Intelligent Setting and Model Predictive Control of Wastewater Treatment Process Based on Case Search Optimization

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***Abstract*—To address the challenges in wastewater treatment processes—namely, the multi-objective conflict between effluent quality and operational energy consumption, complex dynamic characteristics, and the difficulty of applying traditional optimization methods online—this paper proposes an intelligent setpoint method based on case search optimization. This method constructs an optimization framework of "offline construction and online decision-making." In the offline phase, it uses K-means++ to cluster historical operating conditions and employs NSGA-II to screen Pareto-optimal solutions, thereby building a knowledge base. In the online phase, it retrieves optimal setpoints through operating condition matching and similarity calculation. By integrating a dynamic case library maintenance strategy with an Echo State Network-based Model Predictive Controller, the method achieves precise setpoint tracking. Simulation results on the BSM1 platform demonstrate that, while ensuring effluent quality meets discharge standards, this method reduces operational energy consumption by approximately 3.9% compared to the traditional fixed setpoint strategy. It achieves an intelligent dynamic balance between water quality and energy consumption, providing an efficient and reliable new approach for the optimal operation of wastewater treatment processes.**

***Index Terms*—wastewater treatment, case search optimization, multi-objective optimization, setpoint optimization, model predictive controlnstruction**

I. Introduction

A. Research background and significance

Water scarcity and water environmental pollution are global challenges [1]. China's per capita water resources are insufficient, and with the advancement of industrialization and urbanization, the water pollution situation is severe [2-3]. From a process engineering perspective, the activated sludge wastewater treatment process is a typical complex industrial process, characterized by nonlinearity, strong coupling, large time delays, and random disturbances from influent loads [4]. The International Water Association has introduced the Activated Sludge Models (ASM series) and the Benchmark Simulation Models (BSM series), providing a standard framework for mechanistic research. However, these models involve numerous parameters and complex structures, posing significant challenges for their direct application in online optimization control [5-6].

In practical operation, treatment plants frequently encounter fluctuations in both water quality and quantity. The core objective—minimizing energy consumption as much as possible while ensuring effluent quality meets discharge standards—involves an inherent conflict. Traditional operation modes often rely on empirical knowledge or fixed setpoints, making them difficult to adapt to dynamic changes. Model Predictive Control (MPC) and Multi-Objective Evolutionary Algorithms (MOEA) offer potential solutions [7], but they have limitations in practical applications: MPC based on mechanistic models heavily depends on model accuracy and imposes a heavy online computational burden; directly using evolutionary algorithms is also time-consuming and struggles to meet real-time requirements [4,7]. With the widespread adoption of IoT and sensor technologies, massive amounts of historical operational data have laid the foundation for data-driven methods. In view of this, this study introduces case search optimization into the intelligent setpoint determination for the wastewater treatment process. By mining historical optimal operational experiences to build a knowledge base, it achieves rapid and intelligent dynamic adjustment of key setpoints.

B. Main Research Content of the Text

This paper focuses on the intelligent optimal operation of wastewater treatment processes and conducts research about: Optimization Problem Modeling, CSO Framework Design, Closed-Loop Integration and Validation.

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II. Modeling and Analysis of Wastewater Treatment Process Optimization Problems

To effectively study and verify the intelligent setting method for wastewater treatment processes, it is necessary to first clearly and accurately describe the optimization problem mathematically on a recognized and reliable benchmark platform. This chapter will systematically introduce the simulation environment on which the research relies, and based on this, formalize the multi-objective optimization problem centered on water quality and energy consumption, while analyzing key variables and system constraints.

A. BSM1 Benchmark Simulation Platform and System Description

The BSM1 platform is a standardized mathematical model for simulating activated sludge wastewater treatment plants, with its physical layout shown in Figure 1. The system consists of a bioreactor tank and a secondary settler connected in series. The bioreactor comprises five continuous completely mixed reactors (the first two are anoxic zones, and the latter three are aerobic zones). The biochemical kinetics follow the Activated Sludge Model No. 1 (ASM1). The secondary settler uses the Takács double-exponential settling model to simulate the sludge separation process.

