning and high-fidelity ion transport models (Redrawn by [84])

The inherent complexity of operating large-scale chemical plants necessitates considerations of market fluctuations, upstream and downstream scheduling, and long-term maintenance plans. To address the planning and scheduling challenges of large-scale refinery-petrochemical operations, Zhang et.al [85] introduced an enterprise-level hybrid integer nonlinear model that combines heuristic algorithms with convolutional neural networks. This model facilitates the planning and scheduling of the entire manufacturing process from refining to petrochemical products, demonstrating its effectiveness for large-scale problems. Another study examined the impact of employing surrogate models at different levels of abstraction for optimization across various layers, developing deterministic, discrete-time surrogate models [86].

Bridging models across various scales, particularly through the integration of hybrid and data-driven models, significantly enhances simulation speeds. Janus et al. [87]developed a med-scale chemical plant model comprising reactors, separation equipment, and distillation towers. They employed neural networks as surrogate models to streamline evolutionary algorithms, achieving a 50% reduction in the number of required optimization simulations compared to traditional mechanistic models. The effectiveness of different modeling approaches is influenced by their availability, scale, and complexity; therefore, the migrate application of surrogate models is crucial for propelling the chemical industry's digital transformation forward. Research [88] delved into constructing operational decision models for chemical processes at various stages (spatial and temporal) using surrogate models and machine learning. Researchers proposed effective methodologies to address the computational time and reliability issues of high-fidelity models, the real-time decision-making needs of chemical operations, the application of surrogate modeling techniques, and multi-stage process operations. These methodologies aim to achieve precise simulation at all levels, thereby enhancing the effectiveness, accuracy, and efficiency of decision-making.

In summary, the application of digital and intelligent technologies has become deeply integrated at all levels of the chemical industry, facilitating multi-level collaborative applications. The use of surrogate models and big data simplifies chemical process simulations and accelerates digitalization due to their transferable nature. Consequently, the practical implementation of these technologies in industry is increasingly driving the realization of digital twins, bridging the gap between theoretical models and real-world applications.

4 Challenges, Future Research Direction and Conclusion

The integration of information and intelligent technologies, particularly in data analysis, machine learning, and automation control, is a key trend driving industrial activities, especially in the chemical industry. These technologies elevate the demands for precise chemical process predictions, efficient process control, and multi-objective optimization towards sustainable development goals, including minimizing energy consumption, reducing emissions, and optimizing resource utilization.

However, the chemical industry faces significant challenges integrating intelligent and digital technologies due to its complex nature. First, managing and securing the vast array of data from diverse production equipment and systems is critical. Second, the variability in production processes across companies demands highly customized algorithms and models, which require a solid theoretical foundation as well as expertise in data science and AI. Compatibility issues between new intelligent systems and existing infrastructure can hinder digital transformation. Furthermore, the lack of interpretability in some AI models raises safety concerns, especially in areas prone to accidents. Assessing the carbon footprint of chemical enterprises involves analyzing multifaceted data, including regulations and technical reports, to establish appropriate evaluation and calculation methods. Lastly,

the transition towards intelligent operations involves substantial financial investments and personnel changes, making the minimization of payback periods and effective management of workforce transitions key considerations for companies.

In response to these challenges, the research directions for the intelligent transformation of the chemical industry could focus on (Figure 9):

(1) Development of chemical industrial data management platform: The advancement of chemical industry-specific data management platforms is pivotal, focusing on the unique needs of sub-sectors like petrochemical, biochemical, and fine chemical industries. This involves establishing uniform data processing standards and deploying systems for efficient data handling from collection to visualization, thereby ensuring data security and process privacy through cloud computing integration. Such platforms aim to standardize and centralize data management across the chemical industry, enhancing data transferability, usability, and accuracy to support intelligent enterprise transformation.

Incorporating emerging technologies such as blockchain, AI, and edge computing into these platforms will further enhance their capabilities. Blockchain technology could provide a decentralized framework for ensuring data integrity and facilitating secure, transparent data exchanges across the industry. AI and ML algorithms could be employed for predictive analytics and intelligent data discovery, optimizing the efficiency of data analysis and decision-making processes. Edge computing would enable real-time data processing at the source, reducing latency for critical operations and ensuring timely insights. Additionally, privacy-preserving technologies like differential privacy and federated learning could address concerns around data confidentiality and consent management, crucial for maintaining trust and regulatory compliance. These technological integrations aim to amplify the effectiveness of chemical industrial data management platforms, driving innovation, and enabling smarter, data-driven decisions in chemical enterprises, aligning with the broader vision of achieving an intelligent and sustainable chemical industry.

