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EXPERT CONSENSUS ON FUTURE MARKET DEVELOPMENT OF THE "AI + CHEMICAL ENGINEERING INDUSTRY": A DELPHI SURVEY

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ABSTRACT

With the rapid development of the global artificial intelligence (AI) industry, large-scale general AI models are demonstrating diverse potential and distinct development characteristics across the chemical engineering industry chain. Traditional chemical manufacturing relies heavily on physical experiments and validation tests, which are time-consuming, costly, and often involve high safety risks. In contrast, "AI + chemical engineering industry" (i.e., AI-enabled chemical engineering technologies) integrates physical and digital spaces, enabling design, simulation, and verification processes to be efficiently conducted in virtual environments. This approach offers advantages such as near-zero marginal cost, flexible system architecture, and significantly reduced reliance on physical testing. As a result, technological innovation in chemical engineering is shifting from experience-based trial and error toward a data-driven paradigm, substantially improving efficiency and accuracy. This research explores the market potential of the "AI + chemical engineering industry" using the Delphi method, drawing on insights from 20 experts in Henan Province, China. Through case analyses of three representative sectors (AI-driven coal, non-ferrous metals, and new energy industries), the research forecasts emerging market opportunities and future development directions for AI integration within the chemical engineering industry chain. The findings reflect a consensus on the future trajectory of these AI-integrated sectors, suggesting that AI adoption will revitalize the chemical engineering industry, enhance safety and quality management systems, stimulate innovative integration models, and promote the development of industrial clusters.

1. INTRODUCTION

With the rapid growth of new energy, low-altitude industries, robotics, and biomanufacturing, the demand for high-end products such as high-end polyolefins, special engineering plastics, electronic chemicals, and bio-based materials will become more vigorous. General chemicals have changed to a high-end, refined, and differentiated level, which requires the urgent upgradation of the chemical engineering industry. The structural contradictions between this traditional condition environment and the high-tech quality of chemical engineering production have forced the upgrading and acceleration of the development of service-based manufacturing industry, from focusing on general-purpose products to technology innovation as the driving force.

1.1 Main Problems of the Traditional Chemical Engineering Industry

First, from a cost perspective, the research and development cycle for new chemical materials is relatively long. Particularly, developing a new chemical engineering material often requires several years to ensure stable production quality and achieve a return on investment. Additionally, the real-time optimization of

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thousands of process parameters remains difficult, leading to high energy consumption, excessive material usage, and elevated production costs. Second, from a safety perspective, chemical engineering operations involve substantial risks. Traditional technologies place significant limitations on early warning systems for equipment failures and process abnormalities, reducing the effectiveness of accident prevention. Third, from a quality monitoring perspective, maintaining consistent chemical product quality is highly challenging. Product quality is influenced by multiple factors, including raw materials, environmental conditions, and equipment status. As a result, quality stability issues persist across different segments of the chemical industry chain. To address these challenges, the "AI + chemical engineering industry" has emerged, characterized by the integration of artificial intelligence technologies across various stages of chemical engineering. Intelligent chemical engineering systems based on machine learning, deep learning, and reinforcement learning can uncover complex patterns and underlying mechanisms from large volumes of historical and real-time data that are difficult for human experts to identify. These capabilities provide systematic solutions to cost, safety, and quality challenges. Consequently, the "AI + chemical engineering" paradigm represents a transformative integration in which AI acts as a powerful accelerator and innovator across the chemical industry chain.driving force.

1.2 The Inherent Logic of High-quality Development of "AI + Chemical Engineering Industry"

The "AI + chemical engineering industry" (i.e., the AI-enabled chemical engineering industry) represents the application of advanced intelligent algorithms to drive greater innovation, efficiency, and safety in the future chemical engineering sector. Its underlying logic can be summarized in three key aspects:

- To use the penetration of technology to lay a digital base for the innovative chemical industry;
- To build scene reconstruction power and catalyze the innovation of the industrial ecology of the chemical industry;
- To provide organizational evolution and process optimization, innovate the production relationship of the intelligent chemical industry.

