

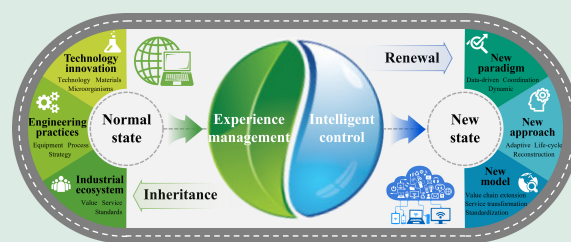
# AI-driven transformation of water treatment technology and industry: toward a new era of comprehensive innovation

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## HIGHLIGHTS

- A tri-axis roadmap is proposed to structure AI integration in water treatment.
- Evolution from local optimization to full-chain AI-enabled coordination is mapped.
- A shift to AI-enabled processes and lifecycle control in water treatment is revealed.
- Extension of the water industry value chain by data-driven services is identified.



**ABSTRACT:** The global water treatment industry urgently demands improved efficiency, energy conservation, and resource recovery. In response to these pressing challenges, artificial intelligence (AI) is rapidly emerging as a driving force for advancing water treatment technology and industry innovation, demonstrating unprecedented potential in data analysis, process prediction, strategy optimization, and resource allocation. However, the application of AI in water treatment currently lacks a systematic theoretical framework and empirical research. In particular, there is a significant gap in the implementation of AI-driven water treatment processes and the evaluation of the water industry, which urgently requires further exploration and resolution. This paper systematically sorts out the transformative logic of AI-driven water treatment technology and industry, analyzing frontier topics in the field from the perspectives of technology development paradigms, engineering application methods, and industry ecosystem models. It also proposes future research priorities and action recommendations, to provide empirical insights for the strategic deployment and execution of smart water management.

**KEYWORDS:** Artificial intelligence, Water treatment, Technological innovation, Industrial transformation, Smart water

## 1 Introduction

Water is a core element of global ecosystems and socio-economic development. According to *The United*

*Nations World Water Development Report*, global water demand will increase by approximately 50% by 2030 compared to current levels, and the world will face a 40% gap in freshwater resources (Loudiere and

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Gourbesville, 2020). Climate change, population growth, and the complex evolution of water usage patterns in industry, agriculture, and urban areas have further exacerbated the risks to water resource security (He et al., 2021; Cui et al., 2023). In this context, traditional water treatment plants (including drinking water treatment plants, wastewater treatment plants, etc.) face numerous challenges. Frequent fluctuations in water quality and quantity can increase the difficulty of process control. The traditional approach, which relies on experience and static parameter settings, struggles to adapt to real-time changes in environmental conditions (Ferraro and Prasse, 2021; Sin and Al, 2021). In addition, water treatment systems often suffer from high energy consumption, excessive use of chemicals, and insufficient potential for resource recovery and reuse (Rani et al., 2022; Zhou et al., 2023; Gong et al., 2024). These challenges make it urgent to promote the innovation and transformation of water treatment systems through new-generation technological solutions.

The wave of the fourth industrial revolution is sweeping the world at an unprecedented speed, and the rapid rise of artificial intelligence (AI) provides a far-reaching opportunity for transformation in the water treatment industry (Vance et al., 2024; Sela et al., 2025). While foundational concepts of machine learning trace back to the late 20th century, their performance has dramatically improved in recent years due to advances in computing power, data availability, and open-source frameworks, making them increasingly relevant to water treatment engineering. Evolving algorithmic paradigms such as deep learning (LeCun et al., 2015), reinforcement learning (Mnih et al., 2015; Sutton and Barto, 2018), transfer learning (Pan and

Yang, 2010), and federated learning (McMahan et al., 2017) can uncover potential rules and patterns from massive online sensor data, historical operational records, meteorological and hydrological data, microbial information of biological processing units, and material genomics databases (Alvi et al., 2023; Richards et al., 2023; Croll et al., 2024; Zhi et al., 2024). Leveraging the powerful natural language understanding, knowledge reasoning, and multimodal data analysis capabilities of large language models also enables intelligent question answering, causal reasoning, and optimization decisions for complex water treatment systems. Furthermore, a deep connection between virtual environments and water treatment plants can be established through digital twin and simulation optimization technology, thereby realizing comprehensive, multi-dimensional intelligent decision support and adaptive control (Li et al., 2024; Shehadeh et al., 2024). This paper will systematically review and forecast from the perspectives of technology development, engineering application, and industry ecology, aiming to offer forward-looking insights for the water treatment field to enter a new era of comprehensive intelligence and sustainability (Fig. 1).

