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Review Article

DECODING PHYSICOCHEMICAL AND OPERATIONAL DRIVERS OF ADSORPTION CAPACITY FOR PROCESS OPTIMIZATION

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Abstract

The adsorption performance depends on the complex interplay of material properties, solution chemistry and processing conditions, and prediction is important for process optimization. In this study, 6,172 observations were analyzed to examine the physicochemical and operational factors affecting the adsorption capacity and included specific surface area, pore volume, material properties, pH, temperature, initial concentration, flow rate, and column height. The statistical association analysis was combined with linear regression and nonlinear machine-learning models. Initial concentration had the highest correlation with adsorption capacity, and contributed to 82.98% of the feature importance for the random-forest, suggesting that it was the most important factor. Random forest has the greatest predictive accuracy (R^2 = 0.9725, RMSE = 13.65 mg/g, MAE = 3.55 mg/g) than gradient boosting and linear regression. Nonlinear effects and interactions between the main adsorption determinants were also found from the response patterns. The results show that combining the physicochemical interpretation with the nonlinear predictive modeling approach is an effective way to identify the main factors that control the adsorption process and offers a practical way to optimize the adsorption process and remove contaminants.

Key Words: adsorption capacity, physicochemical properties, process optimization, machine learning, contaminant removal

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1. Introduction

The capacity to transfer dissolved materials from liquid to solid phases by adsorption via a physicochemical interaction has made adsorption an important separation and remediation process. It has numerous practical applications in wastewater treatment, contaminant recovery, purification and environmental protection, and the performance of adsorption strongly relies on the properties of the materials and the operating conditions. As the effluents from industrial processes have become more complex, there is a greater need for methods of treatment that are able to handle contaminants that have different molecular properties and environmental fate. Moreover, the complexity of wastewater treatment becomes more challenging as contaminant profiles become more diverse, as shown by emerging pollutants like micro plastics – which require flexible and sustainable removal technologies (Badawi et al., 2025). So adsorption is of special interest when its behavior can be explained and improved in a realistic multivariable situation.

The interconnected material and process properties control the adsorption capacity and cannot be controlled by a single experimental parameter. Specific surface area and pore volume have an effect on the availability of adsorption sites, whereas the surface chemistry affects the interactions between the adsorbent and the target species. Solution pH can influence the surface charge of the adsorbent and the speciation of the pollutant, while temperature can have a similar effect on the adsorption energetics and equilibrium behavior. The parameters of the column (flow rate, bed height) influence residence time and contact efficiency, while the initial concentration of the contaminants is the mass-transfer driving force. Mechanistic studies on resin-based contaminated removal have shown that the removal performance depends on the interactions with the surface, the site-energy distributions, the adsorption equilibria, and the kinetic behavior of the process (Chen et al., 2025). Mechanistically similar processes are also found in arsenite sequestration, where the processes of material transformation and composition affect contaminant immobilization under specific aqueous conditions (Liu et al., 2025 A).

These factors are typically assessed in conventional adsorption studies by the use of equilibrium models or by integrating kinetic equations or by varying one parameter at a time. They are still very much needed for mechanistic interpretation but when several material and operating parameters vary at the same time, they may be insufficient to describe nonlinear interactions. This has led to an increased drive to analyse adsorption systems in a data-driven manner, in recent years as a result of advances in computational chemistry and environmental engineering. Machine-learning models are capable of identifying multidimensional relationships without the need for the adsorption behavior to be linear. Previous studies on biochar have validated predictive methods that can relate material properties to P adsorption capacity, and can provide data that can be used in the design of adsorbents and optimization of processes (Lyu et al., 2024). Machine learning has also aided in the prediction and optimization of dye adsorption by biochar, with the outcomes of these models validated by experiments (Liu et al., 2025 B).

These methods are more than just predictive—they can help inform effective marketing strategies. Explainable and chemically informed modelling can be used to identify the material descriptors and process variables that have the largest impact on performance. In the field of porous materials, chemical knowledge has been integrated with deep-learning approaches to enhance the prediction of high-performing materials, demonstrating the potential of chemical-guided deep-learning methods (Ba-Alawi et al., 2024). Machine learning has also been used in the computational design and optimization of disordered nanoporous materials, showing its relevance for establishing the relation between complex properties of the structure and its functional performance (Vishnyakov, 2025). Similar developments in organic framework membrane research suggest that predictive modeling could help in the design, evaluation, and potential industrial applications of these materials (Wu et al., 2025). These advances have elevated data-driven analysis as a tool that works in tandem with applied chemical systems to interpret their behavior, not as an empirical prediction tool.