1.3 The Empowerment Function of the High-quality Development of "AI + Chemical Engineering Industry"

The main function of the "AI + chemical engineering industry" covers the following four aspects:

1. Deep integration of AI, the Industrial Internet, and smart manufacturing: The "AI + chemical engineering" paradigm enables the construction of digital twins that correspond to the industrial Internet and smart manufacturing systems, providing advanced capabilities for digital analysis, simulation, and prediction to optimize the operation of physical and virtual chemical plants;
2. Technological intervention of generative AI: "AI + chemical engineering" supports molecular design and generation, the automated creation of operating procedures, emergency response plans, and training materials, significantly improving the efficiency of knowledge management;
3. "AI + robotics" empowerment of uncrewed chemical plants: AI-driven chemical engineering robots can perform inspection, sampling, and maintenance tasks in high-risk environments, enabling the development of uncrewed or minimally staffed chemical plants;
4. Full life-cycle carbon footprint management: AI technologies enable comprehensive monitoring and recording across the entire product life cycle, from raw material input to end use, allowing precise tracking and reduction of carbon emissions and supporting the achievement of "dual-carbon" goals.

1.4 Research Problem

The research problem addressed is as follows: "What is the expert consensus on the market development prospects and key characteristics of the "AI + chemical engineering industry" based on a Delphi survey?"

2. LITERATURE REVIEW

The chemical industry, a cornerstone of global manufacturing, is undergoing a profound digital transformation (Dutta et al., 2020). Driven by the need for enhanced efficiency, sustainability, and innovation, artificial intelligence (AI) has emerged as a pivotal disruptive force (Govindan, 2022). This literature review synthesizes current academic research and market analyses to explore the key market development trends of the integration of AI and the chemical sectors. To get a more objective prediction of experts on future market development, it is structured around three core domains to review the main achievements of this subject, namely (1) the acceleration of molecular discovery and materials design, (2) the optimization of manufacturing processes and operational excellence, and (3) the advancement of sustainability and safety management.

2.1. Accelerating Molecular Discovery and Materials Design

Traditional research and development (R&D) in the chemical engineering field is often a time-consuming and costly process of trial and error. AI, particularly machine learning (ML) and deep learning, is revolutionizing this paradigm by enabling predictive design and high-throughput virtual screening (Ding et al. 2025).

The application of generative models is a new and significant trend. These algorithms can propose novel molecular structures with desired properties, dramatically expanding the explorable chemical space. Zhavoronkov et al. (2019) demonstrated this empowerment of a deep generative model to design new drug-like molecules, which is directly transferable to the chemical industry for designing novel monomers, polymers, and specialty chemicals. Complementing generative design, predictive ML models are used to map chemical structures to their properties. Butler et al. (2018) detailed how ML techniques are being applied to materials science, using data from quantum mechanics calculations and experiments to predict material properties (e.g., bandgap, conductivity, and catalytic activity), thereby accelerating the development of new functional materials.

The market trend is moving towards integrated “AI-driven discovery platforms” that combine generative AI, predictive models, and robotic high-throughput experimentation, creating a closed-loop system that autonomously proposes, synthesizes, and tests new compounds (Zhao et al., 2025).

2.2 Optimizing Manufacturing Processes and Operational Excellence

Within chemical manufacturing plants, AI is the core enabler of the “Smart Plant,” leading to unprecedented levels of efficiency, yield, and reliability. This trend moves beyond descriptive analytics to prescriptive and predictive operations (Frazzetto et al., 2020).