## 2 Driving factors and transformational logic of AI-driven water treatment

### 2.1 Challenges in water treatment industry and the demand of intelligent solution

Traditional water treatment processes mostly rely on

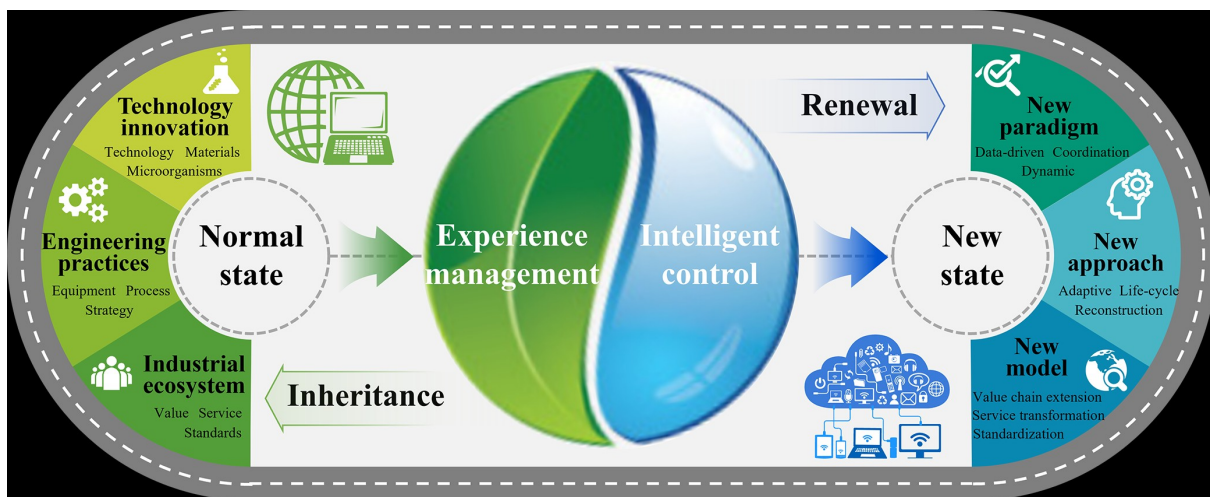


Fig. 1 AI-driven transformation of water treatment technology and industry.

fixed parameters, lacking sufficient resilience and fine regulation of environmental changes (Altowayti et al., 2022). When source water quality, flow, or load suddenly changes, decisions are often based on manual experience and periodic chemical analysis, resulting in delayed responses. This model makes it difficult to meet the demands for increasingly strict water quality standards and efficient resource recovery, and it is particularly passive in responding to climate extremes and sudden pollution incidents (Li et al., 2023; Van Vliet et al., 2023). The increasing complexity of municipal water treatment systems has made comprehensive and real-time process optimization imperative. At the same time, carbon neutrality, ecological civilization construction, and global environmental governance impose new constraints and assessment indicators for the water treatment industry (Du et al., 2023). Therefore, how to utilize emerging intelligent technologies for fine-grained management throughout the entire lifecycle of water treatment systems has become a key path to breaking through traditional limitations and achieving leapfrog development.

## 2.2 The rise of AI creates a new opportunity for water treatment revolution

The rapid development of AI technology in recent years, with breakthroughs in computing power, algorithm depth, and data mining, has laid a solid foundation for the intelligence of water treatment. The advent of AI has enabled more accurate modeling, prediction, and control of complex, multivariable, nonlinear, and time-varying water treatment processes (Li et al., 2021b). In particular, the popularity of big data analysis and cloud computing facilitates machine learning models and intelligent decision algorithms in water treatment systems (Himeur et al., 2023). In addition, AI can also be deeply integrated with emerging technologies such as the Internet of Things, blockchain, and edge computing to build a cross-temporal, cross-hierarchical smart water ecosystem. This integration achieves comprehensive intelligence across all levels, from individual facilities to regional watersheds and even global water cycle management, propelling the water treatment technology industry into a new era of panoramic innovation (Wang et al., 2021a; Liu and Li, 2024).

