

Process Simulation and Reverse Optimization of Modified Biochar Adsorption of Salt and Minerals in Water: Prediction Model of Adsorption Efficiency Based on BP Neural Network

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Research Article

Keywords: Modified Biochar, Salt Adsorption, BP Neural Network, Reverse Optimization, Particle Swarm Optimization, Polyionic System

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1 **Process Simulation and Reverse Optimization of Modified Biochar Adsorption** 2 **of Salt and Minerals in Water: Prediction Model of Adsorption Efficiency** 3 **Based on BP Neural Network**

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8 **Abstract**

9 Removing salts and mineral ions from high-salinity surface water, groundwater, and unconventional resources is a
10 key challenge. Modified biochar offers adjustable structure and low cost, yet studies rarely address synergistic
11 adsorption of multiple ions or provide a complete chain from modification to performance prediction and reverse
12 optimization. Here, corn straw biochar was prepared unmodified (BC), sulfuric acid-modified (SBC), and
13 iron-modified (FeBC). Batch adsorption experiments used Heze farmland drainage to link material structure with
14 adsorption performance. A BP neural network model was built with adsorbent type, dosage, pH, temperature, and
15 reaction time as inputs and adsorption efficiency as output. Hidden layer neurons were optimized to improve accuracy.
16 Particle swarm optimization (PSO) enabled reverse parameter optimization. FeBC gave the best performance due to
17 high specific surface area (315.2 m²/g), oxygen-containing functional groups (3.18 mmol/g), and iron loading
18 (15.6 mg/g). The BP model achieved R² of 0.935 (training) and 0.930 (validation), with prediction relative error below
19 1.2%. Reverse optimization identified optimal FeBC conditions: dosage 0.8 g/L, pH 7.5, 35 °C, 180 min, yielding
20 actual adsorption efficiency of 91.8% and a cost-benefit ratio of 57.4%/yuan. This work provides both an efficient
21 adsorbent and a data-driven optimization method for water salinity removal, with demonstrated engineering feasibility
22 and economic value.

23 **Keywords:** Modified Biochar, Salt Adsorption, BP Neural Network, Reverse Optimization, Particle Swarm
24 Optimization, Polyionic System

25 **1 Introduction**

26 With the increasing demand for the treatment and reuse of high-salinity surface water, groundwater, and
27 unconventional water resources, the efficient removal of salts and mineral ions has become an important issue in
28 water-environment remediation and resource utilization. Modified biochar has attracted attention as an adsorbent
29 because of its abundant surface functional groups, adjustable pore structure, and relatively controllable preparation
30 cost, especially for the removal of inorganic pollutants under complex water-quality conditions [1]. Reviews on
31 engineered biochar have further indicated that modification strategies can enhance interfacial reactivity and selective
32 adsorption capacity, thereby providing a material-design basis for specific ion-removal systems [2]. Meanwhile,
33 studies on water and wastewater treatment have shown that biochar has gradually developed from a single adsorption
34 material into a multifunctional environmental material with adsorption, carrier, and process-enhancement functions;

however, its removal mechanism for salts and mineral ions still requires further clarification [3]. In addition, systematic reviews of anion removal from water demonstrate that adsorption performance depends not only on the intrinsic properties of the material, but also on solution chemistry and competitive ion conditions, suggesting that multi-factor coupling in practical water matrices should be quantitatively examined [4].

In recent years, increasing attention has been paid to the relationship between the structure of engineered biochar and its adsorption performance in realistic aqueous environments. Existing studies have shown that the specific surface area, surface charge, and functional-group distribution of biochar are jointly affected by modification strategy, biomass source, and pyrolysis conditions, and these factors strongly influence adsorption pathways and environmental applicability for different inorganic components [5]. From the perspective of broader material application, biochar is no longer limited to carbon storage; its functions in adsorption separation, ion interception, and resource recovery provide theoretical support for the development of customized adsorbents for salinity control [6]. At the same time, machine-learning studies on the prediction of biochar yield, nitrogen content, and specific surface area have shown that key biochar properties often exhibit nonlinear responses to preparation parameters, making it difficult for empirical trial-and-error approaches to fully reveal the mapping between material preparation and adsorption performance [7]. Modeling studies of adsorption capacity have also indicated that solute type, material characteristics, and operating conditions interact in complex ways, and that robust prediction models can improve experimental efficiency and support the transferability of adsorption results [8].

For salt and mineral-ion removal, existing studies have provided useful but still incomplete evidence. Research on agricultural-waste biochar for sodium-ion adsorption has shown that biomass source can significantly affect adsorption-isotherm characteristics and ion-binding modes, indicating that salt-removal performance is both raw-material dependent and structure sensitive [9]. Machine-learning-assisted studies have also been used to predict the specific surface area and total pore volume of biochar, offering a quantitative tool for interpreting differences in adsorption performance from the perspective of material structure [10]. In specific pollutant systems, studies on Fe-modified biochar have demonstrated that machine-learning models can identify key control variables and improve the prediction accuracy of complex adsorption processes [11]. Moreover, prediction and optimization studies on the adsorption capacity of emerging pollutants have suggested that data-driven methods can be integrated into adsorption-system design to improve model generalization and provide a basis for subsequent parameter optimization and process design [12]. Nevertheless, many of these studies focus on single pollutants, single material properties, or model prediction alone, while fewer studies connect material modification, real multi-ion drainage-water adsorption, model validation, and parameter optimization within the same experimental framework.

However, current research is still mainly concentrated on phosphorus, heavy metals, or organic pollutants, whereas the adsorption of salinity-related mineral ions in realistic multi-ion water matrices has received comparatively limited attention. In particular, there remains a lack of studies that examine the complete chain of “modified biochar preparation–multi-ion adsorption experiment–performance prediction–inverse parameter optimization” under practical drainage-water conditions [13]. Previous work on sodium-ion removal by acid-modified biochar has confirmed that chemical modification can improve ion-removal performance, but the variation pattern and predictability of adsorption efficiency under different operating conditions remain insufficiently explained [14]. Reviews of machine learning in biochar research have also pointed out that data-driven methods have advantages in performance prediction, parameter screening, and mechanism identification, but their integration with adsorption-process optimization in water-treatment applications still needs to be strengthened [15]. Based on these gaps, this study proposes the following scientific hypothesis: iron modification can enhance the adsorption performance of corn-straw biochar for salinity-related mineral ions by improving surface activity and ion-binding sites, while a BP neural-network model combined with

PSO can identify a feasible operating window with improved adsorption efficiency and cost-effectiveness. Therefore, this study focuses on modified biochar adsorption of salt and mineral ions in Heze agricultural drainage water, constructs a BP neural-network prediction model using adsorbent type, dosage, pH, temperature, and reaction time as input variables, and applies PSO-based inverse optimization to identify key process parameters (Figure. 1). The aim is not to claim the novelty of BP or PSO alone, but to evaluate whether their integration with experimentally prepared modified biochar can provide a practical and data-supported optimization framework for salinity-related ion removal in real drainage-water treatment.

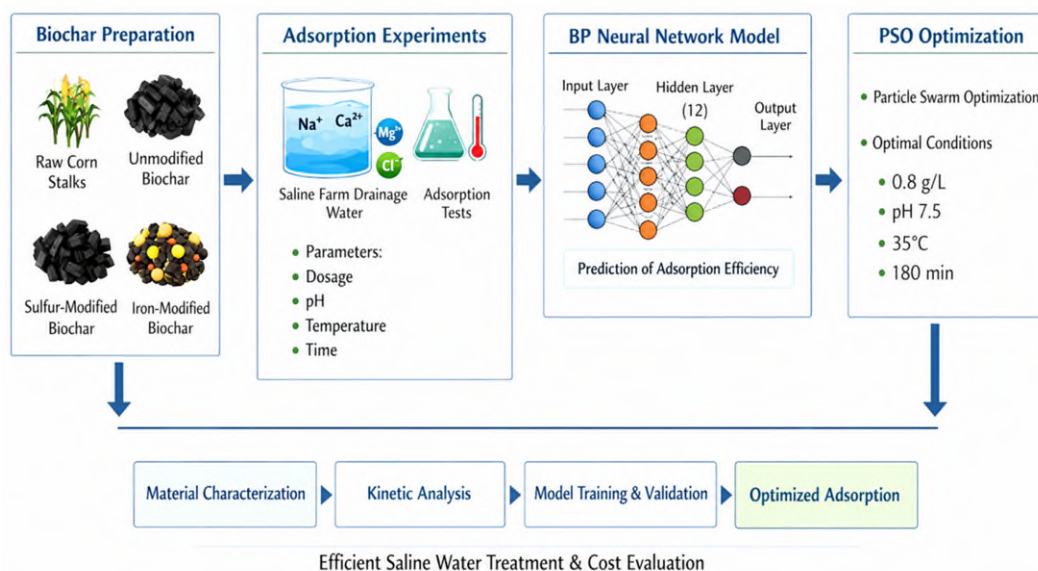


Figure 1. research framework flow chart

2 Material preparation

2.1 Experimental materials

The experimental materials used in this study included biomass feedstock, chemical reagents, and laboratory instruments. Corn stalks (*Zea mays* L.) were used as the biomass feedstock and were collected from farmland in Heze City, Shandong Province, China. To reduce the influence of raw-material heterogeneity, all corn stalks were collected from the same batch. After natural air drying for 7 days, stones, weeds, and other visible impurities were manually removed. The cleaned stalks were then crushed into 2–5 mm particles using an FW100 hammer crusher (Tianjin Taisite Instrument Co., Ltd., China) and stored in sealed polyethylene bags before further treatment.