A widely adopted application is predictive maintenance (PdM). By analyzing real-time sensor data from equipment like reactors, pumps, and compressors, ML algorithms can detect anomalies and forecast failures before they occur. Wu et al. (2020) proposed a hybrid deep learning model for PdM in industrial systems, showcasing its ability to reduce unplanned downtime and maintenance costs, a finding highly relevant to capital-intensive chemical plants. Beyond maintenance, AI is used in revolutionizing process control. Advanced Process Control (APC) systems, enhanced with reinforcement learning (RL), can manage complex, non-linear processes more effectively than traditional PID controllers. Yoo et al. (2019) explored the use of RL for the optimization of a chemical vapor deposition process, a key step in semiconductor manufacturing. Their work, published in Computers & Chemical Engineering, demonstrated that RL could achieve superior control performance, maximizing product quality and yield while minimizing energy consumption.

The chemical engineering market is connecting with a surge deployment of these AI solutions, driven by the tangible return on investment through reduced operational expenditures, improved asset utilization, and consistent product quality (Gamal, 2025).

2.3 Advancing Sustainability and Safety Management

The chemical engineering industry faces mounting pressure to enhance its environmental footprint and operational safety. AI provides powerful tools to address these challenges, making sustainability and safety a key market trend for AI adoption.

In the realm of sustainability, AI is instrumental in optimizing for energy efficiency and carbon footprint reduction. ML models can identify optimal operating conditions that minimize energy use and waste generation (Chauhan et al., 2024). Furthermore, AI aids in the development of circular economy models by optimizing recycling processes and identifying alternative, greener feedstocks. Kumari and Toshniwal (2021) reviewed the role of AI in achieving sustainable development goals in industrial processes, highlighting its use in pollution control, resource optimization, and clean energy, all critical areas for the chemical sector. For safety, AI enhances risk assessment and management. Natural Language Processing (NLP) can analyze vast repositories of incident reports and safety procedures to identify latent risks. More directly, computer vision models can monitor video feeds in real-time to detect unsafe behaviors (e.g., missing personal protective equipment) or hazardous conditions (e.g., leaks using thermal imaging). The work of Ramírez et al. (2022) on using deep learning for intelligent safety management in hazardous environments underscores the potential of AI to create a proactive safety culture, preventing accidents before they happen.

The market for AI in this domain is growing as regulatory frameworks tighten, and corporate ESG (Environmental, Social, and Governance) goals become central to business strategy (Rane et al., 2024).

The integration of AI technology into the chemical engineering industry is fundamentally reshaping its market landscape. The accelerating trends of R&D, intelligent manufacturing, and enhanced sustainability are not isolated developments but mutually reinforcing forces that are collectively driving the chemical industry toward a more efficient, innovative, and responsible future. The competitive landscape will increasingly be shaped by a company’s ability to integrate AI as a core capability across its entire value chain. Future research should therefore focus on addressing key challenges, including data quality assurance, model interpretability related to the “black-box” problem, and the cultivation of a skilled workforce capable of fully realizing the transformative potential of AI in the chemical industry.

3. MATERIALS AND METHODS

In response to the multiple challenges facing the chemical engineering industry, including AI-driven technological disruption, sustainable development pressures, and geopolitical factors, this research adopts the Delphi survey method to identify strategic consensus. By analyzing expert perspectives, the research aims to develop a shared assessment of future market potential and development trends in the “AI + chemical engineering industry.”

3.1 Project Aims of Delphi Survey Design

The Delphi survey is designed to build consensus on the future market potential of the “AI + chemical engineering industry” and its key development drivers. The specific research objectives are as follows:

1. To identify the key AI technologies, market trends, and policy trends of the high-level development of the “AI + chemical engineering industry” in the next

decade;

2. To reach a common consensus on the priority direction of potential market development and the challenges of the "AI + chemical engineering industry."

3.2 Data Collection in the Delphi Survey Conduction

The following are the data collection and analysis in two rounds of the Delphi survey conduction.