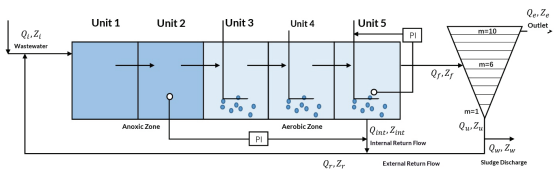


Fig. 1. BSM1 overall layout

The system maintains dynamic balance through material recirculation: the mixed liquor from the aerobic zone is internally recycled to the anoxic zone to provide denitrification substrate, the sludge from the secondary settler is externally returned to maintain biomass, excess sludge is discharged, and the supernatant is discharged as effluent. This platform provides a standardized benchmark for wastewater treatment control research.

B. Formal description of the multi-objective optimization problem

In the BSM1 platform, the operational goal of the wastewater treatment process is to minimize operating costs as much as possible while meeting discharge standards. This is essentially a typical multi-objective optimization problem.

(1) Optimization objective function: The problem can be formalized as finding a set of decision variables that simultaneously optimize the following two conflicting objectives:

$$minF = min\{EQ, EC\} \tag{1}$$

where EQ is the effluent water quality index, with smaller values indicating better water quality; EC is the system's energy consumption index, with smaller values indicating lower energy use. These two objectives are inherently conflicting; for example, increasing aeration to improve treatment efficiency usually results in higher energy consumption.

(2) Effluent water quality constraints: The optimization process must satisfy strict effluent quality constraints, ensuring that the average concentrations of effluent components are below regulatory limits. The core constraints include Ammonia nitrogen concentration, Total suspended solids concentration, Five-day biochemical oxygen demand concentration, Chemical oxygen demand concentration, Total nitrogen concentration.

(3) Key Variables and Constraints: In this study, the dissolved oxygen concentration SO_5 at the outlet of the fifth aerobic zone and the nitrate nitrogen concentration SNO_2 at the outlet of the second anoxic zone are selected as the key setpoints for optimization. The underlying controller tracks these setpoints by adjusting the aeration rate (directly affecting SO_5) and the internal recirculation flow rate (mainly affecting SNO_2). The optimization search must be conducted within the physical boundaries of the system, with the main constraints including Variable range constraints, Actuator constraint, Process dynamic constraints.

III. Design of Optimization Setting Framework Based on Case-based Search

To address the core challenges of multi-objective dynamic optimization in wastewater treatment—namely high online computational complexity and high model dependence—this chapter proposes an intelligent solution driven by data and knowledge—Case Search Optimization (CSO) framework. This framework follows an "offline mining, online reuse" paradigm, transforming complex online optimization problems into efficient knowledge retrieval and decision-making tasks. This chapter systematically explains the overall architecture of the framework and analyzes the algorithm principles and design of its two core components: automated construction of the offline case library and real-time online decision-making.

A. Overall Architecture and Core Process Design

The core idea of the case search optimization framework is to establish and utilize a "knowledge base" (case library) that condenses the best historical operational experience to respond to real-time changing conditions. Its overall architecture is a closed-loop system comprising offline and online stages, with the core process shown in Figure 2, intuitively illustrating the complete information flow from historical data to online decision-making.

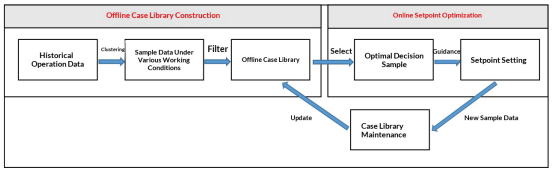


Fig. 2. Data Mining-Based Wastewater Treatment Optimization Steps

(1) Offline Case Library Construction Stage (Knowledge Refinement and Accumulation) The goal of this stage is to automatically learn and structurally store optimal operational experiences under different conditions from massive historical operation data. The input is a long-term collected historical dataset, with each sample formalized as a triplet C=(Z,Y,E). Among them:

- $Z = (S_S, S_I, X_S, X_I, X_{B,H}, X_{B,A}, X_P, S_{NH}, S_{ND}, S_O, S_{NO})$ is the condition feature vector, representing the influent water quality.
- $Y = (y_{d,1}, y_{d,2})$ is the decision scheme, i.e., the dissolved oxygen$SO_5$and nitrate nitrogen SNO_2 setpoints applied under this condition.
- $E = (EQ, EC)$ is the performance evaluation vector, recording the effluent water quality and energy consumption after executing the scheme.

This stage processes data through two key technical steps to ultimately build a Pareto optimal case library $\mathcal{L}$. This case library is the foundation for all subsequent intelligent decision-making.