(2) Development of Chemical Industry's Digital Twin Platform: The development of a digital twin platform for the chemical industry emerges as a promising solution to navigate the challenges of integrating virtual and reality technologies for its green and intelligent transformation. Modular design from microscale to macroscale approach facilitates system compatibility and scalability, enabling seamless integration with existing operational frameworks and eliminating the need for repetitive design from scratch. Moreover, the emphasis on real-time data processing technologies, such as edge computing, AI & ML algorithms, and quantum computing, is crucial. These technologies can process vast amounts of data with unprecedented speed and accuracy, providing insights for predictive maintenance, process optimization, and efficient resource management. Additionally, advanced human-computer interaction techniques play a pivotal role in making these sophisticated systems more accessible and user-friendly for industry professionals. This includes the development of intuitive interfaces and visualization tools that simplify complex data and process models. Lastly,

immersive learning and training simulations, leveraging VR and AR technologies, offer significant potential for workforce development. These simulations can replicate real-world chemical processing environments and scenarios, providing hands-on experience in a risk-free setting.

(3) Customized Evaluation/ Management Framework: The complex interplay of multi-dimensional external factors in chemical industry presents a significant hurdle for the industry's move towards intelligent and sustainable operations. Addressing this challenge necessitates innovative research directions that harness the power of advanced technologies and interdisciplinary approaches. The development of large language model (LLM)-based evaluation frameworks could provide comprehensive analysis tools for assessing compliance and best practices. Digital twins integrated with environmental parameters offer a dynamic monitoring and optimization platform, enabling scenario analysis for policy compliance. Furthermore, blockchain technology promises transparent and sustainable supply chain management, complemented by carbon credit trading platforms. Interdisciplinary research combining economic, environmental, and technological insights is essential for developing holistic strategies. Additionally, socio-technical systems for stakeholder engagement and VR/AR-based educational programs could foster a broader understanding and adoption of sustainable practices.

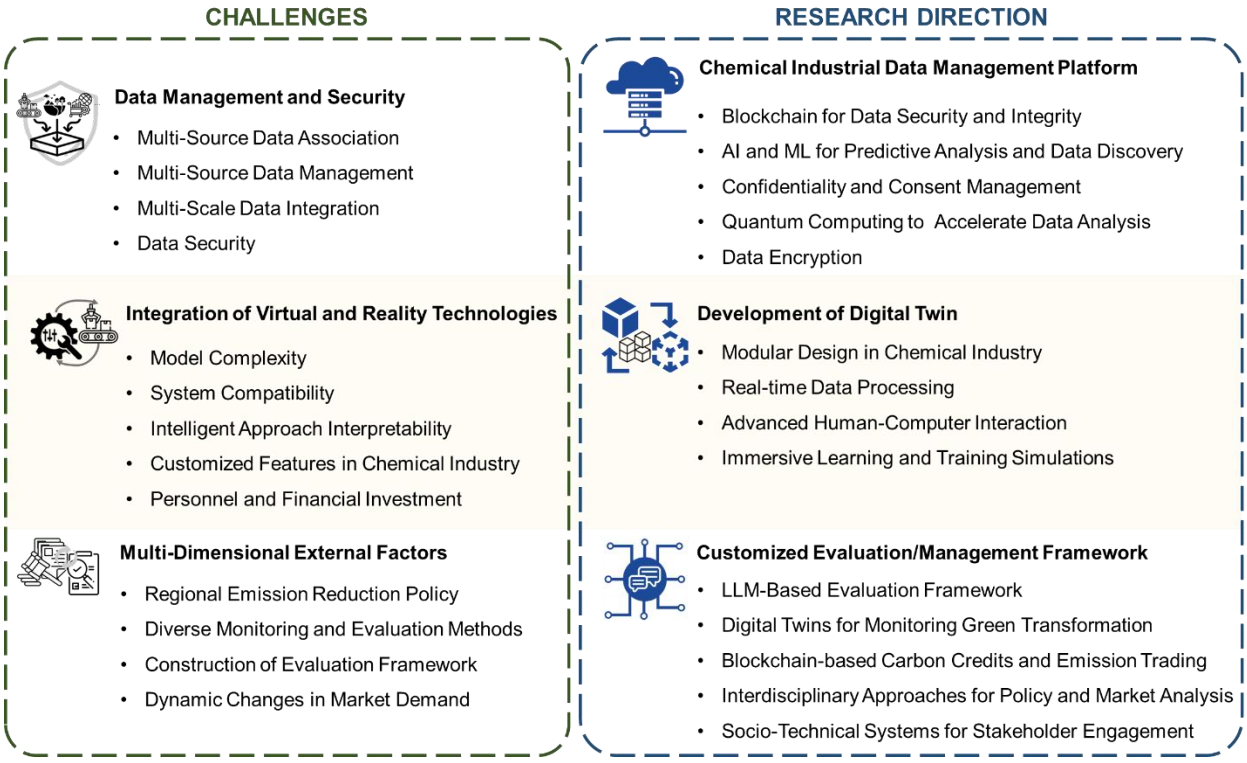

Fig. 9 Challenges and research direction for achieving carbon neutrality through intelligent transformation in the chemical industry.