The chemical reagents used in the experiment included concentrated sulfuric acid (H_2SO_4 , analytical grade, 98%), ferric chloride hexahydrate ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, analytical grade), hydrochloric acid (HCl , analytical grade), sodium hydroxide (NaOH , analytical grade), and silver nitrate (AgNO_3 , analytical grade). All reagents were purchased from Sinopharm Chemical Reagent Co., Ltd., China, and were used without further purification. Deionized water with a resistivity of $18.2 \text{ M}\Omega \cdot \text{cm}$ was used throughout all preparation, washing, and adsorption experiments.

The main instruments used in this study included an SX2-4-10 muffle furnace (Shanghai Yiheng Scientific Instrument Co., Ltd., China), an FA2004 electronic analytical balance (Shanghai Precision Scientific Instrument Co., Ltd., China), a KQ-500DE ultrasonic cleaner (Kunshan Ultrasonic Instrument Co., Ltd., China), a DZF-6050 vacuum drying oven (Shanghai Boxun Industrial Co., Ltd., China), a PHS-3C pH meter (Shanghai Leici Instrument Factory, China), and an XSB-88 vibrating screen machine (Wuhan Geological Instrument Factory, China).

104 2.2 Preparation of modified biochar

105 In this study, pristine biochar (BC), sulfuric-acid-modified biochar (SBC), and iron-modified biochar (FeBC)
106 were prepared from corn stalks. The preparation procedure was designed to keep the biomass source and basic
107 pyrolysis conditions consistent among the three materials, so that the effect of different modification treatments could
108 be compared.

109 For BC preparation, the crushed corn stalk particles were placed in a covered ceramic crucible and pyrolyzed in a
110 muffle furnace under a nitrogen atmosphere. The nitrogen flow rate was maintained at 50 mL/min. The furnace
111 temperature was increased to 500 °C at a heating rate of 5 °C/min and then held for 2 h. After the furnace cooled
112 naturally to room temperature, the obtained biochar was washed with deionized water until the filtrate reached
113 near-neutral pH values of 6.8–7.2. The washed biochar was then dried in a vacuum drying oven at 60 °C for 12 h,
114 ground, and passed through a 100-mesh sieve to obtain BC.

115 For SBC preparation, 10 g of BC was added to 100 mL of 1 mol/L H₂SO₄ solution. The mixture was treated
116 ultrasonically for 30 min to improve the contact between the acid solution and biochar particles, and then stirred in a
117 water bath at 80 °C for 2 h. After the reaction, the solid product was separated by filtration and repeatedly washed with
118 deionized water until the filtrate became neutral. The washed solid was dried under vacuum at 60 °C for 12 h, ground,
119 and passed through a 100-mesh sieve to obtain SBC.

120 For FeBC preparation, 10 g of BC was added to 100 mL of 0.5 mol/L FeCl₃ solution. The pH of the suspension
121 was adjusted to 5.0 using 0.1 mol/L HCl or NaOH, and the mixture was stirred in a water bath at 60 °C for 4 h. After
122 filtration, the solid was washed with deionized water until no Cl⁻ was detected in the filtrate, as verified using 0.1
123 mol/L AgNO₃ solution. The wet solid was dried at 60 °C for 12 h and then calcined in a muffle furnace under a
124 nitrogen atmosphere at 300 °C for 1 h. After cooling, the product was ground and passed through a 100-mesh sieve to
125 obtain FeBC.

126 This preparation procedure provided three biochar materials with different modification treatments under
127 comparable raw-material and pretreatment conditions. BC was used as the pristine control, SBC was used to examine
128 the effect of acid modification, and FeBC was used to examine the effect of iron modification. The prepared materials
129 were subsequently characterized and used in adsorption experiments with Heze agricultural drainage water.

130 3 Research experiment and model design

131 3.1 Adsorption test

132 To evaluate the adsorption performance of pristine biochar (BC), sulfuric-acid-modified biochar (SBC), and
133 iron-modified biochar (FeBC) under a realistic water matrix, agricultural drainage water from Mudan District, Heze
134 City, Shandong Province, China, was used as the experimental water sample. The sampling location was
135 approximately 35°15'N, 115°47'E. Before the adsorption experiments, the collected water sample was filtered through
136 a 0.45 µm microporous membrane to remove suspended particles. The main ion concentrations of the pretreated water
137 sample were Na⁺ 132 ± 6 mg/L, Ca²⁺ 75 ± 4 mg/L, Mg²⁺ 38 ± 2 mg/L, and Cl⁻ 185 ± 8 mg/L, with an initial pH of 7.2
138 ± 0.3. In this study, Na⁺, Ca²⁺, and Mg²⁺ were selected as the main target cations for adsorption evaluation, while Cl⁻
139 was recorded as a background ion reflecting the salinity characteristics of the drainage water.

140 Batch adsorption experiments were conducted in 250 mL conical flasks. For each experiment, 50 mL of the
141 pretreated water sample was added to the flask, followed by a predetermined amount of BC, SBC, or FeBC. The

adsorbent dosage was set at 0.1, 0.2, 0.5, 1.0, and 1.5 g/L to examine the influence of dosage on adsorption performance. The pH of the water sample was adjusted to 3.0, 5.0, 7.0, 9.0, and 10.0 using 0.1 mol/L HCl or NaOH. The reaction temperature was controlled at 25, 30, 35, 40, and 45 °C using a thermostatic oscillator. The reaction time was set at 0, 15, 30, 60, 120, and 240 min to describe the adsorption process over time.

At each predetermined time point, the suspension was sampled and filtered through a 0.22 µm membrane. The concentrations of Na⁺, Ca²⁺, and Mg²⁺ in the filtrate were determined using ion chromatography (Dionex ICS-2100). The adsorption capacity and ion-specific removal efficiency were calculated separately for each target ion. To avoid ambiguity in the model output, the adsorption efficiency used in the BP neural-network model was defined as the arithmetic mean of the removal efficiencies of Na⁺, Ca²⁺, and Mg²⁺, unless otherwise specified. Therefore, the model output represented the overall removal performance of the target cations in the tested agricultural drainage-water matrix, rather than the removal efficiency of a single ion or a mechanistic index of ion competition(Figure 2).

All adsorption experiments were performed in triplicate, and the average value was used for subsequent analysis. The relative standard deviation was controlled within 5%. Because this experimental design used a real multi-ion water matrix without separate single-ion and binary-ion control systems, the results were interpreted as simultaneous adsorption performance under practical drainage-water conditions.

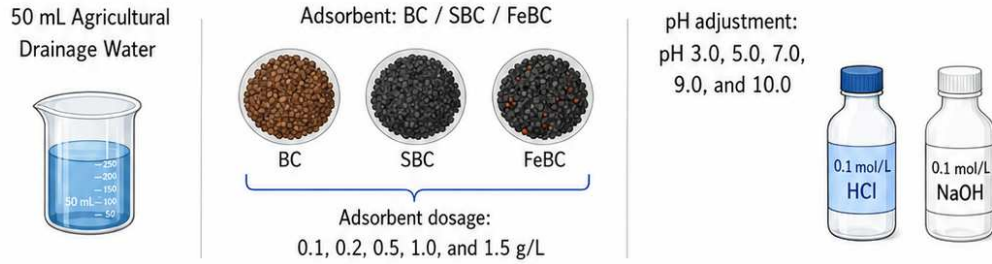
The adsorption capacity (q) is calculated by the following formula:

$$q = \frac{(C_0 - C_t) \times V}{m} \quad (1)$$

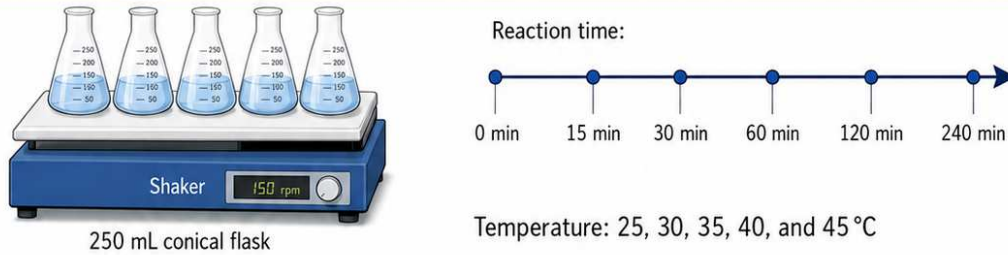
As shown in Formula 1, where: q : adsorption capacity of the adsorbent for the target ion (unit: mg/g); C_0 : initial concentration of target ion in water sample (unit: mg/l); C_t : concentration of target ion in water sample at reaction time t (unit: mg/l); V : water sample volume (unit: l); m : dosage of adsorbent (unit: G).

To ensure the reliability of the data, each group of experiments was repeated three times in parallel, and the average value was taken as the final result, and the relative standard deviation (RSD) was controlled within the range of $\leq 5\%$.