(2) Online Case Search and Decision-Making Stage This stage is the core of the framework's real-time application. At each dispatching moment t, the system obtains the latest influent feature vector Z_t as a query case. The online decision process is as follows:

- Matching: Calculate the similarity between Z_t and all cases in the case library $\mathcal{L}$, quickly locating the most similar subset of cases $\mathcal{L}_{\text{match}} \subset \mathcal{L}$.
- Decision: Based on multi-objective trade-off preferences, select one or more optimal cases from $\mathcal{L}_{\text{match}}$, and generate the recommended setpoints Y_t^* for the current moment through fusion rules (such as weighted averaging).
- Execution and Feedback: Send Y_t^* to the underlying tracking controller for execution. After one operational cycle, new successful run samples (Z_t, Y_t^*, E_t) can be fed back into the system to update the case library.

B. Case Library Construction Method Based on K-means++ and NSGA-II

Constructing a high-quality, high-coverage case library is key to the success of this method. This work adopts a two-step approach of "clustering first, then screening" to ensure the case library can represent typical operating conditions and include the optimal solutions for each condition.

(1) For the high-dimensional and complex influent data, we employ the K-means++ algorithm for unsupervised clustering. This algorithm optimizes the selection of initial cluster centers to achieve more stable results. It partitions the historical operating conditions into K clusters $\{C_1, \ldots, C_K\}$, with each cluster representing a typical type of operating condition.

(2) Pareto optimal case extraction based on NSGA-II: for each cluster C_k, which contains multiple historical samples, each excels in objectives EQ and EC. To extract the most guidance-rich Pareto optimal solutions, we introduce the fast non-dominated sorting genetic algorithm (NSGA-II) with an elitist strategy for screening.

1) Non-dominated Sorting: Treat all samples in cluster C_k as a population. For each individual p in the population, calculate its number of dominating individuals n_p and the set of dominated individuals S_p. First, find all individuals $n_p = 0$ to form the first non-dominated front (Front 1). Then, ignore individuals in Front 1 and repeat the process to obtain the second front (Front 2), and so on. Figure 3 shows an example distribution of Pareto optimal solutions and Pareto front for a bi-objective minimization problem.

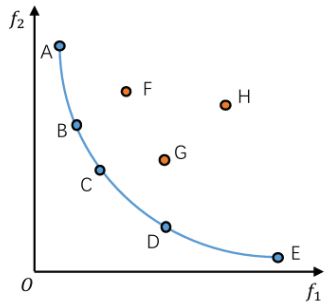


Fig. 3. Multi-objective optimization individual distribution diagram

2) Crowding Distance Calculation and Selection: To maintain the diversity of the solution set, the crowding distance of individuals within the same front is calculated. Individuals from the first non-dominated front within each cluster are selected and stored in the case library.

Ultimately, merge all Pareto optimal solutions from all clusters to form the global Pareto optimal case library $\mathcal{L} = \bigcup_{k=1}^{K} \text{ParetoFront}(C_k)$. Each case in this library is an elite solution that has emerged victorious after multi-objective optimization under its specific working condition.

C. Online Decision Mechanism Design Based on Similarity Matching

The goal of online decision-making is "finding the right person for the right job"—identifying the most suitable experience from the case library based on real-time conditions and applying it. This mechanism consists of matching and decision-making stages. The overall control architecture for wastewater treatment optimization based on data mining is shown in Figure 4.

(1) Real-time Operating Condition Matching and Similarity Calculation

The similarity between the real-time features Z_t and all cluster centers c_k is calculated using a weighted Euclidean distance metric:

$$\text{Sim}(Z_t, c_k) = \frac{1}{1 + \sqrt{\sum_{j=1}^{m} w_j \cdot (Z_{tj} - c_{kj})^2}} \tag{2}$$

Among them, m is the feature dimension, w_j is the weight of the j-th feature (which can be set based on feature importance or inverse variance). The system matches the real-time operating condition to the most similar condition cluster

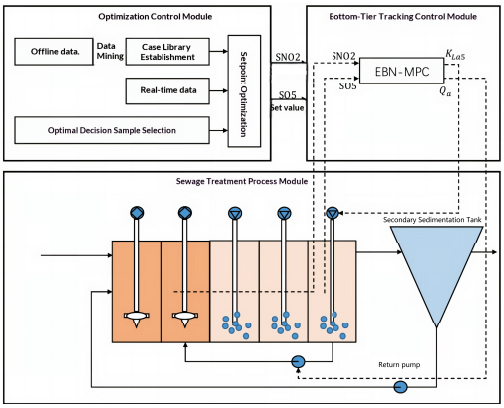


Fig. 4. Overall Control Architecture for Wastewater Treatment Optimization

C_{match}, thereby rapidly narrowing the search scope from the entire case library to the local case subset C_{match} corresponding to that cluster, improving retrieval efficiency.