In conclusion, this review explores the chemical industry's role in global sustainability, emphasizing decarbonization research and strategies from a multi-scale intelligent systems engineering perspective.

It discusses the green transformation of the chemical sector, a significant energy consumer and greenhouse gas emitter, driven by environmental and economic factors. The integration of intelligence approach such as machine learning, knowledge graphs, and digital twin technologies simplifies mechanistic models, enhancing research efficiency and resource conservation. Listed the applications across microscale, mesoscale, and macroscale include material discovery for CO2 capture, reactor design, process simulation, and economic analysis. The key to zero or negative carbon production throughout the chemical industry's lifecycle lies in connecting material design to park construction, leveraging intelligent technologies to reduce complexity and improve model utility. Digital twins bridge the digital and physical worlds, applying multi-level model predictions to optimize park scheduling and adjust production processes based on real data feedback, highlighting the feasibility of interconnected, level-adjusted models for sustainable chemical manufacturing.

Acknowledgements

This work is supported by the National Science and Technology Major Project (No. 2022ZD0117501) and Tsinghua University Initiative Scientific Research Program.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

[1] "Copernicus: September 2023 – unprecedented temperature anomalies; 2023 on track to be the warmest year on record | Copernicus." Accessed: Nov. 09, 2023. [Online]. Available: https://climate.copernicus.eu/copernicus-september-2023-unprecedented-temperature-anomalies

[2] climatechangetracker.org, "Yearly Average Observed Temperature Anomaly: Impacts and Insights." Accessed: Nov. 09, 2023. [Online]. Available: https://climatechangetracker.org/global-warming/yearly-average-temperature-anomaly

[3] W. M. Organization (WMO) *et al.*, "United In Science 2023." Accessed: Nov. 09, 2023. [Online]. Available: https://library.wmo.int/records/item/68235-united-in-science-2023

[4] "Global Warming of 1.5 ºC —." Accessed: Nov. 09, 2023. [Online]. Available: https://www.ipcc.ch/sr15/

[5] "Energy Technology Perspectives 2015 – Analysis," IEA. Accessed: Nov. 09, 2023. [Online]. Available: https://www.iea.org/reports/energy-technology-perspectives-2015

[6] "World Energy Outlook 2017 – Analysis," IEA. Accessed: Nov. 09, 2023. [Online]. Available: https://www.iea.org/reports/world-energy-outlook-2017

[7] "Contributing to UN Sustainable Development Goals | Arkema Global." Accessed: Jan. 12,

2024. [Online]. Available: https://www.arkema.com/global/en/social-responsibility/vision-and-strategy/sustainable-development-goals/

[8] "Chemicals," IEA. Accessed: Nov. 13, 2023. [Online]. Available: https://www.iea.org/energy-system/industry/chemicals

[9] "2019 Guide to the Business of Chemistry," American Chemistry Council. Accessed: Nov. 16, 2023. [Online]. Available: https://www.americanchemistry.com/chemistry-in-america/data-industry-statistics/resources/2019-guide-to-the-business-of-chemistry

[10] "2023 Facts and Figures of the European Chemical Industry," cefic.org. Accessed: Nov. 16, 2023. [Online]. Available: https://cefic.org/a-pillar-of-the-european-economy/facts-and-figures-of-the-european-chemical-industry/

[11] "itp-energy-intensive-processes-energy-intensive-processes-portfolio-addressing.pdf." Accessed: Nov. 16, 2023. [Online]. Available: https://www.energy.gov/eere/amo/articles/itp-energy-intensive-processes-energy-intensive-processes-portfolio-addressing

[12] "Global chemical industry revenue 2022," Statista. Accessed: Nov. 16, 2023. [Online]. Available: https://www.statista.com/statistics/302081/revenue-of-global-chemical-industry/

[13] C. Chung, J. Kim, B. K. Sovacool, S. Griffiths, M. Bazilian, and M. Yang, "Decarbonizing the chemical industry: A systematic review of sociotechnical systems, technological innovations, and policy options," *Energy Res. Soc. Sci.*, vol. 96, p. 102955, Feb. 2023, doi: 10.1016/j.erss.2023.102955.