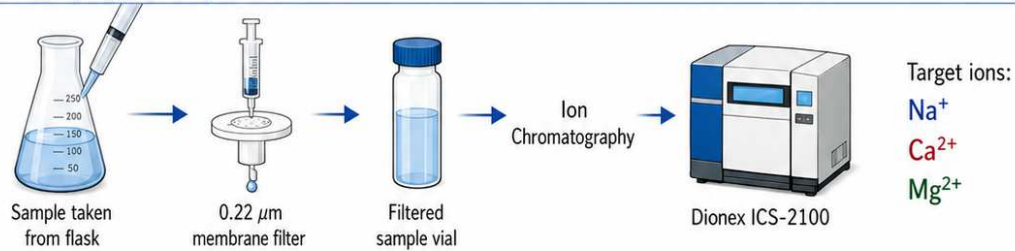
1. Variable Setup



2. Incubation Conditions



3. Sampling & Analysis



4. Representative Ion Chromatogram

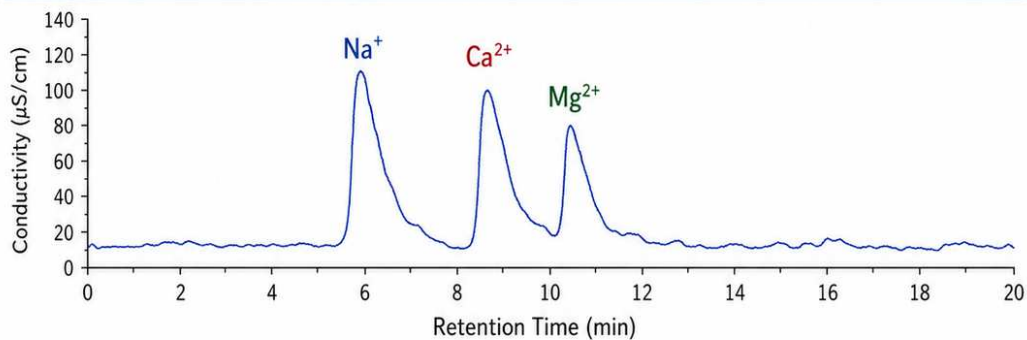


Figure 2. flow chart of batch adsorption experiment

3.2 Construction of BP neural network model

The adsorption of salt-related mineral ions by modified biochar is affected by both material properties and operating conditions. In this study, adsorption efficiency was influenced by the pore structure of the adsorbent, surface functional groups, possible active sites, solution pH, ion concentration, reaction temperature, and contact time [16]. Previous studies have shown that adsorption responses in biochar systems are often nonlinear, because solute characteristics, material structure, and environmental conditions may interact during the adsorption process [17]. Under such conditions, simple linear fitting may be insufficient to describe the relationship between experimental variables and adsorption performance. Machine-learning methods can provide a useful supplementary tool for

identifying nonlinear patterns and key control factors in environmental-material systems [18]. Among these methods, neural-network models have been widely used for predicting adsorption capacity, material properties, and process responses because of their nonlinear approximation ability [19]. In addition, the structured use of experimental variables in prediction models can help reduce empirical trial-and-error work and provide a basis for subsequent process optimization [20].

Based on this consideration, a BP neural-network model was used to predict the adsorption efficiency of modified biochar in the tested agricultural drainage-water matrix [21] (Figure. 3). The input variables included adsorbent type, adsorbent dosage, solution pH, reaction temperature, and reaction time. The adsorbent type was encoded as a categorical variable to distinguish BC, SBC, and FeBC, while the other four variables represented controllable operating conditions. The output variable was adsorption efficiency, denoted as η . To avoid ambiguity, η was defined as the arithmetic mean of the removal efficiencies of the target cations Na^+ , Ca^{2+} , and Mg^{2+} under the same experimental condition. Therefore, η represented the overall cation-removal performance in the real multi-ion drainage-water matrix, rather than the removal efficiency of a single ion. The material characterization results, including specific surface area, pore structure, oxygen-containing functional groups, zeta potential, and iron loading, were used to explain differences among BC, SBC, and FeBC. However, because only three material categories were prepared, these characterization indicators were not directly used as independent model inputs in the main BP model, in order to avoid unstable fitting caused by limited material-category samples [22].

Considering the limited size of the dataset, the model was designed and evaluated with attention to overfitting risk. The 216 valid experimental records were divided into training, validation, and independent test subsets. The training subset was used for parameter learning, the validation subset was used for model selection and hidden-neuron optimization, and the test subset was retained for the final evaluation of predictive performance. In addition, k-fold cross-validation was used during model selection to compare different numbers of hidden-layer neurons and reduce the dependence of the result on a single data split [23]. To further control overfitting, the training process monitored the validation loss, and the final model was selected according to both prediction accuracy and the gap between training and validation performance. Model performance was evaluated using R^2 , MAE, and RMSE, rather than relying only on a single validation-set R^2 value [24].

The BP model was used as the main prediction model because it can describe nonlinear relationships between adsorption conditions and removal performance. However, the purpose of using BP was not to claim methodological novelty of the neural-network algorithm itself. Instead, it was used to build a data-supported link between experimentally prepared modified biochar, adsorption conditions, and process optimization. To examine whether the BP model provided a reasonable prediction advantage, its performance should be compared with benchmark models such as linear regression, polynomial regression, support vector regression, random forest, and gradient-boosting models. Only when the BP model shows stable performance on the independent test set and performs competitively against these benchmark methods can it be used as the prediction basis for the subsequent PSO-driven inverse optimization [25].

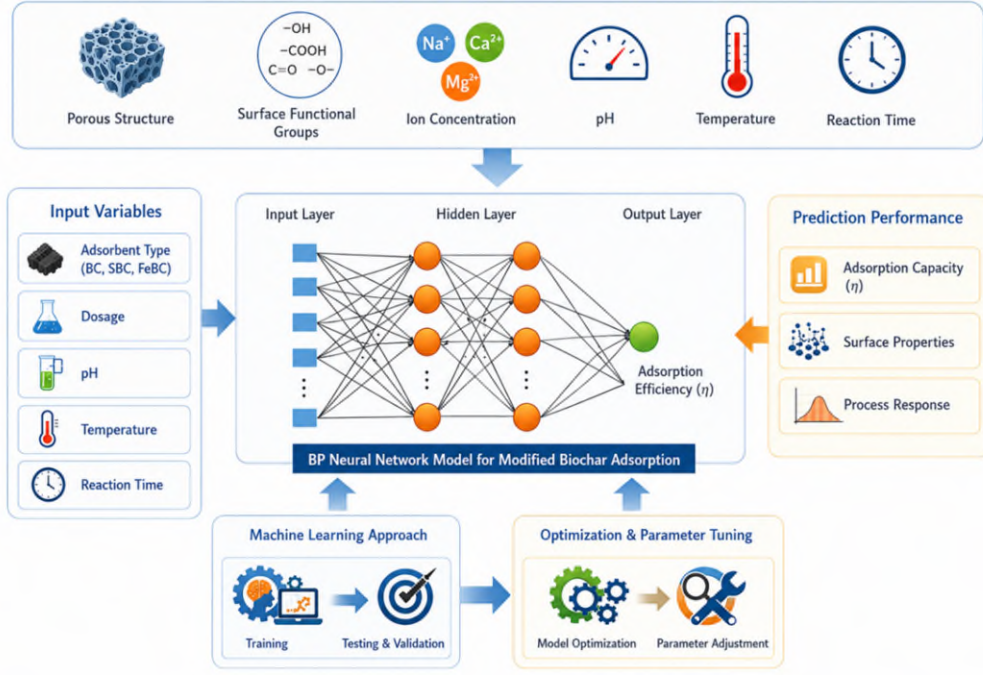


Figure 3. BP neural network model and biochar adsorption

Based on 216 valid experimental records obtained from the adsorption experiments, a three-layer BP neural network with an input layer, one hidden layer, and an output layer was constructed to predict the adsorption efficiency of modified biochar. The input variables included adsorbent type, dosage, solution pH, reaction temperature, and reaction time. The adsorbent type was used to distinguish BC, SBC, and FeBC, while the other variables represented controllable operating conditions. The output variable was adsorption efficiency, denoted as η (%), which was defined as the arithmetic mean removal efficiency of Na^+ , Ca^{2+} , and Mg^{2+} under the same experimental condition. To reduce overfitting risk, the dataset was divided into training, validation, and independent test subsets. Five-fold cross-validation was used to optimize the number of hidden-layer neurons, and 12 neurons were finally selected. Model performance was evaluated using R^2 , MAE, and RMSE.

Hidden layer neuron input calculation:

$$h_i = \sum_{j=1}^5 \omega_{ij} X_j + b_i \quad (2)$$

As shown in formula 2, where: h_i : the input value of the i hidden layer neuron; ω_{ij} : enter the weight coefficient from j layer variable to i hidden layer neuron; X_j : j input layer variable ($j=1 \sim 5$, corresponding to the above five experimental parameters); b_i : the bias term of the i hidden layer neuron; 5: enter the total number of layer variables.

Hidden layer activation function (sigmoid):

$$a_i = \sigma(h_i) = \frac{1}{1 + e^{-h_i}} \quad (3)$$

As shown in Formula 3, where: a_i : the output value of the i hidden layer neuron; σ : sigmoid activation function, which maps input $[0,1]$ to interval to introduce nonlinear relationship; h_i : the input value of the i hidden layer neuron.

Model loss function (mean square error):

$$L = \frac{1}{N} \sum_{k=1}^N (\eta_k^{true} - \eta_k^{pred})^2 \quad (4)$$

As shown in formula 4, where: L : loss value of model training; N : total number of samples; η_k^{true} : actual adsorption efficiency of k sample (measured value); η_k^{pred} : predicted adsorption efficiency of k sample (model output value).

The BP neural network was trained using the Adam optimizer, with a learning rate of 0.001 and a maximum of 1000 epochs. During training, both training loss and validation loss were monitored to examine model convergence and possible overfitting. The final model was not evaluated only by validation-set R^2 ; instead, R^2 , MAE, and RMSE on the independent test subset were used to assess predictive performance. This evaluation strategy provided a more cautious basis for judging whether the model could predict adsorption efficiency beyond the training samples. In this study, the BP model was used as a data-driven tool to link experimental adsorption conditions with subsequent PSO-based parameter optimization, rather than as evidence of methodological novelty alone.