The two rounds of Delphi analysis on market prediction of "AI + chemical engineering industry" include the following:

1. The composition of the expert group (20 participants): The research involved 20 participants from Henan Province, China, drawn from four levels of the chemical engineering ecosystem: universities, AI research teams, local government, and industry. The panel comprised four chemical research experts, four AI technology experts, eight chemical industry practitioners, and four investment and market analysts.
2. Two rounds of quantitative evaluation and consensus statistics: The survey consisted of two rounds of trend-oriented data collection. Following two rounds of structured questionnaires, the core development areas of the "AI + chemical industry" were evaluated across three dimensions: market potential, technology maturity, and implementation barriers. With more than 94% of the questionnaires effectively returned in both rounds, six key development trends with the highest representativeness were identified.

The results are presented in Table 1.

Table 1. Two rounds of quantitative evaluation and consensus statistics

Number	Items	Titles	Market potential	Technology maturity	Potential risks	Consensus Degree
1	AI empowerment as a development trend in the chemical engineering industry	1.1 AI + chemical intelligent safety	4.9(5)	3.9	4.0	H
		1.2 AI + chemical intelligent optimization	4.8(5)	4.2	3.3	H
		1.3 AI + chemical intelligent manufacturing	4.7(5)	4.1	3.2	H
		1.4 AI + chemical intelligent laboratory	4.4(4)	3.8	3.1	M
		1.5 AI + typical professional scenarios	4.3(4)	4.3	3.0	M
		1.6 AI + carbon footprint tracking	4.2(4)	4.4	3.2	M
		1.7 AI + market industry chain forecast scenario	4.1(4)	4.2	3.3	M
2	AI empowerment for the future market of the chemical engineering industry	2.1 AI + new energy chemical engineering industry	4.9(5)	4.5	2.5	H
		2.2 AI + traditional resource products	4.5(5)	4.4	2.7	H
		2.3 AI + high-end chemical materials	4.2(4)	4.3	3.2	H

Source: *Developed by the author.*

As shown in Table 1, the top-ranked development area is "AI + intelligent chemical safety." Experts reached a consensus on advancing the construction of application scenarios such as intelligent video surveillance and behavior recognition, risk prediction and early warning systems, and intelligent emergency decision-support systems. These measures can directly reduce the risk of major industrial accidents.

The second-ranked area is "AI + intelligent chemical optimization." Experts agreed that, under the rigid constraints of the "dual-carbon" goals, the application of AI in energy efficiency optimization and carbon management is closely linked to regulatory compliance and the long-term competitiveness of enterprises. Developing full-process energy efficiency optimization, intelligent monitoring and management of carbon emissions, and intelligent control systems for environmental emissions is considered a core challenge for the sustainable development of the industry.

The third-ranked area is "AI + intelligent chemical manufacturing." Experts emphasized that the development of scenarios such as intelligent quality prediction and control, as well as intelligent production planning and scheduling, is critical for improving operational efficiency and enterprise profitability. The deep integration of AI into production processes is expected to reshape the core competitiveness of chemical enterprises.

Expert interviews further indicate that the three industry segments with the greatest market potential are the new energy chemical industry, traditional resource-based products, and high-end chemical materials. The future market is expected to exhibit the following three main characteristics:

1. New energy industries will lead market growth and direction;
2. Traditional resource-based products will undergo value revaluation and benefit accordingly;
3. High-end substitution will accelerate through the integration of biotechnology.

Experts cited several cases to support these predictions. For example, the rapid expansion of the lithium battery and photovoltaic industry chains signals a surge in demand for new energy materials and strong growth prospects over the next 5–10 years. Traditional resources such as phosphate ore and potash fertilizer have entered a new phase of value reassessment over the past 20–30 years, with significantly improved profitability. Meanwhile, high-end chemicals, including semiconductor materials and bio-based materials, are increasingly being replaced by domestic products, gradually breaking long-standing international market monopolies.

Carbon emission monitoring and forecasting have become core levers for petrochemical and chemical enterprises in implementing the "dual-carbon" strategy, while also serving as a dual safeguard for operational safety and economic performance. The application of AI technologies enables intelligent knowledge retrieval and autonomous process evolution. Chemical domain databases powered by large language models support multimodal retrieval across patent literature and experimental reports within seconds. Additionally, virtual chemical process simulators can achieve globally optimized trade-offs among reactor configurations, operating conditions, and cost and safety indicators, significantly shortening chemical process R&D cycles. Despite these advantages, the "AI + chemical engineering industry" continues to face substantial challenges. Therefore, a third round of the Delphi survey was conducted to rank and assess the key challenges influencing the future market development of the "AI + chemical engineering industry" (Table 2).