(2) Multi-objective trade-off decision and setpoint generation

The matched case subset C_{match} may contain multiple Pareto optimal cases, representing different water quality-energy consumption trade-offs. To make the final decision, a decision function reflecting operational preferences is introduced. This study defines a comprehensive utility function, which calculates for each case i:

$$U_i = \omega \cdot \text{Norm}(EQ_i) + (1-\omega) \cdot \text{Norm}(EC_i) \tag{3}$$

Where Norm$(\cdot)$ indicates normalization of EQ and EC (e.g. scaled to the $[0,1]$ range), $\omega (0 \le \omega \le 1)$ is the preference weight set by the operator.ω close to 1 emphasizes water quality, close to 0 emphasizes energy saving. After computing the utility values for all cases, the case with the highest utility (or several top-ranked cases) is selected. Finally, the setpoints of the selected case are weighted averaged (e.g. based on utility or similarity weights) to generate the recommended setpoints at the current moment Y_t^*:

$$Y_t^* = \frac{\sum_{i \in L_{\text{top}}} \text{Sim}_i \cdot Y_i}{\sum_{i \in L_{\text{top}}} \text{Sim}_i} \tag{4}$$

Where, L_{top} is the set of selected optimal cases, Sim_i is the similarity between case i and the current operating condition. This mechanism respects the objective optimal patterns in historical data while allowing operators to adjust based on practical needs, achieving a combination of intelligence and humanization.

IV. Implementation and Integration of Key System Modules

This chapter elaborates on the specific implementation schemes of two key supporting modules within the case search optimization framework: the dynamic case library maintenance strategy ensures the system's self-evolution capability, while the underlying MPC controller achieves precise tracking of the upper-level setpoints, thereby forming a complete "optimization-control" closed loop.

A. Design of Dynamic Maintenance Strategy for the Case Library

A static case library struggles to adapt to long-term influent characteristic drift or sudden anomalies. The core idea of the online maintenance strategy designed in this paper is to prudently incorporate new knowledge and eliminate outdated knowledge while ensuring the overall stability of the case library.

(1) Real-time update judgment mechanism based on similarity and dominance relations

1) Similarity retrieval: calculate the operational condition similarity between the new sample and all samples in the case library. If the maximum similarity is below the preset threshold θ, indicating that the current case library lacks highly similar experience, then temporarily store the sample in a cache library for subsequent processing. Similarity calculation continues using formula 5:

$$\text{Sim}_{\max} = \max_{C_i \in \mathcal{L}} \text{Sim}(Z_{\text{new}}, Z_i) \tag{5}$$

If $\text{Sim}_{\max} < \theta$, then $C_{\text{new}} \rightarrow$ Cache Cache; otherwise, proceed to performance competition.

2) Performance competition: if the new sample has the highest similarity with a sample in the library and exceeds the threshold (i.e.$\exists C_j \in \mathcal{L}$, then further compare their performance indicators (EQ, EC). If the new sample dominates the historical sample (i.e. $E_{\text{new}} \prec E_j$), replace the old sample with the new one to achieve iterative upgrading of the case; otherwise, retain the original case.

(2) Batch learning and entry mechanism based on the cache library

The cache library $\mathcal{C} = \{C_1, C_2, \ldots, C_M\}$ accumulates samples of "unfamiliar" operating conditions that cannot be immediately matched. When the number of samples reaches a preset capacity N, batch learning is triggered: the offline case library construction process (K-means++ clustering and NSGA-II screening) is re-executed on the samples in the buffer library. The newly generated Pareto-optimal cases are then merged into the main case library, and the buffer library is cleared.

This mechanism transforms the case library from a static knowledge repository into a living knowledge system capable of incremental learning and selective updates, thereby ensuring the long-term adaptability and robustness of the CSO framework.