3.3 Reverse optimization

In the adsorption optimization of modified biochar, relying only on forward batch experiments may require many repeated tests and may not efficiently identify suitable combinations of operating parameters [26]. Previous studies have shown that machine-learning-based adsorption prediction can be combined with optimization algorithms to support parameter screening in nonlinear environmental material systems [27]. Compared with single-factor experimental adjustment, inverse optimization can use a target adsorption performance to search for feasible combinations of adsorbent type, dosage, pH, temperature, and reaction time within a defined parameter space [28]. This approach may reduce experimental blindness and provide a more systematic basis for selecting operating conditions [29]. Therefore, in this study, inverse optimization was used as a supplementary step after BP-model prediction, rather than as an independent proof of adsorption mechanism or algorithmic novelty [30].

Based on the trained BP neural-network model, particle swarm optimization (PSO) was introduced to search for the parameter combination that maximized adsorption efficiency [31]. The optimized variables included adsorbent type, dosage, solution pH, reaction temperature, and reaction time, and their ranges were set according to the batch adsorption experiments. In this way, the BP model provided the prediction function, while PSO searched the feasible parameter space using the predicted adsorption efficiency as the fitness value. The purpose of this design was to identify a practical operating window for the tested drainage-water matrix and to provide candidate conditions for subsequent experimental verification. The overall relationship among experimental data, BP prediction, PSO search, and validation is shown in Figure. 4.

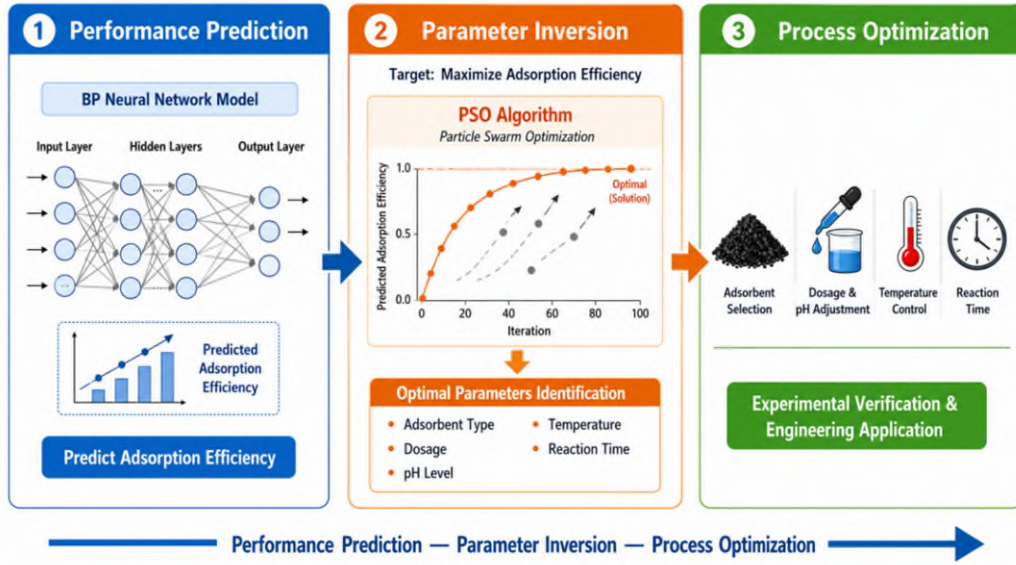


Figure 4. biochar adsorption process optimization framework

Objective function (maximize adsorption efficiency):

$$\max \eta = f(X_1, X_2, X_3, X_4, X_5) \quad (5)$$

As shown in formula 5, where: η : target adsorption efficiency (%; predicted by BP model); f : the mapping function fitted by BP model, the input is 5 process parameters, and the output is adsorption efficiency; X_1 : adsorbent type code (BC=0, SBC=1, FeBC=2, corresponding to the three biochars prepared previously); X_2 : dosage of adsorbent (g/L); X_3 : pH value of solution; X_4 : reaction temperature (°C); X_5 : reaction time (min).

Constraints (parameter feasible region):

$$\begin{cases} X_1 \in \{0,1,2\} \\ 0.1 \leq X_2 \leq 2.0 \\ 3.0 \leq X_3 \leq 10.0 \\ 25 \leq X_4 \leq 45 \\ 30 \leq X_5 \leq 240 \end{cases} \quad (6)$$

As shown in formula 6, the constraint range strictly matches the variable setting of adsorption experiment to ensure that the optimization result is practical and operable. X_1 Limited to three types of biochar; X_2 (dosage) covers the range of 0.1~2.0g/l in the experiment; X_3 (PH) corresponds to the adjustment range of 3.0~10.0 in the experiment; X_4 (temperature) simulate the change of water temperature from 25 °C to 45 °C in Heze area; X_5 (time) covers the reaction period of 30~240Min in the experiment.

PSO speed update formula:

$$v_d^{t+1} = \omega v_d^t + c_1 r_1 (pbest_d - x_d^t) + c_2 r_2 (gbest_d - x_d^t) \quad (7)$$

279 As shown in formula 7, where: v_d^{t+1} : the speed of the d dimension parameter in the $t+1$ iteration; ω :
 280 inertia weight (take 0.7, balance global and local search capabilities); v_d^t : the speed of the d dimension parameter
 281 in the t iteration; c_1, c_2 : learning factor (2.0 for both, guiding particles to move towards individual optimum and
 282 global optimum respectively); r_1, r_2 : random number of interval $[0,1]$; $pbest_d$: the individual optimal value of the
 283 d dimension parameter; x_d^t : the current value of the d dimension parameter in the t iteration; $gbest_d$: the
 284 global optimal value of the d dimension parameter.

285 Figure 5 presents the training-loss trend of the BP neural network and the PSO search process. The gradual
 286 decrease and stabilization of the loss indicate that the model reached numerical convergence during training, while the
 287 PSO curve shows the search tendency toward a higher predicted adsorption efficiency. However, these results were
 288 used only as convergence evidence and were further checked using validation and independent test results. The reverse
 289 optimization step provided candidate operating conditions for experimental verification, and the main procedure is
 290 summarized in Table 1.

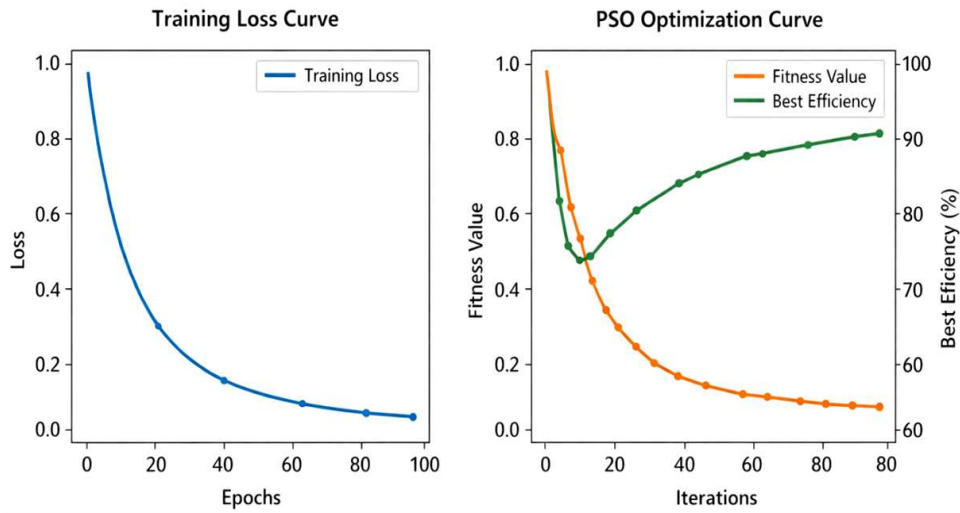


Figure 5. training loss and PSO optimization curve

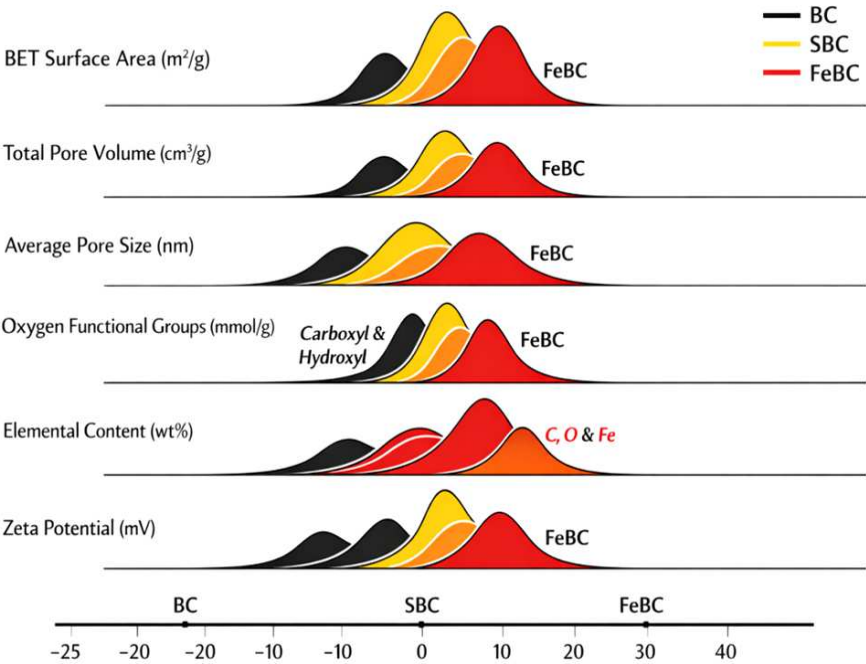
Table 1. core algorithm steps

Step No.	Step Description	Core Code
1	Pretreatment of experimental data (standardized characteristics, coding adsorbent type)	data = preprocess(adsorbent_type, dosage, pH, temp, time, efficiency)
2	Divide training set and verification set (7:3 ratio)	train_data, val_data = split_data(data, test_size=0.3)
3	Build BP neural network model (input 5-D, hidden layer 12 neurons, output 1-D)	model = BPNet(input_dim=5, hidden_dim=12, output_dim=1)
4	Training BP model (minimizing prediction error)	model.train(train_data, epochs=100, lr=0.01)
5	Verify model performance (calculate Mae and R ² indicators)	mae, r2 = model.evaluate(val_data)
6	PSO inverse optimization parameters (prediction based on BP model)	optimal_params = PSO(model, param_bounds)
7	Experimental verification of optimal parameters	actual_efficiency = validate(optimal_params)

294 **4 Results and analysis**

295 **4.1 Characterization results of modified biochar**

296 The physicochemical properties of BC, SBC, and FeBC are summarized in Table 2. Compared with BC and SBC,
297 FeBC showed a larger BET specific surface area of 315.2 m²/g and a higher total pore volume of 0.198 cm³/g. The
298 measured contents of carboxyl, hydroxyl, and carbonyl groups in FeBC were 1.45, 1.08, and 0.65 mmol/g, respectively,
299 which were higher than those of the other two materials. FeBC also showed a more negative zeta potential (-21.2 mV
300 at pH 7) and an iron loading of 15.6 mg/g. These results indicate that iron modification changed the surface and pore
301 characteristics of biochar under the preparation conditions used in this study. Figure 6 provides a visual comparison of
302 these characterization indicators among the three materials. However, these data are used here as supporting
303 characterization results, and the adsorption mechanism should be interpreted together with subsequent adsorption
304 performance and, where available, additional structural evidence.



