Innovations in Water Treatment
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Perspective

Interdisciplinary Integration and Innovation of Hybrid Models for Future Intelligent Wastewater Treatment

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How To Cite: Xu, R.; Cao, J.-S.; Fang, F.; et al. Interdisciplinary Integration and Innovation of Hybrid Models for Future Intelligent Wastewater Treatment. *Innovations in Water Treatment* **2025**, *1*(1), 1.

Received: 9 May 2025
Revised: 6 August 2025
Accepted: 7 August 2025
Published: 12 August 2025

Abstract: The operation of modern wastewater treatment plants has gradually transformed from the empirical paradigm to the computational paradigm. The potential application of mathematical models including mechanistic models and data-driven models have been extensively investigated to predict and improve the performance and efficiency of wastewater treatment processes. However, this paper points out that inherent weaknesses still exist in the standalone model attributed to the high complexity of wastewater treatment processes, emerging prediction targets, limitation of data availability, and lack of critical features in model development. Instead, hybrid models that combine mechanistic models with machine learning models may establish a superior approach to potentially address the limitations of those two modeling strategies mentioned above. Serial, parallel, and circular structures in hybrid models have been proposed to solve issues involved in wastewater treatment processes, whereas closer and deeper cooperation between mechanistic and data-driven models should be explored for solving more important functional scopes involved in the wastewater treatment field. We hope this paper can inspire the idea of developing hybrid models to support intelligent decision-making for wastewater treatment processes.

Keywords: intelligent wastewater treatment; machine learning; hybrid models; carbon neutrality; mechanistic models

1. Introduction

Nowadays, carbon emission, resource recovery, and emerging contaminants have become the central focus of modern wastewater treatment plants (WWTPs) [1,2]. This change not only makes wastewater treatment processes more complicated but also accelerates the calls for the implementation of mathematical models to support decision-making in WWTPs [3]. As a result, the operation of modern WWTPs has gradually transformed from the empirical paradigm to the computational paradigm. In the computational paradigm of WWTPs, mechanistic models and data-driven models are two types of mathematical models that achieve the most attention. Mechanistic models are established based on the verified or hypothetical first principles that have been clarified for specific pathways involved in wastewater treatment processes. Instead, data-driven models such as deep neural networks and random forests can overlook the first principles inside processes and are utilized depending on the big data collected from specific wastewater treatment processes. Although the investigation of mechanistic and data-driven models confirmed their high efficiency in solving lab-scale issues, the growing demand for low carbon emission, high resource recovery, and treatment of emerging contaminants in modern WWTPs limited their practical applications [4,5]. Moreover, mechanistic and data-driven models present inherent weaknesses in designing mechanistic pathways and collecting big datasets, respectively.

To effectively tackle these constraints, it is imperative to develop hybrid models that integrate mechanistic and machine learning models [6]. The mechanistic sub-models play a crucial role in preserving the first principles knowledge and enhancing the extrapolation capabilities of the hybrid models. At the same time, the machine learning sub-models can significantly boost prediction accuracy, thereby compensating for the limitations inherent in mechanistic models. The convergence of machine learning with domain-specific first principles knowledge to address complex problems has emerged as a rapidly growing trend [4,7,8].

In this Making Waves article, we analyze the inherent weaknesses of existing mechanistic and data-driven models. Based on their weakness, we present advantages and the recent development of hybrid models with different combinatorial structures between mechanistic models and data-driven models. The future research points of hybrid modes for wastewater treatment processes are proposed and highlighted. This work reveals the importance of incorporating the advantages of two kinds of mathematical models, which may inspire the idea of developing hybrid models to support intelligent decision-making for wastewater treatment processes.