[14] P. G. Levi and J. M. Cullen, "Mapping Global Flows of Chemicals: From Fossil Fuel Feedstocks to Chemical Products," *Environ. Sci. Technol.*, vol. 52, no. 4, pp. 1725–1734, Feb. 2018, doi: 10.1021/acs.est.7b04573.

[15] Z. Song, H. Shi, X. Zhang, and T. Zhou, "Prediction of CO2 solubility in ionic liquids using machine learning methods," *Chem. Eng. Sci.*, vol. 223, p. 115752, Sep. 2020, doi: 10.1016/j.ces.2020.115752.

[16] X. Yuan *et al.*, "Applied Machine Learning for Prediction of CO2 Adsorption on Biomass Waste-Derived Porous Carbons," *Environ. Sci. Technol.*, vol. 55, no. 17, pp. 11925–11936, Sep. 2021, doi: 10.1021/acs.est.1c01849.

[17] X. Deng, W. Yang, S. Li, H. Liang, Z. Shi, and Z. Qiao, "Large-Scale Screening and Machine Learning to Predict the Computation-Ready, Experimental Metal-Organic Frameworks for CO2 Capture from Air," *Appl. Sci.*, vol. 10, no. 2, Art. no. 2, Jan. 2020, doi: 10.3390/app10020569.

[18] X. Zhu, Y. Li, and X. Wang, "Machine learning prediction of biochar yield and carbon contents in biochar based on biomass characteristics and pyrolysis conditions," *Bioresour. Technol.*, vol. 288, p. 121527, Sep. 2019, doi: 10.1016/j.biortech.2019.121527.

[19] J. Guan *et al.*, "Design and prediction of metal organic framework-based mixed matrix membranes for CO2 capture via machine learning," *Cell Rep. Phys. Sci.*, vol. 3, no. 5, p. 100864, May 2022, doi: 10.1016/j.xcrp.2022.100864.

[20] T. C. Wu *et al.*, “A Materials Acceleration Platform for Organic Laser Discovery,” *Adv. Mater.*, vol. 35, no. 6, p. 2207070, Feb. 2023, doi: 10.1002/adma.202207070.
[21] N. Yoshikawa *et al.*, “Large language models for chemistry robotics,” *Auton. Robots*, vol. 47, no. 8, pp. 1057–1086, Dec. 2023, doi: 10.1007/s10514-023-10136-2.
[22] X. Zhang, K. Zhang, H. Yoo, and Y. Lee, “Machine Learning-Driven Discovery of Metal–Organic Frameworks for Efficient CO2 Capture in Humid Condition,” *ACS Sustain. Chem. Eng.*, vol. 9, no. 7, pp. 2872–2879, Feb. 2021, doi: 10.1021/acssuschemeng.0c08806.
[23] X. Yang, J. Zhang, K. Yoshizoe, K. Terayama, and K. Tsuda, “ChemTS: an efficient python library for de novo molecular generation,” *Sci. Technol. Adv. Mater.*, vol. 18, no. 1, pp. 972–976, Dec. 2017, doi: 10.1080/14686996.2017.1401424.
[24] M. Suvarna, T. P. Araújo, and J. Pérez-Ramírez, “A generalized machine learning framework to predict the space-time yield of methanol from thermocatalytic CO2 hydrogenation,” *Appl. Catal. B Environ.*, vol. 315, p. 121530, Oct. 2022, doi: 10.1016/j.apcatb.2022.121530.
[25] J. Y. Lok, W.-H. Tsai, and I.-C. Cheng, “A hybrid machine learning-genetic algorithm (ML-GA) model to predict optimal process parameters of nanoporous Cu for CO2 reduction,” *Mater. Today Energy*, vol. 36, p. 101352, Aug. 2023, doi: 10.1016/j.mtener.2023.101352.
[26] S. Pablo-García *et al.*, “Fast evaluation of the adsorption energy of organic molecules on metals via graph neural networks,” *Nat. Comput. Sci.*, vol. 3, no. 5, Art. no. 5, May 2023, doi: 10.1038/s43588-023-00437-y.
[27] A. Mazheika *et al.*, “Artificial-intelligence-driven discovery of catalyst genes with application to CO2 activation on semiconductor oxides,” *Nat. Commun.*, vol. 13, no. 1, Art. no. 1, Jan. 2022, doi: 10.1038/s41467-022-28042-z.
[28] “Macroscale - an overview | ScienceDirect Topics.” Accessed: Feb. 12, 2024. [Online]. Available: https://www.sciencedirect.com/topics/engineering/macroscale
[29] A. Shalaby, A. Elkamel, P. L. Douglas, Q. Zhu, and Q. P. Zheng, “A machine learning approach for modeling and optimization of a CO2 post-combustion capture unit,” *Energy*, vol. 215, p. 119113, Jan. 2021, doi: 10.1016/j.energy.2020.119113.
[30] S. G. Subraveti, Z. Li, V. Prasad, and A. Rajendran, “Machine Learning-Based Multiobjective Optimization of Pressure Swing Adsorption,” *Ind. Eng. Chem. Res.*, vol. 58, no. 44, pp. 20412–20422, Nov. 2019, doi: 10.1021/acs.iecr.9b04173.
[31] X. Y. Tai, R. Ocone, S. D. R. Christie, and J. Xuan, “Multi-objective optimisation with hybrid machine learning strategy for complex catalytic processes,” *Energy AI*, vol. 7, p. 100134, Jan. 2022, doi: 10.1016/j.egyai.2021.100134.
[32] L. F. Santos, C. B. B. Costa, J. A. Caballero, and M. A. S. S. Ravagnani, “Framework for embedding black-box simulation into mathematical programming via kriging surrogate model applied to natural gas liquefaction process optimization,” *Appl. Energy*, vol. 310, p. 118537, Mar. 2022, doi:

10.1016/j.apenergy.2022.118537.
[33] S. Amaran, N. V. Sahinidis, B. Sharda, and S. J. Bury, “Simulation optimization: a review of algorithms and applications,” *Ann. Oper. Res.*, vol. 240, no. 1, pp. 351–380, May 2016, doi: 10.1007/s10479-015-2019-x.
[34] H. Xu *et al.*, “Enabling thermal-neutral electrolysis for CO2-to-fuel conversions with a hybrid deep learning strategy,” *Energy Convers. Manag.*, vol. 230, p. 113827, Feb. 2021, doi: 10.1016/j.enconman.2021.113827.
[35] K. G. Kichatov, T. R. Prosochkina, and I. S. Vorobyova, “Principles of creating a digital twin prototype for the process of alkylation of benzene with propylene based on a neural network,” *Fine Chem. Technol.*, vol. 18, no. 5, Art. no. 5, Nov. 2023, doi: 10.32362/2410-6593-2023-18-5-482-497.
[36] J. Li, L. Pan, M. Suvarna, and X. Wang, “Machine learning aided supercritical water gasification for H2-rich syngas production with process optimization and catalyst screening,” *Chem. Eng. J.*, vol. 426, p. 131285, Dec. 2021, doi: 10.1016/j.cej.2021.131285.
[37] S. A. Mazari *et al.*, “Prediction of thermo-physical properties of 1-Butyl-3-methylimidazolium hexafluorophosphate for CO2 capture using machine learning models,” *J. Mol. Liq.*, vol. 327, p. 114785, Apr. 2021, doi: 10.1016/j.molliq.2020.114785.
[38] Y.-D. Hsiao and C.-T. Chang, “Progressive learning for surrogate modeling of amine scrubbing CO2 capture processes,” *Chem. Eng. Res. Des.*, vol. 194, pp. 653–665, Jun. 2023, doi: 10.1016/j.cherd.2023.05.016.
[39] O. Nematollahi, Z. Hajabdollahi, H. Hoghooghi, and K. C. Kim, “An evaluation of wind turbine waste heat recovery using organic Rankine cycle,” *J. Clean. Prod.*, vol. 214, pp. 705–716, Mar. 2019, doi: 10.1016/j.jclepro.2019.01.009.
[40] R. Law, A. Harvey, and D. Reay, “A knowledge-based system for low-grade waste heat recovery in the process industries,” *Appl. Therm. Eng.*, vol. 94, pp. 590–599, Feb. 2016, doi: 10.1016/j.applthermaleng.2015.10.103.
[41] “U.S. energy facts explained - consumption and production - U.S. Energy Information Administration (EIA).” Accessed: Jan. 21, 2024. [Online]. Available: https://www.eia.gov/energyexplained/us-energy-facts/
[42] G. Golkarnarenji *et al.*, “Development of a predictive model for study of skin-core phenomenon in stabilization process of PAN precursor,” *J. Ind. Eng. Chem.*, vol. 49, pp. 46–60, May 2017, doi: 10.1016/j.jiec.2016.12.027.
[43] H. Khayyam, M. Naebe, O. Zabihi, R. Zamani, S. Atkiss, and B. Fox, “Dynamic Prediction Models and Optimization of Polyacrylonitrile (PAN) Stabilization Processes for Production of Carbon Fiber,” *IEEE Trans. Ind. Inform.*, vol. 11, no. 4, pp. 887–896, 2015, doi: 10.1109/TII.2015.2434329.
[44] K. Badii *et al.*, “Energy Saving in Electric Heater of Carbon Fiber Stabilization Oven,” in *2014 4th International Conference on Artificial Intelligence with Applications in Engineering and*