305

306

Figure 6. comparative analysis of biochar properties

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Table 2. core physical and chemical characterization parameters of three kinds of modified biochar

Characterization Index	BC (UNMODIFIED)	SBC (Sulfuric Acid Modified)	FeBC (Iron Modified)
BET Specific Surface Area (m ² /g)	112.5 ± 4.8	238.7 ± 7.6	315.2 ± 9.3
Total Pore Volume (cm ³ /g)	0.072 ± 0.004	0.141±0.007	0.198 ± 0.011
Average Pore Size (nm)	2.5 ± 0.2	2.2 ± 0.1	2.0 ± 0.1
Oxygen Containing Functional Group (mmol/g): Carboxyl/Hydroxyl/Carbonyl	0.45±0.03/0.30±0.02/0.22±0.01	1.12 ± 0.06/0.87 ± 0.05/0.58 ± 0.03	1.45 ± 0.08/1.08 ± 0.06/0.65 ± 0.04
Element Content (wt%): C/O/Fe	78.2 ± 1.2/18.5 ± 0.8/-	75.6 ± 1.1/21.3 ± 0.9/-	73.8 ± 1.0/23.5 ± 1.0/4.5 ± 0.2
Zeta Potential (mV, pH=7)	-12.3 ± 0.5	-18.6 ± 0.7	-21.2 ± 0.8
Iron Load (mg/g)	-	-	15.6 ± 0.9

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4.2 Adsorption test results

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The effect of adsorbent dosage on ion adsorption capacity is shown in Table 3. As the dosage increased from 0.1 to 1.5 g/L, the unit adsorption capacities of Na⁺ and Ca²⁺ decreased for all three biochars. For example, FeBC showed a decrease in Na⁺ adsorption capacity from 25.3 mg/g at 0.1 g/L to 12.1 mg/g at 1.5 g/L, while SBC showed a decrease in Ca²⁺ adsorption capacity from 11.6 to 6.5 mg/g. This trend may be related to the higher availability of active adsorption sites per unit mass at lower dosage and the partial underutilization or overlap of adsorption sites at higher dosage.

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At the same dosage, FeBC generally showed higher adsorption capacity than SBC and BC in the tested drainage-water matrix. For instance, at 0.5 g/L, the Na⁺ adsorption capacities of FeBC, SBC, and BC were 18.5, 14.8, and 9.2 mg/g, respectively. This difference is consistent with the characterization results in Table 2, but the adsorption mechanism should be interpreted cautiously together with further structural evidence. Figure 7 presents the dosage-dependent changes in Na⁺ and Ca²⁺ adsorption capacity, with corrected ion labels and legends.

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Table 3. effect of different dosage on ion adsorption capacity (mg/g)

Dosage (g/l)	BC-Na ⁺	BC-Ca ²⁺	SBC-Na ⁺	SBC-Ca ²⁺	FeBC-Na ⁺	FeBC-Ca ²⁺
0.1	12.8 ± 0.5	7.2 ± 0.3	20.5 ± 0.8	11.6±0.5	25.3 ± 1.0	14.2 ± 0.6
0.2	11.5 ± 0.4	6.8 ± 0.3	18.2 ± 0.7	10.8 ± 0.4	22.6±0.9	13.1 ± 0.5
0.5	9.2 ± 0.3	5.6 ± 0.2	14.8 ± 0.6	9.1 ± 0.3	18.5 ± 0.7	11.2±0.4
1.0	7.6 ± 0.2	4.8 ± 0.2	12.3 ± 0.5	7.8 ± 0.3	15.2 ± 0.6	9.5 ± 0.3
1.5	6.3 ± 0.2	4.1 ± 0.1	10.1 ± 0.4	6.5 ± 0.2	12.1 ± 0.5	8.2 ± 0.3

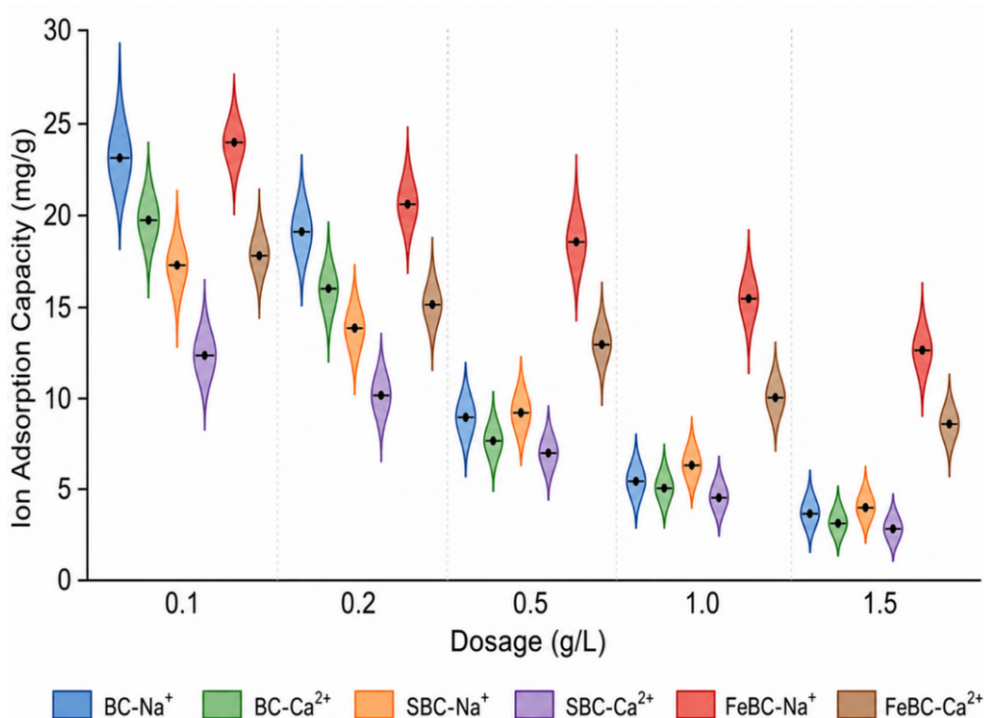


Figure 7. effect of different material doses on ion adsorption capacity

The effect of solution pH on adsorption efficiency is shown in Table 4. For all three biochars, the adsorption efficiency first increased and then decreased as pH changed from 3.0 to 10.0, with the highest values generally observed near pH 7.0. At pH 7.0, the Na^+ removal efficiencies of FeBC, SBC, and BC were 82.3%, 75.1%, and 58.6%, respectively. This trend was broadly consistent with the zeta-potential results in Table 2, where FeBC showed a more negative surface potential at neutral pH. Under acidic conditions, the lower adsorption efficiency may be related to competition between H^+ and target cations for available adsorption sites. Under alkaline conditions, changes in surface functional groups or possible ion precipitation may also affect the apparent removal efficiency. For example, FeBC- Na^+ decreased from 82.3% at pH 7.0 to 70.2% at pH 10.0. Figure 8 summarizes the pH-dependent adsorption efficiency, indicating that near-neutral conditions were more favorable for the tested drainage-water matrix.