## 2.3 The evolutionary pathway of AI-driven water treatment transformation

The AI-driven water treatment revolution has

transitioned from focusing on local optimization of single process steps to a full-chain smart decision-making approach, based on influent prediction, microbial community regulation, and resource recovery strategy design. This shift aims to achieve the lowest energy consumption and optimal comprehensive benefits (Li et al., 2021a). Figure 2 illustrates the evolutionary pathway of AI-driven water treatment. Traditionally, the development of water treatment technology involves multiple stages, including water quality analysis, process trial and error, pilot scaling, and industrial demonstration, which often takes up to 10 to 15 years to put into practical application. AI breaks the isolation between these stages through system optimization methods. For example, digital twin technologies, powered by hybrid process models and real-time data, enable the construction of virtual water treatment plants. These systems not only simulate real dynamics but also learn from historical data to predict failures, optimize energy consumption, and enable emergency response. Unlike conventional simulation tools (e.g., BioWin), which rely on classical static models, AI-based simulators dynamically adapt to changing inputs and learn optimal strategies over time. On this basis, the target of water treatment is no longer limited to meeting discharge standards, but also takes economic costs, greenhouse gas emissions (measured in CO<sub>2</sub> equivalents), and nitrogen and phosphorus recovery rates into decision-making considerations. Under the same treatment scale, AI-driven comprehensive optimization solutions can reduce carbon emission intensity by 21% and lower treatment costs by 19.8% (Lancioni et al., 2024; Wang et al., 2024). In short, AI, with capabilities of self-learning, uncertainty reasoning, and adaptive optimization based on real-time data streams and multi-dimensional constraints, and by offering distinct advantages in process flexibility and systemic intelligence, is acting as the connecting link that is transitioning water treatment technology from “single-point static breakthroughs” to “full-chain precise dynamic control” (Schäfer et al., 2022).