Technology, Dec. 2014, pp. 109–114. doi: 10.1109/ICAIET.2014.27.
[45] H. Khayyam *et al.*, "Improving energy efficiency of carbon fiber manufacturing through waste heat recovery: A circular economy approach with machine learning," *Energy*, vol. 225, p. 120113, Jun. 2021, doi: 10.1016/j.energy.2021.120113.
[46] X. Zhu and Y. Ji, "A digital twin-based multi-objective optimization method for technical schemes in process industry," *Int. J. Comput. Integr. Manuf.*, vol. 36, no. 3, pp. 443–468, Mar. 2023, doi: 10.1080/0951192X.2022.2126013.
[47] S. Rodgers *et al.*, "A surrogate model for the economic evaluation of renewable hydrogen production from biomass feedstocks via supercritical water gasification," *Int. J. Hydrog. Energy*, vol. 49, pp. 277–294, Jan. 2024, doi: 10.1016/j.ijhydene.2023.08.016.
[48] H. Xi, X. Wu, X. Chen, and P. Sha, "Artificial intelligent based energy scheduling of steel mill gas utilization system towards carbon neutrality," *Appl. Energy*, vol. 295, p. 117069, Aug. 2021, doi: 10.1016/j.apenergy.2021.117069.
[49] X. Wang, N. H. El-Farra, and A. Palazoglu, "Optimal scheduling of demand responsive industrial production with hybrid renewable energy systems," *Renew. Energy*, vol. 100, pp. 53–64, Jan. 2017, doi: 10.1016/j.renene.2016.05.051.
[50] T. YANG, "'Six Integrations'of establishing and managing chemical parks in China," *Chem. Ind. Eng. Prog.*, vol. 40, no. 10, pp. 5845–5853, 2021, doi: 10.16085/j.issn.1000-6613.2021-1814.
[51] Y. Zhang, W. Wang, M. Chang, and F. Zhang, "Practice and reflection on safety improvement in chemical industry parks," *Labor Prot.*, no. 1, pp. 56–59, 2023.
[52] M. R. Chertow, "Industrial Symbiosis," in *Encyclopedia of Energy*, C. J. Cleveland, Ed., New York: Elsevier, 2004, pp. 407–415. doi: 10.1016/B0-12-176480-X/00557-X.
[53] K. S. CLMS, "European cluster-led accelerator for digitization of the circular economy across key emerging sectors D 3.6 - Industrial Symbiosis platform," 2021. Accessed: Apr. 24, 2023. [Online]. Available: https://digicirc.eu/
[54] N. Trokanas, F. Cecelja, and T. Raafat, "Semantic input/output matching for waste processing in industrial symbiosis," *Comput. Chem. Eng.*, vol. 66, pp. 259–268, Jul. 2014, doi: 10.1016/j.compchemeng.2014.02.010.
[55] J. Brown *et al.*, "Energetic Limits to Economic Growth," *BioScience*, vol. 61, Jan. 2011, doi: 10.1525/bio.2011.61.1.7.
[56] U. Soytas and R. Sari, "The relationship between energy and production: Evidence from Turkish manufacturing industry," *Energy Econ.*, vol. 29, no. 6, pp. 1151–1165, Nov. 2007, doi: 10.1016/j.eneco.2006.05.019.
[57] G. Zou, "The relationships between energy consumption and key industrial sector growth in China," *Energy Rep.*, vol. 8, pp. 924–935, Nov. 2022, doi: 10.1016/j.egyr.2022.07.112.
[58] C. Chen, Y. Hu, M. Karuppiah, and P. M. Kumar, "Artificial intelligence on economic

evaluation of energy efficiency and renewable energy technologies," *Sustain. Energy Technol. Assess.*, vol. 47, p. 101358, Oct. 2021, doi: 10.1016/j.seta.2021.101358.

[59] M. Riaz, S. Ahmad, and M. Naeem, "Joint energy management and trading among renewable integrated microgrids for combined cooling, heating, and power systems," *J. Build. Eng.*, vol. 75, p. 106921, Sep. 2023, doi: 10.1016/j.jobe.2023.106921.