Table 2. The challenge ranking of "AI + chemical engineering industry" in market development

No.	Items	Contents	Weight
1	Barriers to technology adaptability and system integration	1.1 To focus on high-end, differentiated, and disruptive innovation	0.14
		1.2 To aim for future market trends and invest more R&D resources in areas closely related to global megatrends (e.g., sustainable development, energy transformation, digitization, and nutrition and health)	0.09
2	The contradiction between privacy protection and data compliance	2.1 To achieve the hierarchical integration and understanding of industry general knowledge and expertise data	0.11
		2.2 To transform original data into a deep understanding of production laws and risk trends through artificial intelligence algorithms, thereby providing unified and reliable data support for intelligent decision-making	0.10
3	Interpretability of the model	3.1 To explain the "black box" characteristics of AI for chemical experts.	0.09
		3.2 To develop an interpretable AI model for the chemical engineering industry	0.08
4	Uncertainty about initial investment and ROI	4.1 To cut the high cost of AI system deployment	0.07
		4.2 To cut the long cycle of return on investment that has discouraged many small and medium-sized enterprises	0.07
5	Lack of industrial-grade software	5.1 To encapsulate AI models into stable, easy-to-use, and reliable industrial software	0.08
		5.2 To ensure that AI models create value in the production environment	0.05
6	An imbalance between employee skills and organizational structure	6.1 To cultivate cross-border talents who understand chemical technology and equipment and are proficient in AI algorithms and data	0.07
		6.2 To cultivate talents with an international perspective and the ability to control the comprehensive competitiveness of management, science, technology, and operations	0.05

Source: *Developed by the author.*

According to Table 2 and expert opinions, seven key aspects need to be considered and addressed for chemical enterprises to effectively align with the market development of the "AI + chemical engineering industry." Addressing these aspects requires high-level, customized AI technology empowerment:

1. Cost pressure: The development of new chemical engineering industries and AI-enabled technological transformation requires substantial cost support and diversified investment sources;
2. Capacity optimization: The development and utilization efficiency of traditional resources remain

relatively low, while supply-demand imbalances persist for small and medium-sized enterprises. As a result, production capacity optimization remains a long-term challenge;
3. Trade barriers: The introduction of the EU's Carbon Border Adjustment Mechanism has accelerated the need for Chinese chemical enterprises to strengthen ESG systems in response to evolving international trade rules;
4. ESG and sustainability: Factors such as carbon footprint management, water resource utilization, and community relations are directly linked to financing costs, operating licenses, and brand reputation;
5. Vertical integration and supply chain resilience: End-to-end control of the value chain, from resource extraction to final products and even recycling, can effectively mitigate cyclical fluctuations and enhance supply chain security;
6. Financial health and strategic agility: Enterprises must maintain the resilience to survive industry downturns and the capacity to expand during upswings, while remaining flexible in responding to sudden supply chain disruptions;
7. Management structure and high-end talent: Long-term competitiveness depends on whether enterprises possess an internationally oriented management vision and high-level talent capable of integrating management, technology, and operational excellence.

According to the fourth round of the expert attitude survey, large-scale AI models, supported by deep learning and predictive analytics, have injected new digital momentum into the energy industry through their powerful data-processing capabilities. These models demonstrate significant advantages in energy supply and demand forecasting, energy storage system optimization, charge–discharge management, transformation of energy production processes, smart grid construction, and renewable energy management. The consensus of the fourth round is that representative application scenarios of the AI-enabled new energy chemical industry will play a leading role in stimulating the overall development of the chemical engineering industry in the future.