## 3 AI pioneering technological innovation paradigms in water treatment

### 3.1 AI-enabled innovation and optimization of water treatment materials

By combining materials genomics and high-throughput

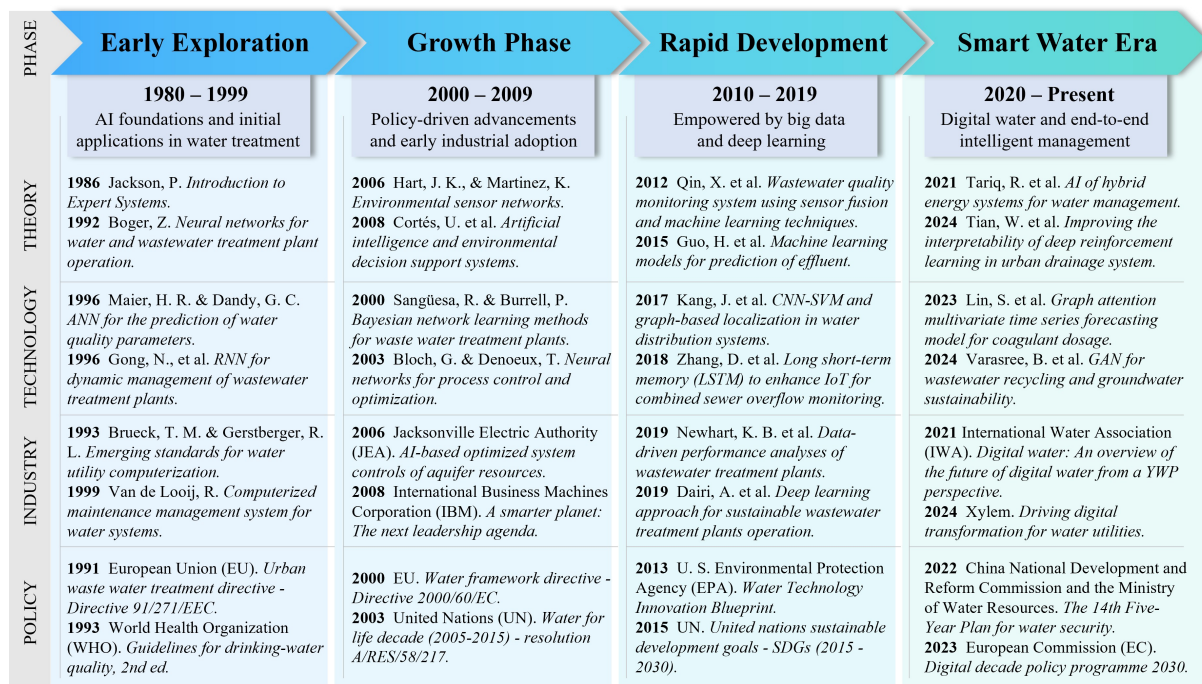


Fig. 2 The evolutionary pathway of AI-driven water treatment transformation.

computing, AI significantly accelerates the design and optimization of new materials (Jablonka et al., 2020). Graph neural networks are used to predict the permeability selectivity of membrane materials (Ignacz and Szekely, 2022), while molecular simulations help optimize the performance of adsorbents such as metal-organic framework (Thaler et al., 2024). The intelligent responsive membranes can dynamically adjust their wettability according to water quality conditions (Gong et al., 2023), and machine learning can realize the design of active sites for water purification materials and the targeted acceleration of non-radical processes (Wang et al., 2023). Self-propelled programmable micro- and nanorobots are also a promising technology, facilitating automated material discovery and efficient iterative optimization (Urso et al., 2023). Beyond pollutant removal performance, emerging studies have begun exploring how AI might assist in evaluating production scalability and practical applicability. Models trained on historical data can forecast operational robustness and cost-performance trade-offs under realistic conditions (Wang et al., 2021b; Pyzer-Knapp et al., 2022; Mahjoubi et al., 2025). Recent efforts explore the AI integration with life cycle assessment frameworks to correlate material composition and parameters with environmental impacts (Romeiko et al., 2024; Balaji et al., 2025). Although AI integration into eco-toxicity modeling, end-of-life impact evaluation, and circularity index

calculation remains nascent, emerging tools are being developed to support sustainability screening in early-stage material design (Jeong and Choi, 2022; Mehrotra, 2024; Recio-Colmenares et al., 2025).

### 3.2 AI-driven microbial intelligent regulation and biological enhancement

AI offers a new lens for decoding, modeling, and even engineering complex, dynamic microbial behavior with precision in biological treatment units. Deep learning combined with metabolic flux analysis can accurately analyze the metabolic networks of microorganisms involved in pollutant degradation (Yang et al., 2024), while algorithms such as convolutional neural networks can predict the dynamic evolution of microbial communities (Sheng et al., 2024). AI can optimize biological enhancement strategies by predicting co-metabolism effects to enhance the removal efficiency of recalcitrant pollutants (Gao et al., 2024). Additionally, it can intelligently regulate microbial electron transfer, improving the stability of microbial treatment units. Furthermore, integrating intelligent microbial regulation with synthetic biology offers an innovative path for constructing efficient and stable artificial microbial communities (Abudayyeh and Gootenberg, 2024). The convergence of AI, synthetic ecology, and microbial systems engineering will enable adaptive bioaugmentation strategies, self-optimizing treatment

consortia, and biosensors capable of autonomous recalibration.

### 3.3 AI-assisted development of self-regulating water ecosystems

Water treatment systems should not only efficiently remove pollutants, but also dynamically adapt to water quality variations, intelligently optimize energy consumption and resource recovery, and predict ecological impacts across different scales (Pham et al., 2022). Smart water models integrate real-time intelligent control and leverage data-driven models to enhance pollutant trend prediction capabilities, even in data-scarce environments (Dai et al., 2025). Focusing on the self-evolution capability of water systems and establishing an integrated intelligent framework for water ecosystem self-regulation can ensure ecological restoration capacity. Ultimately, the goal is to foster resilient, adaptive, and self-evolving water ecosystems, where AI supports not only technical efficiency but also long-term ecological health and social sustainability.