2. Weakness of Standalone Models for Intelligent Wastewater Treatment

Although the separate utilization of mechanistic models and data-driven models for wastewater treatment processes has been extensively studied [9,10], limits still exist in the practical applications of the standalone model in wastewater treatment fields (Figure 1). On one hand, wastewater treatment processes are complicated and influenced by diverse environmental factors and process parameters that may hinder the establishment of effective standalone models. The wastewater composition is highly complex, exhibiting stochastic perturbations and influent variability, which leads to uncertainties in wastewater treatment systems [11]. Then, the influent with fluctuating characteristics will pass through long and complicated multiple-stage treatment processes. The treatment performance of each stage highly depends on influent characteristics and numerous operating parameters, which normally serve as the controlling targets based on the prediction results of mathematical models [12,13]. On the other hand, new predicting targets (e.g., emerging pollutants and resource recovery) further complicate the requirement of model functions, which must be supported by more powerful modeling strategies. Treating emerging pollutants such as pharmaceuticals and personal care products, disinfection by-products, and poly-fluoroalkyl substances in wastewater has achieved increasing attention [14]. Moreover, energy efficiency and resource recovery have emerged as critical priorities in the wastewater treatment industry due to tough challenges such as water scarcity and climate change [15].

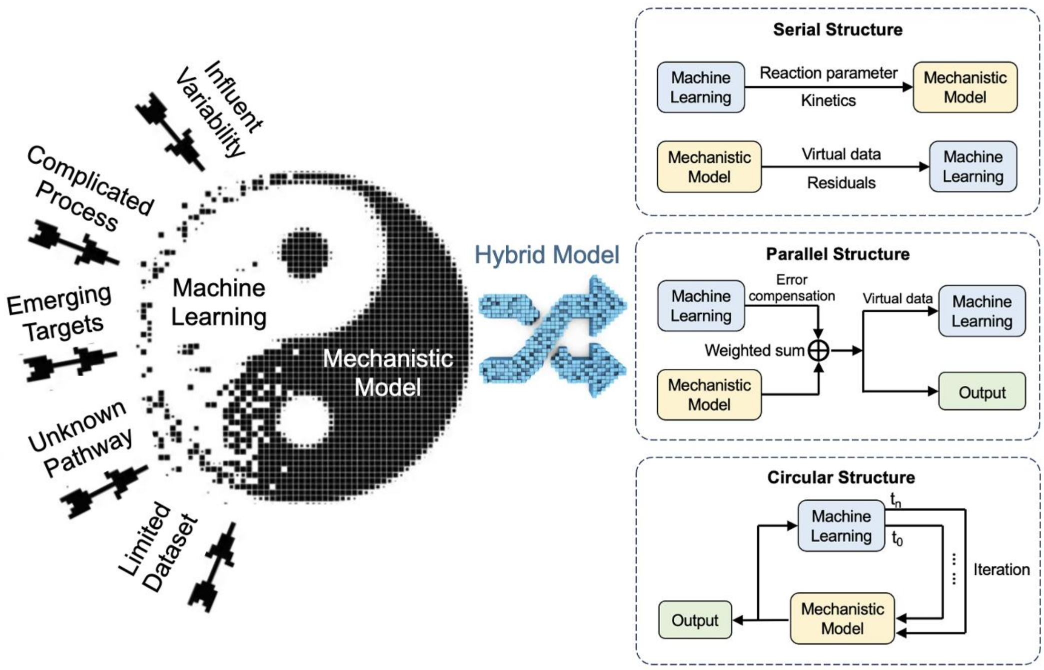

Figure 1. The weakness of standalone models faced in the wastewater treatment field (**left** side) includes influent variability, complicated process, emerging targets, unknown pathway, and limited dataset. Serial, parallel and circular structures of existing hybrid models (**right** side).

From the perspective of models, standalone models may be ineffective in predicting treatment performance and these emerging targets in practical wastewater treatment processes. Mechanistic models are commonly over-parameterized, extremely susceptible to changes in operational conditions, and necessitate substantial calibration and validation efforts. Unknown knowledge of targeted microbial metabolic processes will also hinder the establishment of accurate mechanistic models. Therefore, it is difficult for mechanistic models to be applied singly for practical application, especially for these new targets. The standalone use of machine learning models also suffers from serious drawbacks. First, the limitation of data availability and lack of critical features in WWTPs prevent machine learning models from being widely adopted [13]. The quality of available data from sensors might also be unreliable because these sensors in the wastewater treatment units are exposed to harsh environments [16]. Moreover, the poor mechanistic-based interpretability of the established machine learning models limits their effectiveness and reliability [17]. As a result, machine learning models could predict specific conditions better but lose long-term stability and applicability to distinctly different scenario conditions and new targets supported by poor sensors.