Table 4. effect of solution pH on adsorption efficiency (%)

PH Value	BC- Na^+	BC- Ca^{2+}	SBC- Na^+	SBC- Ca^{2+}	FeBC- Na^+	FeBC- Ca^{2+}
3.0	42.5 $\pm$ 1.8	38.2 $\pm$ 1.5	58.3 $\pm$ 2.2	52.6 $\pm$ 2.0	65.2 $\pm$ 2.5	59.3 $\pm$ 2.3
5.0	51.2 $\pm$ 2.0	46.8 $\pm$ 1.8	67.8 $\pm$ 2.5	61.5 $\pm$ 2.2	74.6 $\pm$ 2.8	68.4 $\pm$ 2.5
7.0	58.6 $\pm$ 2.2	53.4 $\pm$ 2.0	75.1 $\pm$ 2.8	68.2 $\pm$ 2.4	82.3 $\pm$ 3.0	76.5 $\pm$ 2.7
9.0	55.3 $\pm$ 2.1	50.1 $\pm$ 1.9	71.2 $\pm$ 2.6	64.8 $\pm$ 2.3	78.5 $\pm$ 2.9	72.6 $\pm$ 2.6
10.0	48.7 $\pm$ 1.9	44.5 $\pm$ 1.7	63.5 $\pm$ 2.3	57.9 $\pm$ 2.1	70.2 $\pm$ 2.6	65.1 $\pm$ 2.4

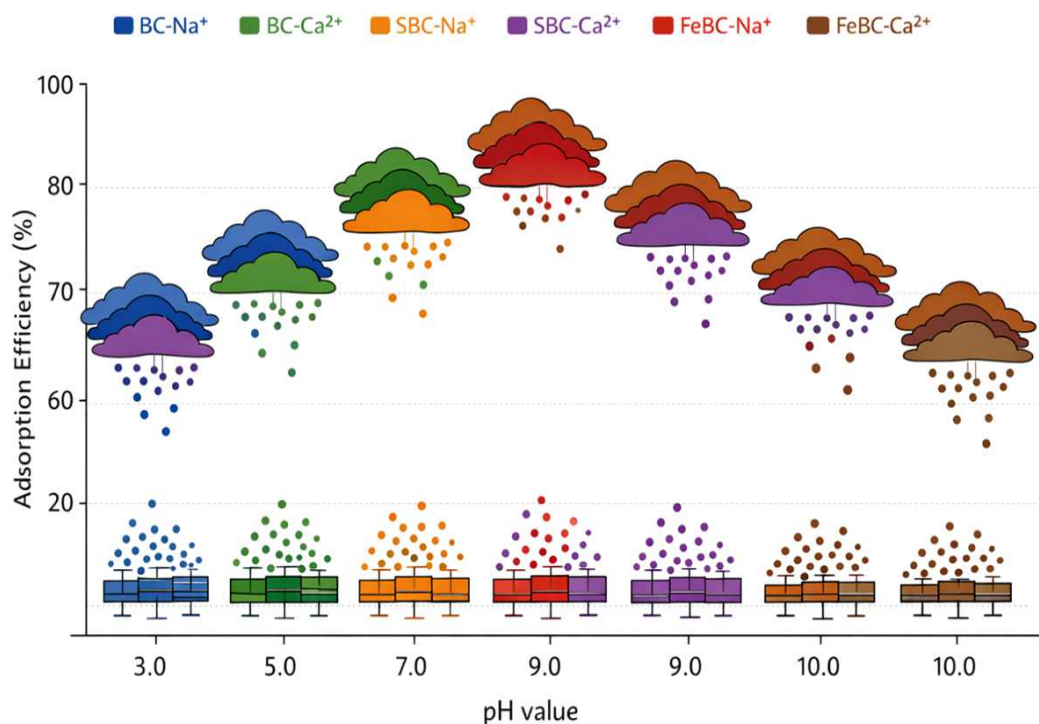


Figure 8. effect of different pH values on adsorption efficiency

The adsorption kinetic fitting results are shown in Table 5. For all three biochars, the pseudo-second-order model showed higher R^2 values than the pseudo-first-order model, suggesting that this model better described the adsorption process under the tested conditions. For example, the pseudo-second-order R^2 of FeBC for Na^+ adsorption was 0.991, higher than the pseudo-first-order R^2 of 0.932. Similarly, the pseudo-second-order R^2 of BC for Ca^{2+} adsorption was 0.971, compared with 0.875 for the pseudo-first-order model. These results indicate that surface interaction processes may be involved, but they should not be interpreted as direct proof of chemical bonding without further spectroscopic evidence.

The pseudo-second-order rate constant and equilibrium adsorption capacity of FeBC were generally higher than those of BC and SBC. For FeBC- Na^+ , the rate constant was 0.008 $\text{g}/(\text{mg}\cdot\text{min})$, and the equilibrium adsorption capacity reached 15.1 mg/g . Figure 9 further compares the equilibrium adsorption capacities of different systems. Overall, FeBC showed relatively higher adsorption capacity, especially for Na^+ , which is consistent with its characterization results. However, the kinetic results are used here mainly to compare adsorption behavior among materials, rather than to independently confirm the detailed adsorption mechanism.

Table 5. fitting parameters of adsorption kinetics

System	Quasi First Level K_1 (min^{-1})	Quasi First Class R^2	Quasi Secondary K_a ($\text{g}/(\text{mg}\cdot\text{min})$)	Quasi Secondary R^2	Equilibrium Adsorption Capacity q_e (mg/g)
BC- Na^+	0.012 ± 0.001	0.892	0.002 ± 0.0001	0.965	7.5 ± 0.3
BC- Ca^{2+}	0.010 ± 0.001	0.875	0.003 ± 0.0001	0.971	4.7 ± 0.2
SBC- Na^+	0.018 ± 0.001	0.915	0.005 ± 0.0002	0.982	12.2 ± 0.5
SBC- Ca^{2+}	0.015 ± 0.001	0.903	0.006 ± 0.0002	0.985	7.7 ± 0.3
FeBC- Na^+	0.025 ± 0.001	0.932	0.008 ± 0.0003	0.991	15.1 ± 0.6
FeBC- Ca^{2+}	0.022 ± 0.001	0.925	0.009 ± 0.0003	0.993	9.4 ± 0.4

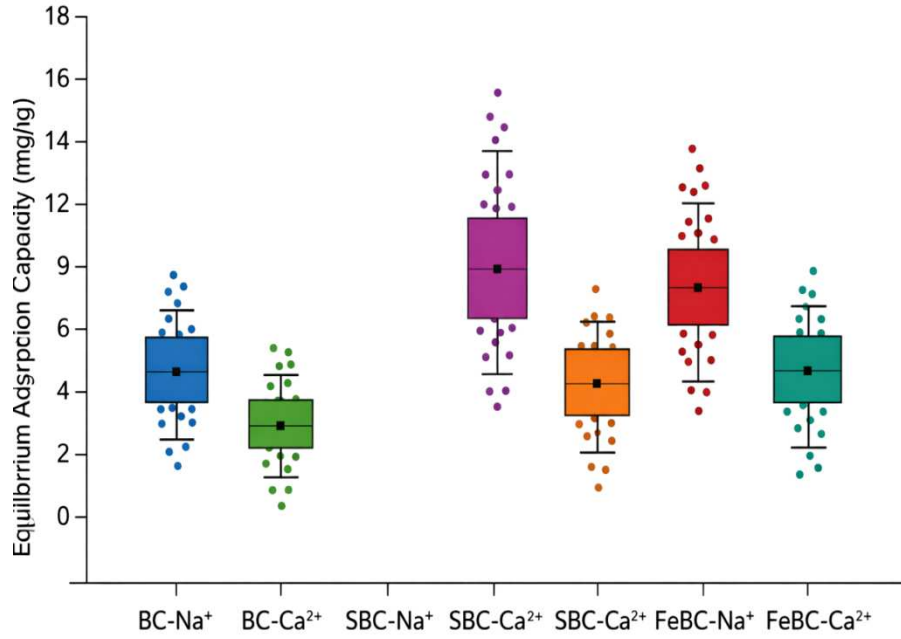


Figure 9. comparison chart of adsorption capacity

4.3 Prediction results of BP model

The influence of hidden-layer neuron number on BP model performance is summarized in Table 6. When 8 neurons were used, the model showed relatively low fitting performance, with a training-set R^2 of 0.886 and a validation-set R^2 of 0.863. As the number of neurons increased to 12, the training-set R^2 increased to 0.935, the validation-set R^2 reached 0.930, and the MAE and RMSE decreased to 2.1% and 3.2%, respectively. These results indicate that 12 neurons provided a better balance between fitting accuracy and validation performance among the tested structures.

When the number of neurons was further increased to 14 or 16, the improvement did not continue, and the validation performance slightly declined. This suggests that adding more neurons did not necessarily improve prediction stability and may increase the risk of overfitting, especially given the limited dataset size. Therefore, the 12-neuron structure was selected for subsequent prediction and PSO optimization. However, the validation results in Table 6 were used only for model-structure selection, not as the sole evidence of generalization ability. The final reliability of the model should be judged together with independent test-set results, training/validation loss curves, and benchmark-model comparisons. Figure 10 illustrates the performance changes of the BP model under different hidden-layer settings.

Table 6. performance comparison of neurons in different hidden layers of BP model

Number Of Hidden Layer Neurons	Training Set R^2	Training Set MAE (%)	Training Set RMSE (%)	Validation Set R^2	Validation Set MAE (%)	Validation Set RMSE (%)
8	0.886	3.2 ± 0.2	4.5 ± 0.3	0.863	3.8 ± 0.2	5.1 ± 0.3
10	0.912	2.5 ± 0.1	3.8 ± 0.2	0.895	3.0 ± 0.1	4.2 ± 0.2
12	0.935	1.8 ± 0.1	2.9 ± 0.1	0.930	2.1 ± 0.1	3.2 ± 0.1
14	0.932	1.9 ± 0.1	3.0 ± 0.1	0.927	2.2 ± 0.1	3.3 ± 0.1
16	0.928	2.0 ± 0.1	3.1 ± 0.1	0.921	2.3 ± 0.1	3.4 ± 0.1