[60] Q. Guo, S. Nojavan, S. Lei, and X. Liang, "Economic-environmental evaluation of industrial energy parks integrated with CCHP units under a hybrid IGDT-stochastic optimization approach," *J. Clean. Prod.*, vol. 317, p. 128364, Oct. 2021, doi: 10.1016/j.jclepro.2021.128364.

[61] Y. Li, W. Yang, P. He, C. Chen, and X. Wang, "Design and management of a distributed hybrid energy system through smart contract and blockchain," *Appl. Energy*, vol. 248, pp. 390–405, Aug. 2019, doi: 10.1016/j.apenergy.2019.04.132.

[62] X. Wei, J. Wang, S. Wu, X. Xin, Z. Wang, and W. Liu, "Comprehensive evaluation model for water environment carrying capacity based on VPOSRM framework: A case study in Wuhan, China," *Sustain. Cities Soc.*, vol. 50, p. 101640, Oct. 2019, doi: 10.1016/j.scs.2019.101640.

[63] R. Shi, X. Fan, and Y. He, "Comprehensive evaluation index system for wind power utilization levels in wind farms in China," *Renew. Sustain. Energy Rev.*, vol. 69, pp. 461–471, Mar. 2017, doi: 10.1016/j.rser.2016.11.168.

[64] M. W. Ryberg, M. Owsianiak, K. Richardson, and M. Z. Hauschild, "Development of a life-cycle impact assessment methodology linked to the Planetary Boundaries framework," *Ecol. Indic.*, vol. 88, pp. 250–262, May 2018, doi: 10.1016/j.ecolind.2017.12.065.

[65] X. Wang, Y. Yu, and T. Wang, "Air pollution prediction in chemical industry park based on improved hierarchical supervised learning strategy," Mar. 2020.

[66] YE Hanyun *et al.*, "Strategies for comprehensive prevention and control of VOCs pollution in fine chemical industrial park," *Enviromental Prot. Chem. Ind.*, pp. 758–765, Dec. 2022, doi: 10.3969/j.issn.1006-1878.2022.06.017.

[67] Q. Zeng, Y. Liang, G. Chen, H. Duan, and C. Li, "Noise prediction of chemical industry park based on multi-station Prophet and multivariate LSTM fitting model," *EURASIP J. Adv. Signal Process.*, vol. 2021, no. 1, p. 106, Oct. 2021, doi: 10.1186/s13634-021-00815-6.

[68] F. Minette and J. De Wilde, "Multi-scale modeling and simulation of low-pressure methane bi-reforming using structured catalytic reactors," *Chem. Eng. J.*, vol. 407, p. 127218, 2021.

[69] H. Jiang *et al.*, "Digital Twin Network (DTN): Concepts, Architecture, and Key Technologies," *Acta Autom. Sin.*, vol. 47, no. 3, Art. no. NREL/JA-5D00-80135, Mar. 2021, doi: 10.16383/j.aas.c210097.

[70] W. Yu, P. Patros, B. Young, E. Klinac, and T. G. Walmsley, "Energy digital twin technology for industrial energy management: Classification, challenges and future," *Renew. Sustain. Energy Rev.*, vol. 161, p. 112407, Jun. 2022, doi: 10.1016/j.rser.2022.112407.