Typical professional scenarios are as follows:

1. Injection and mining linkage model: With the objectives of stabilizing oil output and controlling water injection, this model leverages more than 20 years of accumulated oilfield data and integrates AI technologies with expert knowledge. Through closed-loop management involving intelligent diagnosis, solution formulation, and remote control, it enables precise water injection, failure prevention, and reservoir optimization. As a result, oil recovery rates are improved, equipment life cycles are extended, and cost reduction and efficiency enhancement are achieved;
2. Safe drilling model: By applying machine vision technologies, an intelligent safety monitoring system can be established to identify risks in offshore drilling and completion operations rapidly. This approach significantly reduces unsafe behaviors, replaces traditional manual inspections and screen-based monitoring, enhances operator safety, and improves operational efficiency and quality, thereby providing intelligent support for offshore oil and gas development;
3. Oil and gas trade and marketing model: The integration of AI technologies enables intelligent price prediction for liquefied natural gas (LNG), accelerates import customs clearance, supports intelligent supervision of logistics and transportation, and enables precision marketing of oil and gas products. In resource procurement, the development of intelligent LNG spot price prediction systems improves procurement efficiency across multiple dimensions, significantly shortens tax refund cycles, and reduces compliance risks.

Typical general scenarios are as follows:

1. Intelligent recruitment scenario: By aggregating internal and external data, AI systems can support enterprise capability assessment and risk screening, generate initial drafts of bidding documents within minutes, enable bid comparison and automatic scoring, and rapidly identify abnormal behaviors. This significantly improves the efficiency of bid preparation and evaluation;
2. Intelligent writing scenario: Leveraging natural language processing technologies, AI enables functions such as material retrieval, intelligent formatting, assisted content creation, and precise proofreading. For employees with high demands for multi-type document writing, these capabilities substantially enhance both efficiency and accuracy in document processing;
3. Intelligent meeting scenario: Using speech recognition, voiceprint recognition, and large-scale AI models, AI systems provide real-time transcription and translation, recording transcription, intelligent summarization, and automated generation of meeting minutes. This effectively addresses the challenges of organizing meeting records and improves both the timeliness and quality of meeting outputs.

Overall, the application of AI technologies improves energy utilization efficiency and reduces operating costs, but also significantly enhances power grid stability and the grid integration capacity of renewable energy. Looking ahead, continued algorithm optimization and advances in computing power will further accelerate the intelligent transformation of energy systems, ensuring the transition toward a greener, more efficient, and safer energy era. With ongoing advances in artificial intelligence, large-scale AI models are expected to play an increasingly important role in the energy industry, driving its digitalization, intelligence, and low-carbon development.

4. RESULTS

With ongoing optimization of algorithms and continuous improvements in computing power, large-scale AI models are expected to accelerate the intelligent transformation of the chemical engineering industry and energy systems, promoting the global transition toward a new era of green, efficient, and safe energy. Based on four rounds of surveys, the results indicate that AI large models will play an increasingly important role in the energy industry, driving its digitalization, intelligent upgrading, and green development as artificial intelligence technologies continue to advance. The results of this study are presented in the following aspects.

First, "AI + chemical industry" empowers technology innovation in the market: from "trial and error" to "precise design," including the following. According to the survey, 90% of experts think "AI + chemical engineering technology can benefit the intelligent molecular design. By learning the structure and performance relationship of known chemical molecules, the AI model quickly generates millions of new molecular structures that meet specific requirements (e.g., higher strength and better electrical conductivity) and predicts the synthesis path, shortening the research and development time of new materials from a few years to weeks or even days. Moreover, most industry experts agree that AI can analyze the relationship between reaction conditions (temperature, pressure, catalyst, etc.) and yield and selectivity, recommend optimal reaction parameters, and greatly improve R&D efficiency.