In this coupling, adsorption systems are especially suitable because of the effect of the

coupling between the characteristics of the adsorbent, the solution chemistry and the operating conditions. In recent years, machine-learning methods have been shown to be useful in unveiling important adsorption mechanisms in oxyanions when experimental data are combined with literature data (Yuan et al., 2025). Predictive modeling has also been used to describe the amount of phosphate that can be adsorbed, the capacity for adsorption, and the rates of adsorption and desorption, while also incorporating physically meaningful information into the predictive model framework (Zhou et al., 2024). A multi-model approach has proven to be useful for decoding interactions between biochar, microbial regulation, and pathways for pollutant removal, leading to more complex remediation systems benefiting from this approach (Tao et al., 2025). Such results demonstrate the potential of computational analysis beyond simple prediction–response relationship, to a more comprehensive representation of adsorption process.

This need increases in complex wastewater systems with multiple pollutants and operating conditions interacting. Multi-factor adsorption studies showed that coupled effects can be successfully highlighted by using machine learning alongside optimization algorithms, and that the behavior of the process can be successfully validated by experimental tests (Yang et al., 2025 A). The co-adsorption of oils and phenols has also been explored using multi-task deep-learning models, where interactions between contaminants can be modeled concurrently with the selective separation of oils and phenols (Yang et al., 2025 B). Also, the development of new adsorbents is still progressing well for pharmaceutical contaminants, such as efficient adsorption systems based on aerogels for diclofenac (Wang et al., 2025 A), which can be used for mechanistic interpretation. Taken together, these advances highlight the necessity of the adsorption performance as a multi-variable chemical process that needs integrated analytical treatment.

Although these advances have been made, there is a practical need to understand the interplay between physicochemical properties of the adsorbent and operating conditions and how they affect adsorption capacity in heterogeneous observations. The predictive accuracy is part of the process value only if dominant drivers, nonlinear responses and their significance for optimization are identified at the same time. The correlation of the specific surface area, pore volume, material properties, solution properties, and column properties with adsorption capacity can then be more firmly founded on an integrated framework. The implications of converting predictive relationships into practically useful operating strategies are further emphasized by the use of optimization-oriented machine-learning frameworks developed in complex adsorption systems (Yang et al., 2025 A). This is an opportunity to improve linkage between adsorption chemistry, data-driven modeling, and applied process decision-making. Accordingly, this research pursues three objectives:

1. To quantify relationships between physicochemical properties, operational conditions, and adsorption capacity across heterogeneous adsorption observations
2. To develop and compare predictive models for accurately estimating adsorption capacity from available process variables
3. To identify dominant adsorption drivers and characterize nonlinear response patterns relevant to practical process optimization

2. Materials and Methods

2.1 Study Design and Data Framework

To explore physicochemical and operational parameters that affect adsorption capacity, a quantitative analytical design was used. Analytical framework included 6,172 observations of adsorption and focused on adsorption capacity (Q) as the main response variable. The predictor variables included the material properties, solution condition, and the column operating parameters (Yang, 2025). These were specific surface area, pore volume, pH,

temperature, initial concentration, flow rate and column height. The framework was designed to model individual relationships, identify dominant adsorption drivers, and create predictive models which can be used to support process level optimization.

2.2 Variables and Data Preparation

Pre-processing was carried out on the dataset to remove noise and outliers and make it ready for statistical analysis and predictive modeling.Systematic screening of the data was performed prior to the statistical analysis and predictive modelling. Specific surface area (SSA), pore volume (PV), material characteristic (MC), pH, temperature (T), initial concentration (IC), flow rate (FR) and column height (CH) were listed as explanatory variables, while adsorption capacity (Q) was listed as response variable. The variable formats, measurement consistency, missing values, duplicate records and implausible values were explored. The numerical variables were transformed into suitable analytical data and categorical data was coded when necessary. The data were then prepared and put into a uniform matrix of models for repeatable analysis.