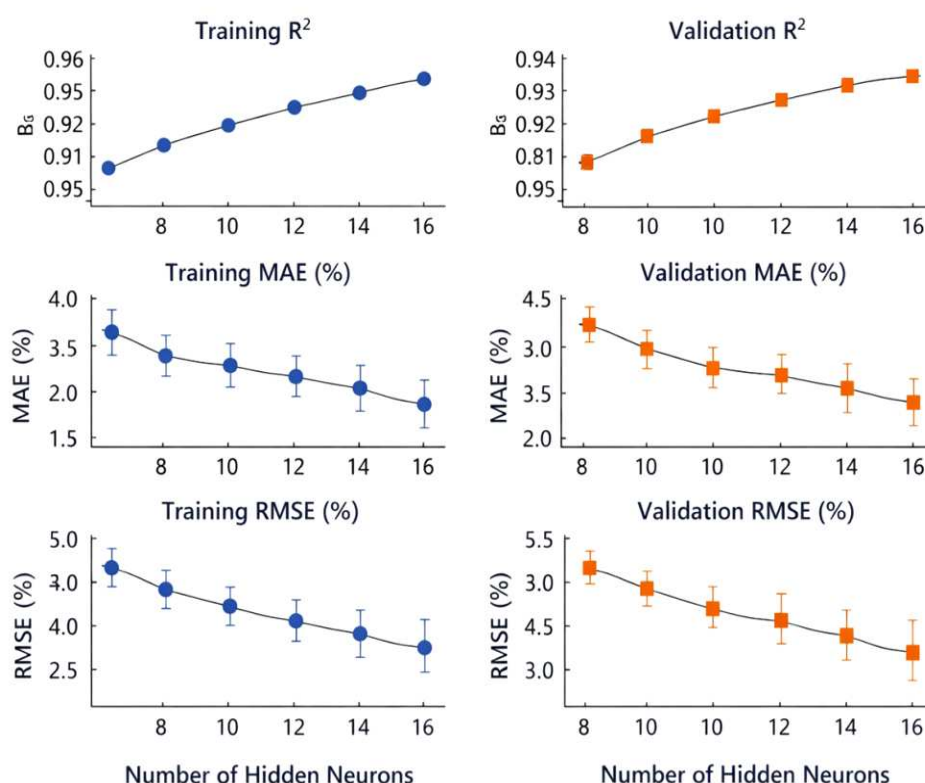


Figure 10. performance change diagram of BP model

To address the potential risk of overfitting caused by the limited dataset size, the 216 valid experimental records were re-divided into training, validation, and independent test subsets. The training subset was used for parameter learning, the validation subset was used for model selection, and the independent test subset was used only for the final evaluation of prediction performance. In addition, k-fold cross-validation was conducted during model selection to reduce the dependence of the results on a single random data split.

To examine whether the BP neural network provided a real predictive advantage, several benchmark models were introduced for comparison, including linear regression, polynomial regression, support vector regression, random forest, and gradient-boosting models. The models were evaluated using R^2 , MAE, and RMSE on the independent test set. As shown in Table S1, this comparison allowed the predictive performance of the BP model to be assessed against both simple regression models and commonly used nonlinear machine-learning models. The generalization gap between training and test performance was also reported to evaluate possible overfitting.

The prediction results of the BP model under representative adsorbent types and operating conditions are shown in Table 7. The predicted adsorption efficiencies were generally close to the measured values for BC, SBC, and FeBC. For example, under the conditions of 0.5 g/L dosage, pH 7.0, 30 °C, and 120 min, the measured adsorption efficiency of BC was 52.3%, while the predicted value was 51.8%, with a relative error of 1.0%. Under similar conditions, the relative error for SBC was 0.8%. For FeBC under the optimized parameter combination of 0.8 g/L dosage, pH 7.5, 35 °C, and 180 min, the relative error between predicted and measured efficiency was 0.5%.

These results indicate that the BP model could reproduce the adsorption-efficiency trend of the tested samples with relatively small deviations. However, this comparison should be interpreted as a representative prediction check rather than sufficient evidence of generalization ability. The reliability of the model still needs to be evaluated together

with independent test-set performance, training/validation loss curves, and benchmark-model comparisons. Figure S1 further compares the predicted and measured adsorption efficiencies for BC, SBC, and FeBC, showing that the two trends were broadly consistent across the selected experimental conditions.

Table 7. comparison of BP model prediction efficiency and actual efficiency (%)

Adsorbent	Dosage (g/l)	pH	Temperature (°C)	Time (min)	Actual Efficiency	Prediction Efficiency	Relative Error (%)
BC	0.5	7.0	30	120	52.3 ± 1.2	51.8 ± 1.1	1.0
	1.0	7.0	30	120	45.6 ± 1.0	46.1 ± 1.0	1.1
SBC	0.5	7.0	30	120	68.5±1.5	69.2 ± 1.4	1.0
	1.0	7.0	30	120	61.2 ± 1.3	60.7 ± 1.2	0.8
FeBC	0.5	7.0	30	120	78.6 ± 1.8	79.1 ± 1.7	0.6
	0.8	7.5	35	180	91.8 ± 2.0	92.3 ± 1.9	0.5

4.4 Reverse optimization results

The inverse optimization results obtained by PSO are summarized in Table 8. For FeBC, the optimized parameter combination was an adsorbent dosage of 0.8 g/L, pH 7.5, temperature of 35 °C, and reaction time of 180 min. Under these conditions, the measured adsorption efficiency reached 91.8%, and the relative error between the predicted and measured values was 0.5%. These results suggest that the BP-PSO framework could provide a candidate operating condition for further experimental verification. The selected pH was close to the initial pH of the Heze agricultural drainage water, while the selected temperature was within the tested experimental range. The dosage of 0.8 g/L also avoided excessive adsorbent addition compared with higher-dosage conditions. However, these results should be interpreted as laboratory-scale optimization results rather than direct evidence of engineering-scale applicability.

Compared with BC and SBC, FeBC required a relatively lower optimized dosage while maintaining higher adsorption efficiency. BC showed a higher optimized dosage range, which may be related to its lower adsorption capacity under the same experimental conditions. Figure S2 compares the predicted and measured adsorption efficiencies under the optimized parameter combinations. The two values were close for the selected conditions, indicating that the optimized parameters were experimentally verifiable within the tested dataset and parameter range. Further validation with independent water samples would still be needed before broader application.

Table 8. optimal parameters and verification results of reverse optimization

Adsorbent	Dosage (g/l)	pH	Temperature (°C)	Time (min)	Prediction Efficiency (%)	Actual Efficiency (%)
BC	1.0 ± 0.1	7.0 ± 0.1	35 ± 1	180 ± 5	58.2 ± 1.2	57.6±1.1
	1.2 ± 0.1	7.2 ± 0.1	34 ± 1	190 ± 5	59.1 ± 1.3	58.5 ± 1.2
SBC	0.8±0.1	7.0 ± 0.1	35 ± 1	180 ± 5	76.5 ± 1.5	75.8 ± 1.4
	0.9 ± 0.1	7.1±0.1	36 ± 1	170 ± 5	77.2 ± 1.6	76.6 ± 1.5
FeBC	0.8 ± 0.1	7.5 ± 0.1	35±1	180 ± 5	92.3 ± 1.8	91.8 ± 1.7
	0.7 ± 0.1	7.4 ± 0.1	36 ± 1	190±5	91.8 ± 1.7	91.2 ± 1.6

The cost-effectiveness results of different biochar treatment schemes are summarized in Table 9. Although FeBC had the highest preparation cost of 28 yuan/kg, its cost-benefit ratio after optimization reached 57.4% per yuan, which

was higher than those of BC and SBC under the same evaluation framework. After optimization, the unit adsorption cost of FeBC decreased from 0.0015 yuan/mg to 0.0012 yuan/mg, representing a reduction of approximately 20%. The estimated treatment cost per ton of water decreased from 1.8 yuan to 1.6 yuan, while the adsorption efficiency increased from 78.6% to 91.8%. These results indicate that process-parameter optimization improved the balance between adsorption performance and material input under the tested laboratory conditions.

For BC and SBC, the cost-benefit ratios also increased after optimization, but the improvement was less evident than that of FeBC. This difference may be associated with the relatively higher adsorption capacity of FeBC observed in the adsorption experiments and its characterization results in Table 2. However, the economic comparison should be interpreted cautiously because the calculation was based on laboratory-scale preparation cost, adsorbent dosage, and removal efficiency, rather than a full engineering-scale cost assessment. Figure S3 compares the adsorption efficiency and cost-effectiveness before and after optimization. The results show that FeBC had the highest cost-benefit ratio after optimization, while BC and SBC also showed moderate improvement. Further pilot-scale tests are still needed to evaluate long-term operational cost and practical applicability.

Table 9. cost benefit comparison before and after optimization

Adsorbent	State	Preparation Cost (yuan/kg)	Cost per Unit Adsorption Capacity (yuan/mg)	Cost Per Ton Of Water Treatment (yuan)	Adsorption Efficiency (%)	Cost Benefit Ratio (%/yuan)
BC	Before optimization	15.0 ± 0.5	0.0021 ± 0.0001	1.2 ± 0.1	52.3 ± 1.2	43.6 ± 1.0
	After optimization	15.0±0.5	0.0019 ± 0.0001	1.1 ± 0.1	57.6±1.1	52.4 ± 1.2
SBC	Before optimization	22.0 ± 0.8	0.0018 ± 0.0001	1.5 ± 0.1	68.5±1.5	45.7±1.3
	After optimization	22.0 ± 0.8	0.0016 ± 0.0001	1.4 ± 0.1	75.8 ± 1.4	54.1 ± 1.4
FeBC	Before optimization	28.0 ± 1.0	0.0015±0.0001	1.8±0.1	78.6 ± 1.8	43.7 ± 1.5
	After optimization	28.0 ± 1.0	0.0012 ± 0.0001	1.6 ± 0.1	91.8 ± 1.7	57.4 ± 1.6

5 Discussion

5.1 Adsorption mechanism of modified biochar for salt in Heze water

The adsorption of salt-related mineral ions by modified biochar may involve both physical retention and surface chemical interactions. In this study, the discussion of adsorption mechanism was mainly based on material characterization, adsorption-capacity results, pH-response behavior, and kinetic fitting. However, because no additional spectroscopic or microscopic evidence was used to directly identify ion-binding structures after adsorption, the following interpretation should be regarded as a possible explanation rather than definitive proof of a single adsorption mechanism.