Second, "AI + chemical industry" empowers the chemical production process optimization market: from "empirical control" to "intelligent optimization." It optimizes process parameters. According to 85% of experts, AI technologies can significantly benefit the market for chemical production process optimization. By applying reinforcement learning algorithms, AI functions as a "super operator," continuously adjusting production parameters in real time, 24/7, to minimize energy and material consumption while ensuring product quality and improving overall yield. Moreover, it ensures predictive maintenance. Most technology experts agreed that AI technology can benefit the more difficult, dangerous, and complicated production procedures. Through real-time monitoring and analysis of equipment operating data (vibration, temperature, pressure, etc.), AI can accurately predict the probability of failure and remaining life of key equipment (e.g., fans, pumps, compressors, etc.) and change "post-maintenance" to "pre-maintenance" to avoid unplanned shutdowns and ensure production safety. Additionally, AI ensures intelligent PID control. Traditional PID control is difficult to cope with complex non-linear processes. AI can establish more accurate soft measurement models and advanced process control models to achieve smoother and more accurate control.

Third, "AI + chemical industry" empowers the chemical safety and environmental protection market: from "passive response" to "active early warning." According to 80% of experts, AI can enhance early warning of safety risks across different operational procedures. AI models can integrate multisource data, including production data, equipment status, and video surveillance, to identify subtle anomalies that may lead to safety incidents, enabling timely warnings and effective prevention before accidents occur. It ensures emission management and optimization. Most university research teams and management representatives agree that AI can optimize the operation of environmental protection facilities by, for example, calculating the optimal dosage of desulfurization and denitration agents in real time. This approach reduces operating costs while ensuring regulatory compliance. At the same time, data analysis enables effective tracing of pollution sources.

Fourth, "AI + chemical industry" empowers the chemical supply chain and marketing market: from "chain" to "network collaboration". According ot 75% of experts, future development of the chemical engineering market will increasingly require "networked collaboration." By integrating market, seasonal, macroeconomic, and other data, AI can more accurately forecast product demand and guide production planning. Additionally, most technology teams believe that AI can dynamically optimize complex warehousing and transportation resources, thereby reducing inventory and logistics costs. Furthermore, according to downstream customer requirements, most university researchers agree that AI can provide personalized recommendations for chemical formulations or product solutions, improving market responsiveness and customer satisfaction.

5. DISCUSSION

The integration of AI and the chemical engineering industry is widely regarded as a core driving force of a new round of industrial transformation. However, as researchers and industry actively embrace this trend, most experts emphasize the need to examine potential problems and challenges from a prudent and comprehensive perspective to ensure that technological development remains stable, sustainable, and far-reaching.

At the technical implementation and data foundation level, chemical process data are often affected by noise, missing values, and outliers, while in large chemical enterprises, data systems across departments such as R&D, production, warehousing, and operations and maintenance are typically isolated, forming serious "data silos." In addition, the chemical industry involves numerous physical parameters, equipment models, and complex process descriptions, and the lack of unified data standards makes data integration and AI model generalization extremely difficult. Many advanced AI models, such as deep neural networks, also suffer from limited interpretability in their decision-making processes. When chemical processes involve extreme operating conditions or new materials beyond the training scope of the models, predictions may become inaccurate or unpredictable, posing significant safety risks. Moreover, industrial AI applications require dedicated algorithms and substantial computing power, and high-fidelity process simulations and digital twin systems place heavy demands on enterprise IT infrastructure.

At the organizational and talent level, a major bottleneck in the "AI + chemical industry" is the severe shortage of interdisciplinary professionals who are proficient in AI algorithms while also possessing deep knowledge of chemical processes, equipment, and safety. The integration of AI fundamentally changes traditional working modes, requiring enterprises to undertake significant organizational transformation and business process reengineering; otherwise, new technologies risk being constrained by outdated organizational structures. Traditionally, the chemical industry has been conservative, emphasizing experience-based decision-making and strict operational norms, whereas AI-driven approaches encourage rapid iteration, trial and error, and data-driven decision-making, creating challenges in organizational adaptation and cultural alignment.