2.3 Descriptive and Distributional Analysis

The variability of the adsorption system was described in descriptive analysis prior to assessment of inferential and prediction. Continuous variables were summarized as the mean, the standard deviation, the median, the minimum, the maximum and the interquartile range, depending on their distribution. The adsorption capacity was studied in detail to determine its central tendency, dispersion, range and distributional behavior. Skewness and potential influential observations were identified graphically. This preliminary analysis was provided to enable interpretation of the subsequent correlations between adsorption performance and adsorbent properties, solution chemistry, and operational conditions.

2.4 Physicochemical Association Analysis

The association analysis of bivariate was performed to elucidate the relationships between material, physicochemical and operational parameters and adsorption capacity. Correlations between Q and specific surface area, pore volume, pH, temperature, initial concentration, flow rate and column height were calculated after choosing the method of correlation according to the distribution characteristics. The intercorrelations between the predictors were also computed to look for redundancy and multicollinearity. The adsorption performance was compared with the appropriate procedures, and the characteristics of the materials were evaluated. The statistical significance was determined at $p < 0.05$, in addition to the effect size and direction.

2.5 Predictive Modeling of Adsorption Capacity

The available physicochemical and operational predictors were used to create predictive models to estimate the adsorption capacity. Analytical data was divided into training and testing sets to allow for the evaluation of the model's generalization ability. The use of conventional regression methods was contrasted with the nonlinear machine-learning algorithms that can capture the complex adsorption relationships. To prevent overfitting, hyperparameters of the model were optimized using cross validation in the training data. The model performance was assessed using the coefficient of determination (R2), root mean squared error (RMSE) and mean absolute error (MAE), for prediction on unseen (held-out) observations, providing objective model comparison.

2.6 Driver Importance and Process Optimization

The vigorous predictive model was questioned to find out which variables are most significant for adsorption capacity. Physicochemical and operational determinants were ranked by their feature-importance values, and response profiles investigated to describe the nonlinear effects over the relevant range of the variables. Interactions between the properties of the adsorbent, solution and the column parameters that may affect the adsorption performance were given special consideration. The following favourable combinations for

higher predicted Q values were then identified. These analyses converted the predictions into chemotoxic pieces of evidence that would be useful for adsorption-process control, operating-condition selection, and practical process optimization.

3. Results

3.1 Dataset and Adsorption Characteristics

The analytical data consisted of 6172 complete observations for nine physicochemical, operational and adsorption variables. The adsorption capacity (Q) values exhibited significant heterogeneity from 0.048 to 592.45 mg/g with a mean value of 32.89 ± 77.63 mg/g and a median of 8.84 mg/g, and a right-skewed distribution. The initial concentration (0-2,000 mg/L) also varied widely, as did the specific surface area (0.43-2,311 m^2/g) along with material characteristics, pH, temperature, flow rate and height of the column (Table 1).

Table 1. Descriptive characteristics of adsorption variables

Variable	Mean ± SD	Median	Min–Max
SSA (m^2/g)	390.37 ± 473.25	229.00	0.43–2311.00
PV (cm^3/g)	0.40 ± 0.38	0.30	0.00–3.37
MC	3.39 ± 2.34	2.40	0.00–14.60
pH	6.32 ± 1.47	6.50	2.00–11.00
T (°C)	25.34 ± 5.69	25.00	10.00–70.00
IC (mg/L)	81.84 ± 155.45	30.00	0.00–2000.00
FR (mL/min)	4.78 ± 3.71	4.00	0.40–25.00
CH (cm)	9.47 ± 5.86	8.00	1.00–50.00
Q (mg/g)	32.89 ± 77.63	8.84	0.048–592.45

3.2 Relationships Governing Adsorption Capacity

The initial concentration had the highest positive association with the adsorption capacity (Spearman's ρ = 0.839), while the other two bivariate variables (pore volume and temperature) had weak positive associations (ρ = 0.118 and 0.087, respectively). There was a slight positive correlation (ρ = 0.014) between flow rate. The pH (rho = −0.003), material characteristic (rho = −0.007), column height (rho = −0.015) and specific surface area (rho = −0.018) showed much lower monotonic correlation with the adsorption capacity (Table 2) (Figure 1).

