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Mechanism-Driven Modelling and Plant-Specific Calibration of a Full-Process Wastewater Treatment Model Adapted to Chinese Influent Characteristics

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Abstract: Optimisation of wastewater treatment processes relies on mechanistic models that accurately describe biochemical reactions. However, the parameters of the internationally dominant Activated Sludge Model (ASM) family are calibrated against European and North American influent concentrations, and their direct application to Chinese plants—characterised by low-strength influent, combined-sewer infiltration and frequent industrial shocks—produces systematic distortion, while their elaborate component fractionation is difficult to measure in practice. This paper proposes a full-process mechanistic model, termed Helix-Core, adapted to Chinese influent characteristics, together with a plant-specific calibration method. Built upon the activated sludge mechanism, the model assembles 32 governing equations along the process chain covering six process units, namely the primary clarifier, anaerobic tank, anoxic tank, aerobic tank, secondary clarifier and filter. A five-step calibration pipeline (process parsing, data correction, parameter calibration, measured back-testing, online service) is proposed, which requires only routinely monitored indicators. The adjoint sensitivity method is introduced to make the whole equation system differentiable, turning parameter inversion from manual trial-and-error into gradient-driven optimisation, and a Fourier neural operator is trained as a millisecond-level surrogate of the model. Validation on more than 31 million operating records from 27 wastewater treatment plants shows that the relative deviations of the simulated effluent COD, ammonia nitrogen, total nitrogen and total phosphorus are all below 10%, providing a trustworthy high-fidelity evaluation environment for process optimisation algorithms.

1. Introduction

Refined operation of wastewater treatment plants (WWTPs) depends on the quantitative modelling of biochemical processes. The ASM1/ASM2d/ASM3 models issued by the International Water Association established the classical paradigm of organising components and reaction processes in

matrix form [1], and the benchmark simulation platforms BSM1/BSM2 further standardised test scenarios and evaluation protocols [2]. Nevertheless, three limitations hinder their application in China. First, the kinetic and stoichiometric parameters are calibrated against European and North American influent concentrations, whereas Chinese plants commonly face low-strength influent, rain-sewage mixing and industrial shocks, so direct adoption leads to systematic distortion. Second, the models rely on elaborate component fractionation that most domestic plants cannot measure. Third, commercial simulators (GPS-X, WEST, BioWin) are closed-source and run offline, which prevents them from entering control loops. Purely data-driven models, on the other hand, lack physical conservation constraints and fail to extrapolate under shock loads outside the training distribution [3], so neither plant engineers nor regulators trust them with control authority.

To address these problems, this paper develops the self-built mechanistic model Helix-Core and an engineering-oriented calibration method. The main contributions are as follows:

1) An equation system and parameter set reconstructed for Chinese influent characteristics, forming a full-process model of 32 governing equations covering six process units along the process chain;

2) A five-step calibration method that only requires routinely monitored indicators, compressing the modelling cycle from months to a standardised and replicable pipeline;

3) The introduction of the adjoint sensitivity method, which makes the entire model differentiable and upgrades parameter inversion from a manual craft into an algorithm, thereby supporting online evolution applications.

2. Construction of the Helix-Core Mechanistic Model

2.1 Full-Process Equation System

Helix-Core organises the whole plant as a network of reactors connected in series along the process chain, where the effluent of one unit is the influent of the next. For the k-th unit, the component concentration vector c_k satisfies the mass-conservation equation

$$\frac{dc_k}{dt} = \frac{Q_k}{V_k}(c_{k-1} - c_k) + r_k(c_k, \theta) \tag{1}$$

where Q_k is the influent flow rate of the unit, V_k is the effective volume, r_k is the biochemical reaction rate vector, and θ denotes the set of kinetic and stoichiometric parameters. The growth rate in the aerobic unit adopts a Monod-type dual-substrate limitation expression

$$\mu(S, S_O) = \mu_{max} \cdot \frac{S}{K_S + S} \cdot \frac{S_O}{K_O + S_O} \tag{2}$$

and the denitrification rate in the anoxic unit introduces nitrate and readily biodegradable carbon source limitations together with the anoxic correction factor η_g:

$$r_{DEN} = \mu_{max} \cdot \eta_g \cdot \frac{S_S}{K_S + S_S} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot \frac{K_O}{K_O + S_O} \cdot X_{BH} \tag{3}$$

Oxygen supply by aeration is described by the oxygen-transfer equation, in which the volumetric oxygen transfer coefficient K_La follows a power law of the air flow rate G_s, forming the physical basis for aeration optimisation:

$$\frac{dS_O}{dt} = K_{La}(G_s)(S_O^* - S_O) - OUR, K_{La} = a \cdot G^b \tag{4}$$

where the exponent b of G_s is written as a superscript. The distribution of the 32 governing equations along the process chain is listed in Table 1; the effluent component vector of each unit directly serves as the influent boundary condition of the next unit.

Table 1 Distribution of the 32 governing equations

Process unit	Equations	Modelled processes
Primary clarifier	3	Hydraulic loading and primary removal
Anaerobic tank	7	Phosphorus release and sludge loading
Anoxic tank	3	Denitrification
Aerobic tank	8	Nitrification and carbon oxidation (model core)
Secondary clarifier	6	Sludge-water separation (layered settling flux)
Filter	5	Advanced treatment polishing
Total	32	Full-process coupled system

2.2 Five-Step Calibration Method

Parameter calibration is formulated as a nonlinear least-squares problem that minimises the deviation between simulated and measured effluent series:

$$\theta^* = argmin_\theta \sum_{i=1}^{N} \sum_{j=1}^{J} w_j (\hat{y}_j(t_i;\ \theta) - y_j(t_i))^2 \tag{5}$$

where ŷ_j and y_j are the simulated and measured series of the j-th effluent indicator (COD, NH3-N, TN, TP) respectively, and w_j is the indicator weight. The five-step calibration method engineeringises this problem into: (i) process parsing, which determines the unit division and equation topology from process flow diagrams and design parameters; (ii) data correction, which removes sensor drift and abnormal records using mass-conservation redundancy among monitoring fields; (iii) parameter calibration, which solves Eq. (5) to obtain a plant-specific parameter set; (iv) measured back-testing on a held-out period, where the model is not released until the deviations reach the threshold; (v) online service, where the model is deployed as a service and runs on a 5-minute cycle. The key innovation is that the data required by calibration are restricted to routinely monitored indicators, avoiding the special component fractionation required by ASM-type models.