## 4 AI revolutionizing engineering practices approaches in water treatment

### 4.1 Smart equipment manufacturing and process unit coordinated control

AI is transforming both equipment design and process architecture in water treatment systems. On the equipment level, adaptive control strategies enable dynamic adjustment of equipment parameters based on real-time monitoring data, thereby maintaining optimal efficiency and operational stability. Additionally, AI facilitates the rapid iteration of intelligent equipment manufacturing, significantly reducing equipment manufacturing costs through modularization and automation while enhancing the precision and reliability of intelligent equipment (Koziel et al., 2024). Moreover, integrating AI with edge computing platforms and smart sensors enables modular hardware to function not just as passive components, but as intelligent agents capable of autonomous feedback-driven optimization.

Beyond individual equipment, AI facilitates the coordination and control of treatment process units to enhance operational efficiency and environmental performance. For example, intelligent aeration control systems powered by reinforcement learning algorithms

such as Deep Q-Network or Proximal Policy Optimization can reduce aeration energy consumption by 34% while ensuring stable compliance with effluent quality standards (Nam et al., 2020). Rather than merely tuning operational parameters, AI leverages data-driven simulations and influent characteristics to reconfigure process flows and treatment logic, enabling process unit optimization, energy consumption prediction, and the identification of valuable resources under corresponding conditions. For instance, a biological aeration tank based on the particle swarm optimization algorithm can reduce process energy consumption by approximately 37.6% (Muloiwa et al., 2024). Through hierarchical modeling, AI can map the relationships between process units, evaluate trade-offs across energy and chemical use, and simulate treatment efficacy under varied scenarios. Model libraries incorporating membrane bioreactors, anaerobic ammonia oxidation, and advanced oxidation can be flexibly assembled and optimized. Employing hybrid bio-inspired machine learning control technology to optimize reallocation of treatment functions across anaerobic and aerobic units, the aeration energy cost index and sludge production cost index can also be reduced by 488.96 kWh/d and 3620.08 kg/d, respectively, achieving a win-win outcome for economic and environmental benefits (Ateunkeng et al., 2024). This capability supports the emergence of design platforms in which AI co-designs and continuously refines the interlinkages among equipment, module, process, and operation under varying constraints, effectively transforming water treatment from a static system into a responsive, learning infrastructure.

### 4.2 Intelligent scheduling and full lifecycle management

AI facilitates system-level coordination and lifecycle-based decision-making in water treatment. Full-chain intelligent decision-making in water treatment includes raw water allocation, coordination and optimization among process links, collaborative scheduling of water treatment plants, and intelligent model optimization of distribution network layout (Yan, 2021; Tsai et al., 2022). In industrial parks aiming for zero-discharge, AI plays a critical role in the orchestration of wastewater recycling and reuse. AI makes its realization more feasible through accurate forecasting, adaptive control, and collaborative resource scheduling. Water quality forecasting models and predictive maintenance algorithms guide the allocation of treated effluent for reuse, minimizing downtime and maximizing system efficiency. In some cases, centralized AI systems

manage effluent quality monitoring, treatment routing, and feedback regulation across facilities, ensuring the safe return of treated water to industrial users after advanced processes like ultrafiltration and reverse osmosis. Optimization algorithms also support emergency response planning and resilience under extreme events, providing dynamic guidance for reconfiguration of treatment strategies under uncertainty. Such AI-enabled frameworks are essential for the development of smart, circular water systems that align with long-term environmental and operational goals.

## 5 AI reshaping industry ecosystem models in water treatment

### 5.1 Industrial chain extension

AI-driven value creation in water treatment has expanded from equipment supply, engineering construction, and operational maintenance to include data value-added services and intelligent decision support. From virtual simulation and optimization in the design phase to predictive precision control during operation and maintenance, and ultimately to value-added services of resource recovery in the later stages, the value chain has been significantly extended (Zhang et al., 2020). Big data analysis enterprises, cloud platform service providers, and consulting firms are embedded in various links of the water treatment industry. Through data sharing and collaborative innovation, the industrial chain is evolving from a linear extension to a networked ecosystem.