Table 2. Association with adsorption capacity

Predictor	Spearman's ρ
IC	**0.839**
PV	0.118
T	0.087

FR	0.014
pH	−0.003
MC	−0.007
CH	−0.015
SSA	−0.018

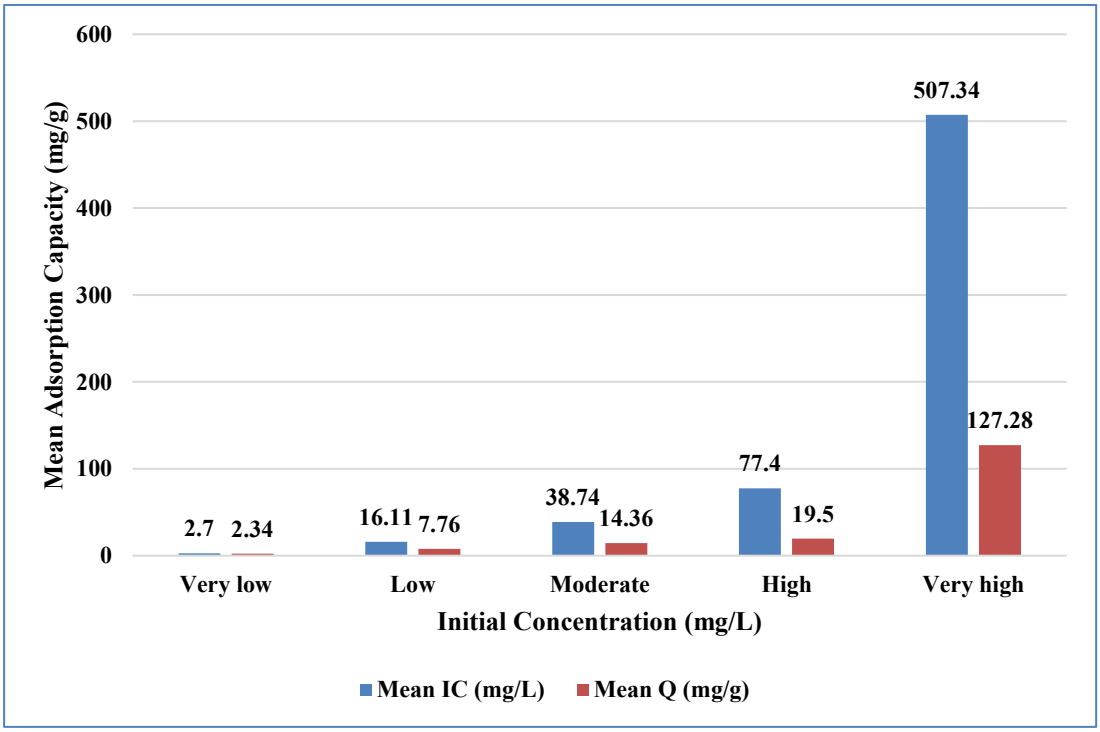

Figure 1. Adsorption capacity across initial-concentration groups

3.3 Predictive Performance

The power of the nonlinear approach over the traditional linear regression was clearly shown by the predictive modeling. Linear regression accounted for 78.83% of the variance in R, and the RMSE and MAE values were 37.90 and 13.99 mg/g, respectively. Gradient boosting produced the best results with $R^2 = 0.9714$, RMSE = 13.93 mg/g and MAE = 6.07 mg/g. The held-out test data results indicated that random forest gave the best overall prediction with $R^2 = 0.9725$, RMSE = 13.65 mg/g and MAE = 3.55 mg/g (Table 3).

Table 3. Predictive model performance

Model	R^2	RMSE (mg/g)	MAE (mg/g)
Linear regression	0.7883	37.90	13.99
Gradient boosting	0.9714	13.93	6.07
Random forest	0.9725	13.65	3.55

3.4 Dominant Drivers of Adsorption

Random-forest feature importance analysis showed that initial concentration was the most important factor affecting the adsorption capacity with 82.98% of the total predictive importance. Specific surface area ranked second at 11.62%, implying that there is another contribution from the material level which was not detected in the weak monotonic

correlation with Q, with column height contributing 2.19%, and pH 1.26%, and pore volume 0.89%. The combined effect of material characteristic, temperature and flow rate was comparatively weak. Strongly hierarchical driver structure, with concentration and surface properties as dominating drivers, as is demonstrated in these results (Table 4) (Figure 2).