B. Implementation of Setpoint Tracking Controller Based on MPC

The setpoint instructions output by the upper-level optimization module must be converted into actual control variables (aeration volume, internal reflux) through a fast, stable lower-level control loop, thereby affecting the process variable (SO_5,

SNO_2). This study adopts Model Predictive Control (MPC) as the lower-level tracking controller, with its structure shown in Figure 4.

(1) Controller role and interface with upper and lower layers The setpoints for dissolved oxygen SO_5 and nitrate nitrogen SNO_2 output by the upper-level CSO module need to be transformed into actual operational variables by the lower-level controller. The input to the MPC is the upper-level setpoint vector $\mathbf{y}_{\text{set}} = (SO_5^{\text{set}}, SNO_2^{\text{set}})$. Its outputs are the control actions applied to the physical equipment: the oxygen transfer coefficient in the fifth zone $K_{La,5}$ for adjusting aeration, and the internal recirculation flow rate Q_{int}. The controlled variables are $\mathbf{y} = (SO_5, SNO_2)$.

To address the nonlinearity and large time delays in the wastewater treatment process, we adopt an Echo State Network (ESN) to establish a data-driven predictive model. In each control cycle, the MPC solves an optimization problem to make the controlled variables track the upper-level setpoints as closely as possible while satisfying the actuator constraints. It then applies the first element of the calculated control sequence to the system, achieving rolling optimization. Simultaneously, we introduce a feedback correction mechanism that utilizes the error between actual measured values and model predictions to correct the model's forecasts online. This compensates for model uncertainties and unknown disturbances, thereby forming a complete closed-loop control system.

V. Simulation Verification and Performance Comparison Analysis

To verify the effectiveness and superiority of the proposed "Case Search Optimization-Based Intelligent Setpoint Method," comprehensive comparative experiments were conducted on the BSM1 international benchmark simulation platform. The experiments are conducted on three levels: first, an introduction to the simulation environment and specific parameter configurations; second, an illustration of the core effects of the case search optimization method; finally, a comprehensive performance comparison with various benchmark strategies to evaluate performance from multiple perspectives.

A. Simulation Platform and Parameter Settings

We conduct all simulation experiments within the BSM1 environment. We run various typical operating conditions (dynamic influent data such as dry weather and rain events) on the platform to collect historical operational data. Each record contains the influent component vector Z, the control setpoints Y, and the performance evaluation E. Applying the methodology from Chapter 3, we use K-means++ to divide the influent characteristics into five typical operating condition clusters and employ NSGA-II to extract Pareto-optimal solutions from each cluster, thereby constructing the initial case library.

The comparison strategies include:

- Fixed setpoint strategy (BSM1 default strategy): The setpoints for SO_5 and SNO_2 are fixed at 2.0 mg/L and 1.0 mg/L, respectively. This is the benchmark operation strategy in the BSM1 report, representing traditional empirical operation.
- Traditional multi-objective evolutionary algorithm (e.g. NSGA-II): In each optimization cycle, NSGA-II is directly invoked online to solve the multi-objective optimization problem under the current conditions to obtain setpoints.
- The method in this paper (CSO): a dynamic setpoint method based on case search optimization.

We evaluate performance using the total energy consumption (EC), the comprehensive effluent quality (EQ), and the compliance rate of key effluent quality parameters.

B. Effect verification of case search optimization (CSO)

This section aims to intuitively demonstrate the core operational features and direct effects of the CSO method.

(1) Dynamic optimization trajectory of setpoints

Figure 5 illustrates the dynamic changes in the SO_5 and SNO_2 setpoints output by the CSO method over multiple consecutive days. Unlike the horizontal lines representing the fixed setpoint strategy, the CSO setpoints adjust dynamically in response to variations in the influent load. This demonstrates that the method can effectively perceive changes in operating conditions and reuse historical optimal experiences for intelligent decision-making.

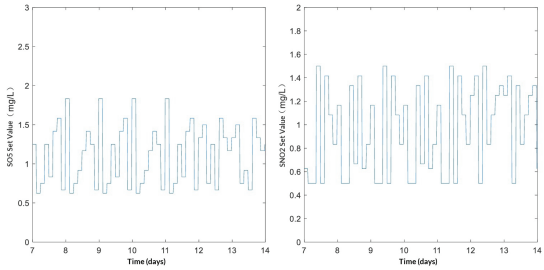


Fig. 5. Optimization results of dissolved oxygen and nitrate nitrogen concentration setpoints in wastewater treatment based on data mining

(2) Effectiveness in ensuring water quality compliance

Under the CSO optimization strategy, the daily average values of all effluent quality parameters remained stably below the discharge standard limits (Table 1). Figure 6 shows the dynamic variations of five effluent quality parameters: $BOD_{5,e}$, COD_e and TSS_e consistently met the standards throughout the entire period. Although $S_{Ntot,e}$ and $S_{NH,e}$ exhibited instantaneous peak values, their daily averages still complied with the assessment standards.