From the perspectives of safety, ethics, and ecological sustainability, robust verification, validation, and reliability assessment mechanisms for AI systems are essential. When safety incidents arise from AI-driven decision-making, responsibility allocation among algorithm developers, system integrators, equipment manufacturers, and end users remains unclear, with existing legal frameworks containing significant gray areas that hinder AI adoption in high-risk chemical engineering scenarios. Ethical risks may also emerge from narrowly defined optimization objectives; for example, AI systems trained solely to maximize short-term economic benefits may adopt opportunistic strategies that compromise long-term environmental sustainability or equipment health. Therefore, constraints related to safety, environmental protection, and energy consumption must be explicitly embedded in AI objective functions. At the same time, although AI can accelerate the discovery of chemicals with specific functions, strong ethical review mechanisms are necessary to prevent misuse, such as the development of hazardous substances, including new toxins or explosives.

satisfaction.

6. CONCLUSION

The following conclusions summarize this study's findings on accelerating market development and application in the "AI + chemical engineering industry."

First, the construction of high-standard petrochemical and chemical industry datasets is essential. Priority should be given to developing comprehensive datasets for subdivided petrochemical and chemical sectors, integrating public industry data, private enterprise data, general educational data, specialized datasets, as well as structured and unstructured data. By fostering standardized industry data systems and implementing rigorous data screening, labeling, and management mechanisms, the industry can be provided with high-quality, professional data support. This approach ensures reliable training data and correct value orientation, fully unlocks the application potential of AI across vertical industries, establishes a virtuous "data-model-data" cycle, and promotes industrial upgrading and innovation-driven development.

Second, the construction of industry-specific and modular scenario models is a key pathway for scalable AI applications. Based on general-purpose large models, modular scenario models should be developed for the operation of common chemical units in areas such as distillation, extraction, mass transfer, and separation, creating a demonstrative "point-to-area" empowerment effect. Through standardized and reusable knowledge cores, prefabricated operational scenario models can be flexibly assembled to reflect enterprise-specific process chains, enabling a "building-block" approach to model deployment. This ecological modeling framework can break the industry's long-standing problem of repetitive development, significantly enhance total factor productivity, and support long-term growth. At the same time, it is necessary to focus on strategic, long-term objectives by building large-scale petrochemical and chemical industry models trained on high-quality industry corpora to meet the shared needs of the entire sector.

Third, establishing an ecosystem for AI model testing and evaluation in the raw materials industry is crucial. Once industry-scale models reach a certain level of maturity and adoption, systematic testing and evaluation mechanisms should be launched. Clear evaluation standards, automated evaluation toolchains, and practical, measurable, and scalable assessment methodologies should be developed, alongside the regular publication of quality rankings for industry- and enterprise-level large models.

Fourth, strengthening AI literacy and talent development across the industry is fundamental. Universities are encouraged to introduce interdisciplinary programs such as "Artificial Intelligence + Raw Materials" and to collaborate with enterprises in training master's and doctoral-level talent in AI engineering. Industry digital transformation promotion centers can deliver tiered and targeted AI training, including advanced case studies, technology trend analysis, and full-process engineering training for large enterprises facing high collaboration costs and severe data silos. For small and medium-sized enterprises, training should focus on AI awareness, foundational application skills, and the effective use of mainstream models to address concerns about implementation feasibility and practical outcomes.

In summary, AI breaks through traditional time and space constraints and drives a transformation of the manufacturing paradigm in the "AI + chemical engineering industry." From a temporal perspective, it enables "boundaryless" utilization of historical data, optimization of production and operations, and predictive maintenance. From a spatial perspective, it supports "boundaryless" multi-factory collaboration, regional capacity complementarity, industrial chain coordination, shared technical capabilities, and remote operation and maintenance services, fundamentally reshaping manufacturing models. Nevertheless, significant uncertainties remain in the future development of the "AI + chemical engineering market." Whether AI technologies can ultimately achieve the anticipated market forecasts and economic returns requires continuous observation, dynamic evaluation, and ongoing improvement.

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