Table 4. Importance of adsorption-capacity drivers

Rank	Predictor	Importance (%)
1	IC	82.98
2	SSA	11.62
3	CH	2.19
4	pH	1.26
5	PV	0.89
6–8	MC, T, FR	<1 each

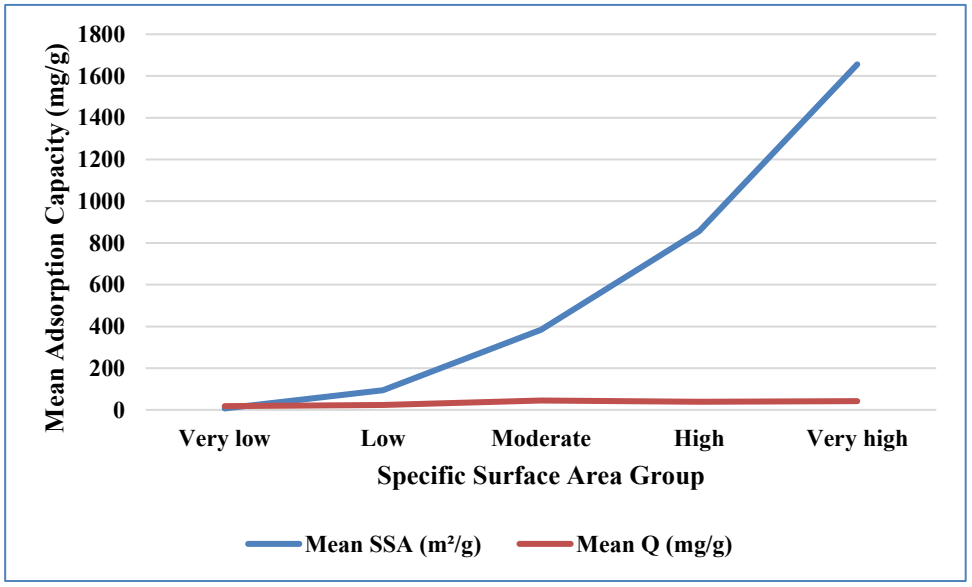

Figure 2. Adsorption response across specific-surface-area groups

3.5 Process Response and Optimization

The analytical results were combined revealing that initial concentration was a primary factor in influencing the adsorption performance while specific surface area also played an important secondary role in the nonlinear framework for predicting the adsorption performance. The negative bivariate relationships of a number of variables and the good performance of the nonlinear models indicated that the adsorption capacity was dependent on complex response patterns, rather than merely simple monotonic effects. Additional contributions were smaller from the column height, pH and pore volume. Thus, optimizing the process should focus on optimizing the concentration conditions and the characteristics of the adsorbent surface, while taking into account secondary operating variables in an integrated multivariable process optimization (Table 5) (Figure 3).

Table 5. Numerical prioritization of adsorption process variables

Rank	Process variable	Importance (%)
1	Initial concentration (IC)	**82.98**
2	Specific surface area (SSA)	**11.62**
3	Column height (CH)	**2.19**

4	pH	**1.26**
5	Pore volume (PV)	**0.89**
6	Material characteristic (MC)	**0.48**
7	Temperature (T)	**0.38**
8	Flow rate (FR)	**0.20**