In summary, the mechanistic model or data-driven model alone is unlikely to satisfy the growing modeling needs of wastewater treatment or answer specific scientific questions.

3. Hybrid models with Diverse Structures and Their Advantages Outperform Standalone Models

Hybrid models that combine mechanistic models with machine learning models may establish a superior approach to potentially address the limitations of those two modeling strategies mentioned above. To utilize the complementary nature of these two modeling strategies, hybrid models with diverse structures (i.e., serial, parallel, and circular structures) have been proposed to solve issues involved in wastewater treatment processes (Figure 1).

In the serial structure, the first model will generate useful information to support the establishment of the second model. For example, machine learning models can output functional parameters required by mechanistic models, such as the reaction parameters of emerging micropollutants degradation [18] and oxygen off-gas fraction in aeration systems [19]. Then, the mechanistic models can be established based on the parameters predicted by the machine learning models. In this way, the hybrid model serves as a parameter simulator that statistically infers kinetic parameters, which can then be fed back to the mechanistic models for predicting targets.

Instead, outputs of the mechanistic model can also be embedded into or used by a machine learning model. First, the output of mechanistic models can serve as an important source of datasets for machine learning models. In practical wastewater treatment systems, the data of some important variables cannot be collected intensively but they can be generated by the well-calibrated mechanistic models. The virtual data generated by mechanistic models can capture large fluctuations and critical features related to the domain knowledge, which supports the training of following machine learning models [8]. The resulting hybrid model needs lower data requirements than the standalone machine learning model and fewer calibration efforts than the standalone mechanistic model. Also, the residuals (i.e., differences between the measured data and predicted data of mechanistic models) of important variables can be utilized as the input variables of the following machine learning models [20]. The hybrid model can capture sufficient residual information to compensate for the inaccuracy of the standalone mechanistic model and improve the extrapolative capability of the standalone machine learning model.

In the parallel structure, the mechanistic model and machine learning model can be combined in several ways. First, the weighted sum of the outputs of the two models can be used as the output of the hybrid model. The weights of the two models are adjusted according to the prediction error [21]. Moreover, the prediction results of a mechanistic model and a machine learning model can be integrated and utilized as the input of the following machine learning model [22]. In this way, the parallel hybrid model and the following machine learning model form a serial hybrid model, where the parallel hybrid model serves as a data generator. The virtual data generated by the parallel hybrid model combines the biochemical mechanism and hidden features of monitoring data, providing better training efficiency for the machine learning model. In parallel structure, machine learning models can also be used as the error compensation model, which compensates the predictive error between the mechanistic model output and measured data [23]. In this parallel hybrid mode, the machine learning model is utilized in parallel with the mechanistic model to reduce the error of the mechanistic model predictions. The outputs of this parallel hybrid model are obtained by summing the outputs from the two models. The resulting parallel hybrid model not only supplies an adequate explanation of the process kinetics but also improves the prediction accuracy.

In the circular structure, the predicted results of the machine learning model are incorporated into the establishment of the mechanistic model [24]. Then, the predicted results of the mechanistic model were utilized as the input to the machine learning model for the next iteration. In this loop, the predicted results of the machine learning model and the mechanistic model are continuously fed to each other to reduce the prediction errors of the circular hybrid model.

Except for these three structures, Schneider et al. (2022) considered surrogate models as hybrid models in view of a loose definition [6]. However, we don't embed the surrogate models into the concept of hybrid models because surrogate models don't contain two or more sub-models in their final modeling structures.