Simultaneously, AI empowers a new generation of service-oriented business models. Although the concept of “selling services and solutions” has existed in the water industry for years, AI significantly enhances the effectiveness and adaptability of service-based models. Smart water platforms support “Water Treatment as a Service” (WaaS), where billing is based on real performance metrics such as pollutant removal efficiency, energy consumption reduction, or water reuse volumes (Lapointe and Rochman, 2023). AI systems enable remote diagnostics, real-time performance benchmarking, and predictive maintenance, allowing services to be tailored to local treatment conditions. Moreover, emerging trends such as microservice-based platforms and smart contracts allow for modular, on-demand delivery and billing of water treatment functions, making services more

transparent, customizable, and scalable.

### 5.2 Standardization and development

Water issues have transboundary characteristics, making unified standards crucial for the orderly development of the global smart water market. With the increasing application of AI in water treatment, there is an urgent need to establish uniform data standards, testing and validation mechanisms, and transparency regulations for algorithms (Szczekocka et al., 2022; Um et al., 2022). The International Organization for Standardization, the International Water Association, and other international organizations are spearheading the development of standards and the establishment of data-sharing platforms. These initiatives promote international mutual learning and resource integration, enhancing the sustainability of the intelligent water treatment industry on a global scale.

## 6 Strategic frontiers and future trajectories for AI-driven water innovation

Despite the impressive momentum surrounding AI applications in water treatment, the landscape remains disjointed, often focused on discrete cases and disconnected from system-level innovation, rarely culminating in integrated, scalable, and resilient frameworks. Several strategic imperatives must be addressed to transition from proof-of-concept to transformational impact. The first shift involves moving from perception to interpretation: while monitoring is widespread, translating raw data into actionable intelligence remains underdeveloped. AI must evolve from pattern recognition to reasoning, bridging the gap between measurements and mechanistic understanding. Second, AI models must move from narrow prediction to broader universalization, functioning reliably across regions, seasons, and infrastructure types. Furthermore, AI should expand from an analytical tool to a systemic platform embedded throughout the water treatment process, including design, simulation, control, and feedback. Finally, AI deployments must move beyond short-term pilot projects to permanent integration into engineering and industrial codes, requiring standardization, interpretability, and reliable performance.

Alongside these imperatives lie several technical and structural obstacles. Variability in data quality and structure hinders cross-site learning. Model brittleness

under the water treatment emergency or edge conditions and mismatches with legacy infrastructure prevent real-time actuation. Engineering constraints (e.g., response time and material compatibility) often lag behind AI recommendations. Overcoming these obstacles calls for a three-axis developmental trajectory (Fig. 3):

1) The foundational axis focuses on building verifiable, translatable, and hybridized intelligence. High-resolution, multisource data sets (e.g., microbial omics, process logs) should be standardized and shared via open-access platforms, underpinned by benchmarking protocols aligned with real process dynamics. AI models built upon these data sets should go beyond black-box predictions and integrate knowledge through neural networks, mechanistic data fusion, and simulation-validated architectures.