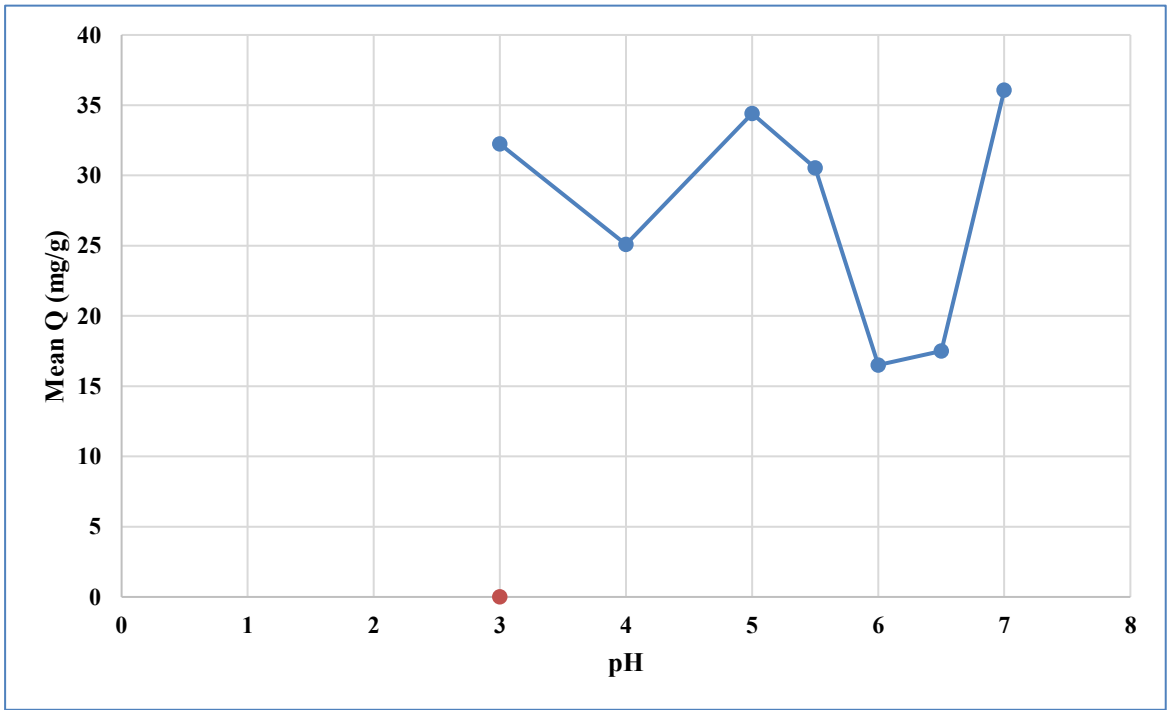

Figure 3. Adsorption capacity under different pH conditions

4. Discussion

The adsorption capacity showed significant differences between the conditions tested indicating the adsorption performance depended on the combination of physicochemical characteristics and operation parameters; it did not exhibit a uniform response. This was followed by initial concentration which was strongly and positively correlated with adsorption capacity and had the largest percentage of predictive importance. This is chemically logical as the higher the concentration, the higher the driving force for mass transfer between the aqueous phase and the adsorbent's surface, until eventually all the adsorption sites on the surface are completely filled. The adsorption performance can also be described by the synergistic effects of the physicochemical properties and process-related variables rather than the individual properties of the adsorbents, as shown in similar data-driven studies (Wang et al., 2025 B).

Specific surface area was second most influential predictor, although it was not a strong monotonic correlation with adsorption capacity. This apparent contradiction is significant since it suggests a nonlinear or nonmonotonic relationship over the entire range of observations for the surface area. The effectiveness of the extra surface area depends on the solution conditions and competing process effects, as well as the chemical accessibility/compatibility of available surface sites to the adsorbate. The machine learning investigations of heavy metal adsorption by biochar have also focused on the fact that adsorption mechanisms are a result of the interplay of multiple material and environmental parameters instead of being limited to individual structural descriptors (Zeng et al., 2025). Chemical modification can also significantly affect biochar physicochemical properties, highlighting the need to understand the surface properties in the context of the general

material (Song et al., 2025).

The effect of column height, pH, and pore volume were minor but still important for the multivariable adsorption model. Available contact areas and residence time may be altered by column height, and the pH may influence the surface charge, the speciation of the adsorbates and the interactions between the adsorbates and the adsorbent. Pore volume is a parameter that measures how much space is available within the pores for the diffusion and retention of molecules, but it is not the only parameter, as the availability of the pores depends on molecular dimensions. The adsorption behavior for perfluorooctanoic acid, showing the importance of chemically specific interactions in determining adsorption behavior, has also been demonstrated, through experiments and molecular dynamics simulations (Gu et al., 2025). These factors contribute to the reason why the predictions of individual small predictors can still be enhanced when used together.