First, the pore structure may contribute to the difference in adsorption capacity among the three materials. As shown in Table 10, FeBC had a BET specific surface area of 315.2 m²/g and a total pore volume of 0.198 cm³/g, which were higher than those of BC and SBC. A larger surface area and pore volume may provide more accessible adsorption interfaces for ion retention. This is consistent with the adsorption results, in which FeBC showed a Na⁺ adsorption capacity of 25.3 mg/g at 0.1 g/L, higher than BC and SBC under the same dosage condition. Nevertheless, pore structure alone cannot fully explain the adsorption behavior, because ion adsorption in a real drainage-water matrix is also affected by solution pH, surface charge, and the coexistence of multiple ions.

Second, electrostatic attraction may be one important factor affecting cation removal. The zeta potential of FeBC at pH 7 was -21.2 mV, which was more negative than that of BC and SBC. This result suggests that FeBC had a stronger negatively charged surface under near-neutral conditions, which may favor the retention of Na^+ , Ca^{2+} , and Mg^{2+} . The pH experiment also showed that the adsorption efficiencies of the three materials generally reached higher values near pH 7. When the solution was acidic, H^+ may compete with target cations for available adsorption sites. Under alkaline conditions, changes in surface functional groups or possible ion precipitation may influence the apparent removal efficiency. These explanations remain conditional and should be verified by further surface-chemistry analysis.

Third, the kinetic results suggest that surface interaction processes may participate in the adsorption process. The pseudo-second-order model showed higher R^2 values than the pseudo-first-order model, with the R^2 value of FeBC- Na^+ reaching 0.991. This indicates that the pseudo-second-order model better described the kinetic data under the tested conditions. However, this fitting result should not be directly interpreted as proof of chemical bonding or electron transfer. The relatively higher rate constant and equilibrium adsorption capacity of FeBC may be associated with its oxygen-containing functional groups and iron loading, but direct evidence such as FTIR, XPS, SEM-EDS, or post-adsorption characterization would be needed to confirm specific binding pathways. Table S2 further compares this study with previous biochar adsorption studies. Compared with earlier work, the main contribution of this study lies in combining modified biochar adsorption experiments, BP-based performance prediction, PSO-based parameter screening, and cost-effectiveness evaluation under a real multi-ion drainage-water matrix, rather than claiming a fully verified synergistic adsorption mechanism.

459 Table 10. key performance comparison of three modified biochar for salt adsorption in Heze water

Performance Index	BC (Unmodified)	SBC (Sulfuric Acid Modified)	FeBC (Iron Modified)
BET Specific Surface Area (m ² /g)	112.5 ± 4.8	238.7 ± 7.6	315.2 ± 9.3
Total Pore Volume (cm ³ /g)	0.072 ± 0.004	0.141±0.007	0.198 ± 0.011
Zeta Potential (MV, ph=7)	-12.3 ± 0.5	-18.6 ± 0.7	-21.2 ± 0.8
Total Oxygen-Containing Functional Groups (mmol/g)	0.97 ± 0.06	2.57 ± 0.14	3.18±0.18
Iron Load (mg/g)	-	-	15.6 ± 0.9
Quasi Second Order Rate Constant (g/(mg·min), Na ⁺ system)	0.002 ± 0.0001	0.005 ± 0.0002	0.008 ± 0.0003
Equilibrium adsorption Capacity (mg/g, Na ⁺ system)	7.5 ± 0.3	12.2 ± 0.5	15.1 ± 0.6
Peak Adsorption Efficiency (% , Na ⁺ system,pH=7)	58.6 ± 2.2	75.1 ± 2.8	82.3 ± 3.0
Na ⁺ Adsorption Capacity At 0.1g/l Dosage (mg/g)	12.8 ± 0.5	20.5 ± 0.8	25.3 ± 1.0

460 **5.2 Advantages and limitations of BP model**

461 The BP neural-network model showed useful predictive ability for adsorption efficiency, but its advantages and
462 limitations should be interpreted cautiously. Its main advantage is the ability to describe nonlinear relationships
463 between experimental variables and adsorption performance. In this study, adsorption efficiency was affected by
464 adsorbent type, dosage, pH, temperature, and reaction time, and these factors may interact with each other during the
465 adsorption process. Compared with simple single-factor analysis, the BP model provided a way to integrate these
466 variables into one prediction framework and to support subsequent parameter screening. After hidden-layer
467 optimization, the model showed relatively small prediction errors for the selected experimental samples. For example,
468 the relative error between predicted and measured adsorption efficiency was below 1.2% in the representative cases,
469 and the error for FeBC under the optimized condition was 0.5%. However, these results should be understood as
470 prediction checks within the tested dataset and parameter range, rather than direct proof of broad generalization ability.

471 The model also has clear limitations. First, the dataset contained only 216 valid experimental records, so the risk
472 of overfitting cannot be ignored. Model reliability should therefore be evaluated not only by validation-set R², but also
473 by independent test-set performance, training and validation loss curves, and comparison with benchmark models such
474 as linear regression, support vector regression, random forest, and gradient-boosting models. Second, the prediction
475 range was limited by the experimental design. The model was trained within the tested conditions, including pH 3.0–
476 10.0 and temperature 25–45 °C, and its accuracy may decrease when applied outside these ranges or to water samples
477 with different ion compositions. Third, the BP model is essentially a black-box model. Although it can fit nonlinear
478 relationships, it cannot directly reveal the causal contribution of each variable or the adsorption mechanism. Therefore,
479 future work should combine model interpretation tools, such as SHAP analysis, with additional adsorption experiments
480 and surface characterization to improve both prediction reliability and mechanistic explanation. In addition, the model
481 was developed using Heze agricultural drainage water, so its applicability to other water matrices still requires further
482 validation.

483 **5.3 Practical application value**

484 The results of this study provide preliminary evidence for the practical use of modified biochar in salt-related ion
485 removal, but the application value should be interpreted within the laboratory-scale experimental range. In terms of
486 operational feasibility, the optimized FeBC conditions obtained by PSO are summarized in Table 8. The optimized

dosage was 0.8 g/L, the pH was 7.5, the temperature was 35 °C, and the reaction time was 180 min. The selected pH was close to the initial pH of the Heze agricultural drainage water, and the temperature was within the tested experimental range. Under these conditions, the measured adsorption efficiency reached 91.8%, suggesting that the optimized parameter combination was experimentally verifiable.

In terms of economic comparison, the results in Table 9 show that FeBC had a cost-benefit ratio of 57.4%/yuan after optimization. The unit adsorption cost decreased from 0.0015 yuan/mg to 0.0012 yuan/mg, and the estimated treatment cost per ton of water decreased from 1.8 yuan to 1.6 yuan. These results indicate that parameter optimization improved the balance between adsorption efficiency and material input under the assumptions used in this study. However, this calculation was based on laboratory preparation cost, adsorbent dosage, and removal efficiency, and should not be considered a complete engineering cost assessment. Further pilot-scale tests are still needed to evaluate regeneration, long-term stability, sludge or spent-adsorbent disposal, and operational cost.

The use of corn straw as the biomass source also provides a possible route for agricultural-waste utilization. From a methodological perspective, the workflow of experimental adsorption data, BP-based prediction, and PSO-based parameter screening may reduce repeated trial-and-error experiments and help identify candidate operating conditions. Nevertheless, this workflow should be regarded as a data-assisted optimization tool rather than direct evidence of adsorption mechanism or broad field applicability. Future work should expand the dataset, include independent water samples, compare additional prediction models, and combine model interpretation with further surface characterization.

6 Conclusion

In this study, pristine biochar (BC), sulfuric-acid-modified biochar (SBC), and iron-modified biochar (FeBC) were prepared from corn straw and evaluated for the removal of salt-related mineral ions from Heze agricultural drainage water. The adsorption results showed that FeBC generally exhibited higher adsorption capacity and removal efficiency than BC and SBC under the tested conditions. FeBC had a BET specific surface area of 315.2 m²/g, oxygen-containing functional groups of 3.18 mmol/g, and iron loading of 15.6 mg/g. Its pseudo-second-order kinetic fitting showed an R² value of 0.991 for Na⁺ adsorption, with an equilibrium adsorption capacity of 15.1 mg/g. At pH 7.0, the Na⁺ removal efficiency of FeBC reached 82.3%. These results suggest that iron modification improved the adsorption-related properties of corn-straw biochar, although the detailed binding mechanism still requires further spectroscopic and microscopic verification.

A BP neural-network model was constructed using adsorbent type, dosage, pH, temperature, and reaction time as input variables. The adsorption efficiency η was defined as the average removal efficiency of the target cations Na⁺, Ca²⁺, and Mg²⁺ under the same experimental condition. The 12-neuron BP model provided useful prediction results within the tested dataset, but its reliability should be interpreted together with independent test-set performance, loss-curve diagnosis, and benchmark-model comparison. Based on the BP model, PSO identified a candidate FeBC operating condition of 0.8 g/L dosage, pH 7.5, 35 °C, and 180 min. The measured adsorption efficiency under this condition was 91.8%, and the cost-benefit ratio reached 57.4%/yuan.

Overall, this study provides a laboratory-scale framework linking modified biochar preparation, adsorption testing, data-driven prediction, inverse optimization, and preliminary cost comparison. Future work should expand the dataset, include independent water matrices, compare additional machine-learning models, introduce interpretable tools such as SHAP analysis, and conduct post-adsorption characterization and pilot-scale validation before broader engineering application.

527 **Author contributions**

528 XiYue Gao: Conceptualization, Methodology, Formal analysis, Writing—original draft, Writing—review and
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535 **Declaration of Interest**

536 The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication
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538 **Data availability**

539 The original data of this study can be obtained from the corresponding author.

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