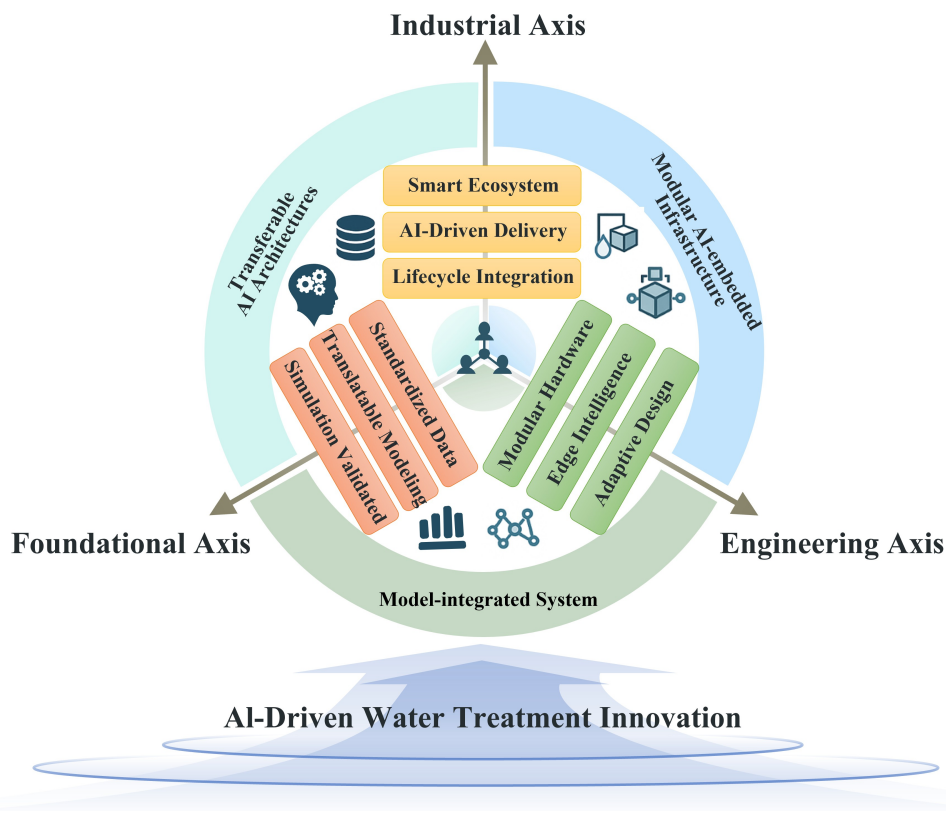
2) The engineering axis focuses on embedding intelligence into the physical infrastructure of water treatment, including equipment and processes. Equipment should support real-time sensing and modular reconfiguration through AI-compatible interfaces, edge processors, and pre-integrated control models. Design strategies must shift from static specification to adaptive capability, and support pre-

deployment testing across diverse water treatment processes, influent types, and stress conditions.

3) The industrial axis accelerates AI integration across the value chain, from planning to operation. Project delivery models must incorporate AI-driven simulation in planning and performance learning during operation to achieve lifecycle integration. Specifically, this shift entails transitioning from fixed-function products to AI-ready units, where control logic, feedback, and data interfaces are co-designed with the process to enable a plug-and-play ecosystem of water treatment modules.

## 7 Outlooks

AI presents transformative opportunities for the water treatment industry, enabling quantifiable improvements in key indicators such as energy consumption, chemical dosage, effluent stability, resource recovery rates, and system resilience. Notably, the rise of foundation models and large-scale cognitive systems offers a new transformational dimension of intelligent water treatment technology and industry. These models can integrate interdisciplinary knowledge, quickly analyze



**Fig. 3** Strategic frontiers and future trajectories for AI-driven water innovation.

complex water quality monitoring data, assist in decision-making, and provide real-time optimization recommendations, thereby accelerating the implementation of smart water management. In the future, with the continuous expansion of data resources, ongoing innovation in model algorithms, upgrading in sensing equipment, and the gradual improvement of the industrial ecology, a fully integrated smart water management framework is expected to be established, achieving a transition from local optimization to system panoramic coordination.

In this process, technological challenges and regulatory hurdles coexist. AI can be effectively implemented in water treatment by continuously enhancing data reliability, interpretability, and generalization capabilities. By further promoting the deep integration of AI and water treatment, exploring interdisciplinary innovations through the convergence of AI with emerging technologies such as synthetic biology and materials informatics, and building an intelligent water ecosystem that integrates monitoring, analysis, decision-making, and execution, the industry can drive full-process optimization in water treatment with carbon neutrality as the goal. Based on standardized quantitative indicators, continuous improvement in system performance and stability will ensure that smart water management is no longer just a blueprint but a solid foundation for the global water treatment industry to achieve high-quality growth and green transformation in the 21st century.

#### CRediT Authorship Contribution Statement

**Lili Jin:** Investigation, Methodology, Data curation, Formal analysis, Visualization, Writing-original draft. **Hui Huang:** Conceptualization, Funding acquisition, Supervision, Writing-review and editing. **Hongqiang Ren:** Conceptualization, Resources, Supervision, Funding acquisition.

**Conflict of Interests** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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