2.3 Adjoint Sensitivity and Operator-Based Acceleration

Conventional calibration depends on expert trial-and-error for each plant. We introduce the adjoint sensitivity method so that all 32 equations become differentiable. For the objective functional L(θ) defined as the time integral of a loss over the state trajectory, the adjoint variable λ(t) is introduced and the gradient of the objective with respect to the parameters is obtained as

$$\frac{\partial L}{\partial \theta} = -\lambda^T \frac{\partial F}{\partial \theta} \tag{6}$$

where F is the residual of the state equations. One forward solve of the state equations plus one backward substitution of the adjoint equations yields the gradients with respect to all parameters, with a cost essentially independent of the parameter dimension; calibration thereby changes from per-plant manual tuning into gradient-driven optimisation [4].

To support the rapid evaluation of massive candidate strategies, a Fourier neural operator (FNO) is trained to learn the solution operator of Helix-Core in the spectral domain: the input field is truncated to m modes by the Fourier transform, a linear transform is applied in the spectral domain, and the inverse transform returns to the physical domain. The layer-wise iteration reads

$$v_{l+1}(x) = \sigma(W \cdot v_l(x) + \mathcal{F}^{-1}(R_\varphi \cdot \mathcal{F}(v_l))(x)) \tag{7}$$

The trained operator performs millisecond-level inference and acts as an operator-level student of the mechanistic model for fast screening, while its output must finally be re-verified inside the mechanistic boundary [5]. In addition, the Koopman operator lifts the nonlinear biochemical

dynamics into an approximately linear system z_{t+1} = K z_t through observable functions, providing a globally linearised representation for model predictive control [6].

3. Experiments

3.1 Datasets and Evaluation Metrics

The experimental data come from 27 WWTPs covering seven regions of China, whose statistics are summarised in Table 2. The evaluation metric is the relative deviation of simulated effluent indicators, $\delta_j = |\hat{y}_j - y_j| / y_j \times 100\%$.

Table 2 Statistics of the data foundation

Item	Value
Number of plants	27 (21 overloaded)
Dominant process	AAO and its variants
Time span	approx. 10.9 years (2015.05–2026.03)
Sampling interval / fields	5 min / 20 fields
Total operating records	approx. 31 million
Cumulative treated volume	approx. 16.6 billion m ³

3.2 Experimental Setup

Each plant is modelled independently following the five-step calibration method: twelve consecutive months of data form the training segment for solving the parameter-inversion problem of Eq. (5), with the optimiser being a batch gradient method and the initial values taken as the midpoints of the ASM-recommended parameter ranges; the following three months form the back-testing segment, with a release threshold of $\delta_j < 10\%$. The adjoint equations are solved by implicit backward integration on the same time grid as the forward solve.

3.3 Experimental Results

By April 2026, all 27 plants had completed calibration and measured back-testing, and the simulated deviations of key effluent indicators all satisfied the release threshold. Typical results are shown in Table 3, and the calibration efficiency and inference performance are compared in Table 4.

Table 3 Measured back-testing results of typical plants (relative deviation, %)

Indicator	Plant A (100,000 m ³/d)	Plant B (200,000 m ³/d)	Plant C (50,000 m ³/d)	Threshold
COD	6.8	7.5	8.1	<10
NH3-N	7.2	6.4	8.6	<10
TN	8.3	8.9	9.2	<10
TP	7.9	8.2	8.8	<10

Table 4 Comparison of calibration and inference performance

Item	Manual trial-and-error	Adjoint gradient inversion
Calibration cycle per plant	Several months	Standardised five-step pipeline (hour-level gradient solve)
Gradient computation	Per-parameter perturbation, O(n) forward solves	1 forward solve + 1 adjoint backward substitution
Inference latency	Mechanistic forward solve (second level)	FNO operator (millisecond level)

The calibrated models were further used in optimisation verification: Helix-Core-based process optimisation achieved about 10% energy saving in a series-CSTR conceptual experiment; intelligent dosing combining Helix-Core with AI parameter search achieved about 18%–20% chemical saving, while the effluent orthophosphate remained stably below 0.2 mg/L; and, together with published calibration practice of stable terminal dissolved-oxygen control in biochemical tanks, blower energy consumption decreased by 18%–25% with an ammonia nitrogen compliance rate no lower than 99.5%. These results verify the engineering effectiveness of the mechanistic model in its three usages of prediction, optimisation and control.

4. Conclusion

This paper has proposed the full-process mechanistic model Helix-Core and its five-step calibration method, adapted to Chinese influent characteristics. The model couples six process units through 32 governing equations along the process chain, requires only routinely monitored indicators for plant-specific calibration, and is made fully differentiable by the adjoint sensitivity method, which automates parameter inversion; a Fourier neural operator provides a millisecond-level inference surrogate. Validation on 27 WWTPs shows that the relative deviations of key effluent indicators are below 10%, qualifying the model as a high-fidelity and trustworthy evaluation environment for process optimisation algorithms. Future work will proceed along cross-plant parameter transfer and microbiome-sequencing calibration of biological state variables.

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