C. Comparative Analysis of Overall Performance

To quantitatively evaluate the comprehensive performance advantages of the CSO method, We compared the CSO method with the fixed setpoint strategy over a complete 14-day operational cycle, with the results shown in Table 2. While ensuring effluent quality meets the discharge standards, the CSO method reduced total energy consumption (EC) by approximately 3.9% compared to the fixed setpoint strategy.

TABLE I
WATER QUALITY INDICATORS BASED ON DATA MINING OPTIMIZATION ALGORITHMS

Water quality indicators	Optimization algorithm based on data mining	Limit value
TSS_e	***13.021***	$< 30mg/L$
$BOD_{5,\mathrm{e}}$	***2.7628***	$< 10mg/L$
COD_e	***48.2658***	$< 100mg/L$
$S_{\mathrm{Ntot,e}}$	***16.3039***	$< 18mg/L$
$S_{\mathrm{NH,e}}$	***2.9555***	$< 4mg/L$

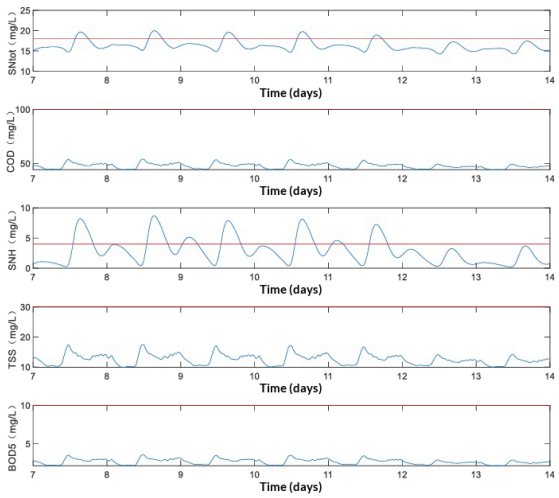


Fig. 6. Changes in Water Quality Parameters at Outlets

This demonstrates that intelligent dynamic optimization can unlock energy-saving potential without compromising effluent quality.

TABLE II
COMPARISON OF WATER QUALITY AND ENERGY CONSUMPTION INDICATORS

Strategy	EQ	EC
BSM1 Default	***6034.5129***	***3936.9527***
Strategy Data	***6167.0983***	***3783.3425***

Compared with online NSGA-II optimization, the two methods achieve similar optimization results. However, CSO demonstrates a significant advantage in computational efficiency: NSGA-II requires a full population iteration at each decision point, leading to long computation times. In contrast, CSO only requires a single case retrieval, resulting in extremely short computation times that meet real-time requirements. Furthermore, CSO decisions are based on historical optimal experiences, providing clear physical meaning and strong interpretability, which makes them easier to integrate and implement within existing control systems.

VI. SUMMARY AND OUTLOOK

This paper addresses the challenge of multi-objective dynamic optimization in wastewater treatment processes by proposing an intelligent setpoint method based on case search optimization. It establishes a new paradigm of "offline case library construction - online search decision-making." By mining Pareto-optimal operational experiences from historical data to form a knowledge base, it transforms complex online optimization into efficient case matching and integrates this with a closed-loop, lower-level model predictive control system. Simulation validation on the BSM1 platform demonstrates that, while ensuring effluent quality meets discharge standards, this method reduces operational energy consumption by approximately 3.9% compared to traditional fixed setpoint strategies, effectively reconciling the multi-objective conflict between water quality and energy consumption.

Future research can delve deeper in three main areas. First, enhancing method safety by incorporating the suppression of instantaneous effluent quality peaks into the optimization constraints to improve the algorithm's robustness under extreme operating conditions. Second, advancing the method from simulation validation to practical engineering applications, addressing challenges related to real data quality, online adaptive learning, and engineering integration. Third, exploring integration with technologies such as digital twins and deep reinforcement learning to expand towards the coordinated optimization of multiple treatment units across the entire plant, achieving system-level global energy efficiency improvements.

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