Overall, the hybrid models with multiple structures present greater flexibility, more powerful functions, and better interpretability than the standalone models (Figure 1). The hybrid models could handle the issues (e.g., influent variability, complicated processes, and limited datasets) that affected the standalone models. On the other hand, the diverse combinations in hybrid models may be confusing for users and inevitably increase the complexity of the hybrid model. The trade-offs between hybrid model complexity and real-time decision support need to be considered in the development and applications of hybrid models involved in the intelligent control of WWTPs.

4. Hybrid Models for Intelligent Wastewater Treatment Require Further Development

Due to the high diversity of hybrid structures, the appropriate structure of hybrid models should be selected carefully according to the predicted targets, data availability, and prior knowledge (Figure 2). The quick development of computational power and computer science provides a strong foundation for establishing hybrid models incorporating mechanistic models and machine learning models. The establishment of hybrid models can effectively improve the model's ability to develop the digital representation of wastewater treatment processes and support automated decision-making [3,25].

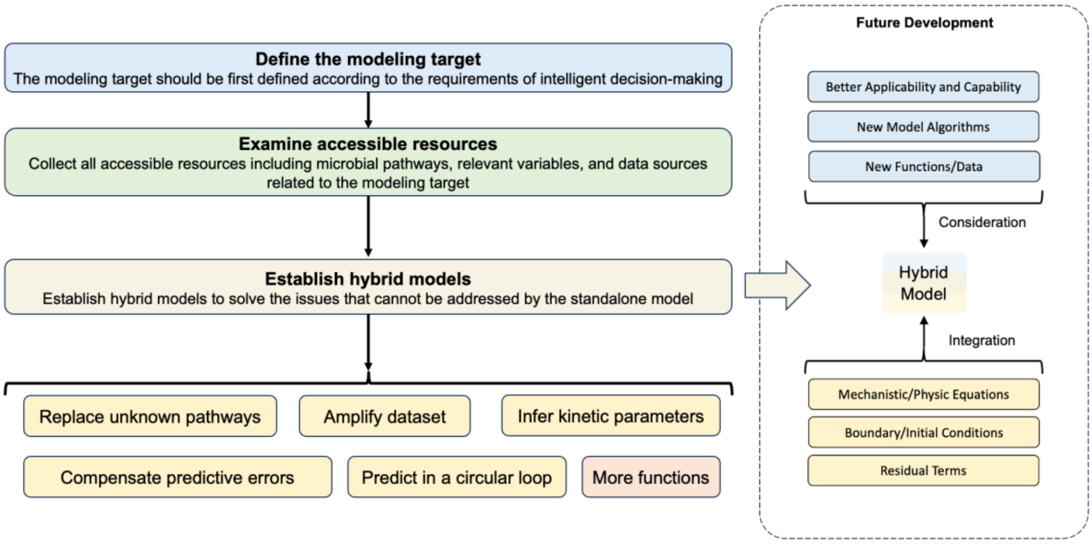

Figure 2. The procedure and future development of establishing hybrid models.

Undoubtedly, hybrid models with diverse structures present better prediction performance and stronger implementation capability than standalone models. However, there are still some limitations in the current development of hybrid models (Figure 2):

(1) In existing hybrid models, the combination between mechanistic models and machine learning models is relatively independent. For understandable processes, the knowledge concept supported by mechanistic models should be truly integrated into the architecture of machine learning models to endow machine learning models with high interpretability. The concept of physics-informed neural network (PINN) and machine learning interatomic potentials (MLIPs) may inspire us. PINNs can incorporate both measured data and physical laws in the training process by integrating differential equation residual terms, initial and boundary conditions into the architecture of machine learning models [26]. MLIPs support the potential of first-principles multiscale modeling with quantum mechanics accuracy and flexibility to study the properties of structures and materials [27]. For example, Koksal et al. [28] utilized the equations from the activated sludge model No.1 (ASM1) to strengthen the physics-informed models for predicting the dissolved oxygen (DO) concentration in the activated sludge and the chemical oxygen demand concentration at the clarifier outlet of an industrial wastewater treatment plant. Specifically, the physics loss related to DO concentration in ASM1 could be integrated into the objective function, compelling the training process to adhere to the underlying physics principles [29]. Moreover, Guo et al. [30] predicted the urban nonpoint source (NPS) persistent pesticide pollution by developing a hybrid physical