[71] Y.-R. Li, C.-J. Yang, H.-W. Zhang, and J.-F. Li, “Discussion on key technologies of digital twin in process industry. Acta Automatica Sinica,” *Acta Autom. Sin.*, vol. 47, no. 3, pp. 501–514, 2021, doi: 10.16383/j.aas.c200147.
[72] E. A. Costa, C. M. Rebello, L. Schnitman, J. M. Loureiro, A. M. Ribeiro, and I. B. R. Nogueira, “Adaptive digital twin for pressure swing adsorption systems: Integrating a novel feedback tracking system, online learning and uncertainty assessment for enhanced performance,” *Eng. Appl. Artif. Intell.*, vol. 127, p. 107364, Jan. 2024, doi: 10.1016/j.engappai.2023.107364.
[73] B. Bayer, R. Dalmau Diaz, M. Melcher, G. Striedner, and M. Duerkop, “Digital Twin Application for Model-Based DoE to Rapidly Identify Ideal Process Conditions for Space-Time Yield Optimization,” *Processes*, vol. 9, no. 7, Art. no. 7, Jul. 2021, doi: 10.3390/pr9071109.
[74] M. Eklund, S. A. Sierla, H. Niemistö, T. Korvola, J. Savolainen, and T. A. Karhela, “Using a Digital Twin as the Objective Function for Evolutionary Algorithm Applications in Large Scale Industrial Processes,” *IEEE Access*, vol. 11, pp. 24185–24202, 2023, doi: 10.1109/ACCESS.2023.3254896.
[75] S. Hu, S. Wang, N. Su, X. Li, and Q. Zhang, “Digital twin based reference architecture for petrochemical monitoring and fault diagnosis,” *Oil Gas Sci. Technol. – Rev. D’IFP Energ. Nouv.*, vol. 76, p. 9, 2021, doi: 10.2516/ogst/2020095.
[76] Á. Bárkányi, T. Chován, S. Németh, and J. Abonyi, “Modelling for Digital Twins—Potential Role of Surrogate Models,” *Processes*, vol. 9, no. 3, Art. no. 3, Mar. 2021, doi: 10.3390/pr9030476.
[77] T. Zhou, R. Gani, and K. Sundmacher, “Hybrid Data-Driven and Mechanistic Modeling Approaches for Multiscale Material and Process Design,” *Engineering*, vol. 7, no. 9, pp. 1231–1238, Sep. 2021, doi: 10.1016/j.eng.2020.12.022.
[78] D. McLaughlin, M. Bierling, B. Mayerhöfer, G. Schmid, and S. Thiele, “Digital Twin of a Hierarchical CO2 Electrolyzer Gas Diffusion Electrode,” *Adv. Funct. Mater.*, vol. 33, no. 10, p. 2212462, 2023, doi: 10.1002/adfm.202212462.
[79] V. Alves, V. Gazzaneo, and F. V. Lima, “A machine learning-based process operability framework using Gaussian processes,” *Comput. Chem. Eng.*, vol. 163, p. 107835, Jul. 2022, doi: 10.1016/j.compchemeng.2022.107835.
[80] J. Straus and S. Skogestad, “A new termination criterion for sampling for surrogate model generation using partial least squares regression,” *Comput. Chem. Eng.*, vol. 121, pp. 75–85, Feb. 2019, doi: 10.1016/j.compchemeng.2018.10.008.
[81] S. Jog, D. Vázquez, L. F. Santos, J. A. Caballero, and G. Guillén-Gosálbez, “Hybrid analytical surrogate-based process optimization via Bayesian symbolic regression,” *Comput. Chem. Eng.*, vol. 182, p. 108563, Mar. 2024, doi: 10.1016/j.compchemeng.2023.108563.
[82] R. E. Franzoi, B. C. Menezes, J. D. Kelly, J. A. W. Gut, and I. E. Grossmann, “Cutpoint Temperature Surrogate Modeling for Distillation Yields and Properties,” *Ind. Eng. Chem. Res.*, vol. 59,

no. 41, pp. 18616–18628, Oct. 2020, doi: 10.1021/acs.iecr.0c02868.
[83] W. Zhu, J. Chebeir, and J. A. Romagnoli, "Operation optimization of a cryogenic NGL recovery unit using deep learning based surrogate modeling," *Comput. Chem. Eng.*, vol. 137, p. 106815, Jun. 2020, doi: 10.1016/j.compchemeng.2020.106815.
[84] D. Rall, A. M. Schweidtmann, M. Kruse, E. Evdochenko, A. Mitsos, and M. Wessling, "Multi-scale membrane process optimization with high-fidelity ion transport models through machine learning," *J. Membr. Sci.*, vol. 608, p. 118208, Aug. 2020, doi: 10.1016/j.memsci.2020.118208.
[85] L. Zhang, H. Hu, Z. Wang, Z. Yuan, and B. Chen, "Enterprise-wide optimization of integrated planning and scheduling for refinery-petrochemical complex with heuristic algorithm," *Front. Chem. Sci. Eng.*, vol. 17, no. 10, pp. 1516–1532, Oct. 2023, doi: 10.1007/s11705-022-2283-7.
[86] K. Ma *et al.*, "Data-driven strategies for optimization of integrated chemical plants," *Comput. Chem. Eng.*, vol. 166, p. 107961, Oct. 2022, doi: 10.1016/j.compchemeng.2022.107961.
[87] T. Janus, A. Lüubbers, and S. Engell, "Neural Networks for Surrogate-assisted Evolutionary optimization of Chemical Processes," in *2020 IEEE Congress on Evolutionary Computation (CEC)*, Jul. 2020, pp. 1–8. doi: 10.1109/CEC48606.2020.9185781.
[88] A. Shokry Abdelaleem Taha Zied, "A contribution to chemical process operation support: new machine learning and surrogate models based approaches for process optimization, supervision and control," Doctoral thesis, Universitat Politècnica de Catalunya, 2021. doi: 10.5821/dissertation-2117-349568.