One of the key findings was the superiority of the nonlinear predictive models. Linear regression had an R^2 of 0.7883 while the gradient boosting and random forest models achieved higher R^2 values of 0.9714 and 0.9725 respectively. The lowest RMSE and MAE were also obtained by random forest as 13.65mg/g and 3.55mg/g, respectively. The significant improvement suggests that the adsorption capacity was explained as being nonlinear, threshold or interactive, which could not be adequately represented by a simple additive linear structure. Similar advantages of machine learning have been achieved for the study of the coupling effect of process parameters in ion-adsorption rare-earth ore leaching, where computational methods were used to optimize the process and interpret the coupling effect of the process parameters simultaneously (Liu et al., 2025 C). This evidence is applicable to processes with highly interdependent variables, such as chemically complex processes, that can be modeled as nonlinear processes.

The process-response patterns lend support to this interpretation. The adsorption capacity was found to be significantly increased with increasing initial concentrations, whereas the initial surface area showed a non-monotonic response. The combined concentration-surface area analysis indicated that the maximum concentration and surface area quartiles yielded a mean adsorption capacity of 214.83 mg/g with significantly more adsorption than in lower concentration conditions. This interaction should make it clear why feature importance and response analysis provide more useful information about the process than correlation coefficients alone. A similar line of research in the field of environmental processes has been implemented in recent years that uses machine-learning approaches to find nonlinear combinations of either catalyst or operational parameters that best achieve decontamination performance (Wang et al., 2025 C). Multi-objective computational optimization has also shown to be valuable in electrochemical separation systems that are influenced by multiple operating conditions, but not just operating parameters alone (Moon et al., 2025).

The results have important implications for optimization of adsorption process. The initial concentration should be considered as a special case when determining treatment loading and adsorption requirements, and the specific surface area should be taken into account when selecting an adsorbent and/or engineering the material. The column configuration and solution pH can then be varied as secondary control factors without any interpretation. The hierarchical approach follows a general trend of process engineering evidence that simultaneous consideration of the kinetics, feed characteristics and operational variables is necessary for successful optimization (Aworanti et al., 2023). The analytical approach can then provide a useful decision support tool to evaluate operating conditions prior to more costly experimental optimization.

Overall, the method provides a helpful combination of predictive accuracy and chemical interpretability. Prediction models on their own may offer only a small amount of scientific information that does not show which factors control the observed response. The present analysis, on the other hand, shows how feature ranking, response profiling, and interaction evaluation can be used in conjunction with predictive modeling to link the computational results to the adsorption chemistry. Extension of this interdisciplinary style is also being applied to decipher complex environmental systems, where direct coupling and indirect coupling both contribute to the observed phenomena, such as microbial aggregation and

contaminant related processes (Zhu et al., 2025). Data-driven interpretation can thus serve as a tool for hypothesis generation while maintaining the mechanistic context for applied chemical research.

Some caveats are warranted, however. The analysis was limited to the physicochemical/operational parameters present in the compiled adsorption data set, and additional solution-chemistry properties or detailed surface functional groups were not explicitly included. Relationships between the machines are also obtained through machine learning and are valid only for the domain of experiments observed, and should not be automatically extended outside of that domain. Future work will confirm experimental validation of the high performance regions identified and will incorporate molecular, structural and mechanistic descriptors. Developing similar multiscale integration may help to better understand material properties and environmental processes, and could be more useful for understanding complex transformations in heterogeneous systems (Fu et al., 2025).

5. Conclusion

The adsorption capacity is controlled by the interplay of several physicochemical and operational parameters, and the initial concentration is the most important and specific surface area is the secondary. The highly nonlinear relationships between the former variables were captured well by nonlinear modeling methods, with random forest having the highest R^2 (0.9725), RMSE (13.65 mg/g), and MAE (3.55 mg/g). Further, there were contrasting effects of specific surface area, column height, pH and pore volume, demonstrating that adsorption behavior cannot be explained simply by considering linear relationships. Process-response analysis revealed that the concentration and the adsorbent surface characteristics are important to consider together if the best adsorption performance is desired. Thus, combining physicochemical interpretation with data-driven modeling is an effective process for determining critical process variables and helping with adsorption optimization. These results could be further validated in the lab with controlled conditions in the future and would help to utilize the results in practical contaminant removal systems.

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