mechanism and an artificial intelligence–based model in the absence of urban pipeline network data and using easily accessible traditional NPS model parameters. Therefore, there is potential to incorporate mechanisms and physics into the structure of machine learning models by imposing equations, which form the "differentiable modeling" and offer better interpretability, generalizability, and extrapolation capabilities than purely data-driven models [31]. Moreover, the rapid development of machine learning algorithms (e.g., Transformer, graph neural network, and active learning) may provide new chances for better integration with mechanistic models.

(2) The functional scopes of the existing hybrid models are still limited. Although hybrid models have been studied to solve several issues in wastewater treatment fields such as pollutant degradation [32], effluent prediction [33], and microbial analysis [8], the model prediction of some important targets in intelligent wastewater treatment is still missing. For example, we should establish hybrid models for predicting and optimizing anaerobic fermentation and digestion processes to improve the efficiency and stability of resource recovery, which are essential to the carbon neutrality of WWTPs. The establishment of hybrid models for new functions may provide significant process improvements through prediction, optimization and intelligent decision-making.

(3) Last but not least, practical applications of hybrid models in the intelligent wastewater treatment field are still few. The applicability and capability of hybrid models should be further evaluated with full-scale WWTPs. To truly apply hybrid models in practical WWTPs, the standard benchmarking protocols across full-scale plants for evaluating the efficiency of hybrid models need to be established. The establishment of hybrid models with new structures and functions must be verified by both experimental data and practical data. The gradual adoption of hybrid models in full-scale WWTPs requires the cooperation among data scientists, wastewater treatment engineers and the faculties of WWTPs

5. Conclusions

- Standalone models have been extensively investigated for wastewater treatment fields, whereas inherent weaknesses exist in the standalone models due to the high complexity of wastewater treatment processes, emerging prediction targets, limitation of data availability and lack of critical features.
- Hybrid models with different combined structures present a stronger capacity for handling the requirements of intelligent wastewater treatment. The limitation of data availability and unclear microbial metabolism could be solved by the combination of mechanistic models and data-driven models.
- More research should focus on establishing hybrid models with new structures and realizing more important functional scopes involved in the wastewater treatment field.
- To reduce carbon emissions and enhance treatment performance, wastewater treatment utilities must adapt to embedding the intelligent wastewater treatment system based on hybrid models. Advanced sensors, industrial computers, communication networks, cloud platforms, and well-calibrated hybrid models are required in intelligent WWTPs.

Author Contributions

R.X.: conceptualization, methodology, writing—original draft preparation, writing—review & editing, Funding acquisition; J.-S.C.: conceptualization, writing—review & editing, funding acquisition; F.F.: data curation, Software, validation; C.S.: writing—review & editing, visualization; B.-J.N.: writing—review & editing, supervision; J.L.: writing—reviewing and editing, methodology. All authors have read and agreed to the published version of the manuscript.

Funding

This research was funded by Fundamental Research Funds for the Central Universities (B240201132), National Natural Science Foundation of China (52400032), Natural Science Foundation of Jiangsu Province (BK2041534), China Postdoctoral Science Foundation (2024M750744), Jiangsu Funding Program for Excellent Postdoctoral Talent (2024ZB687), Jiangsu Carbon Peaking and Neutrality Science and Technology Innovation Fund (BE2022861), Anhui Provincial Key Laboratory of Environmental Pollution Control and Resource Reuse (2023EPC01).

Institutional Review Board Statement

Not applicable.

Conflicts of Interest

Given the role as Editor-in-Chief, Bing-Jie Ni had no involvement in the peer review of this paper and had no access to information regarding its peer-review process. Full responsibility for the editorial process of this paper was delegated to another editor of the journal.

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