

Comparative Study of Machine Learning Algorithms for Cr(VI) Adsorption Optimization: A Case Study Using KOH-Activated Wood Charcoal

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ABSTRACT. The removal of toxic Cr(VI) ions from industrial wastewater remains a pressing environmental concern due to their high mobility and carcinogenic nature. This study presents a data-driven approach for modeling and optimizing Cr(VI) adsorption onto KOH-activated wood charcoal using various machine learning (ML) algorithms. A dataset derived from batch adsorption experiments was used, involving three operational parameters: initial Cr(VI) concentration (10–50 mg/L), contact time (40–120 min), and adsorbent dose (0.5–1.5 g). Six supervised regression models such as Linear Regression, Decision Tree, Random Forest, Support Vector Machine (SVM), Gradient Boosting, and k-Nearest Neighbors (kNN) were evaluated. Model performance was assessed using the coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE) dan mean square error (MSE). Gradient Boosting and Decision Tree showed superior predictive accuracy, with R^2 values of 0.89 and 0.87, respectively. Feature importance analysis revealed initial concentration as the most influential factor, followed by contact time and adsorbent dosage. These findings highlight the potential of ML as an effective tool for predicting and optimizing adsorption processes in environmental remediation. The integration of ML methods supports efficient decision-making, particularly under constraints of limited experimental data, and aligns with digital transformation strategies in wastewater treatment.

1. INTRODUCTION

Environmental pollution from heavy metal waste, particularly hexavalent chromium Cr(VI), presents a significant concern in global water resource management [1,2]. Cr (VI) demonstrates toxic, carcinogenic, and persistent attributes which create potential hazards to human health and disrupt ecosystem balance [3-5]. Therefore, an efficient technique is required to eliminate Cr (VI) from the environment, one of which involves the adsorption process. Adsorption was selected because to its simplicity, cost-effectiveness, efficiency, and compatibility with both natural and synthesized materials [6-8]. One of the adsorbents with promising prospects is activated wood charcoal using potassium hydroxide (KOH) solution, which is able to expand the surface area and improve the pore structure of the adsorbent so that its performance in binding heavy metal ions becomes more suitable [9,10].

In our earlier investigations [11], the adsorption process of Cr (VI) using KOH-activated wood charcoal has been carried out, providing experimental data that evaluates the influence of various process parameters such as initial Cr (VI) concentration, contact time, and adsorbent mass on removal efficiency[11]. However, despite the experimental results discovered, attempts to systematically optimize the adsorption process still encounter challenges, especially in forecasting adsorption effectiveness based on various parameter combinations. Conventional methods often require multiple extra trials, which are time-consuming, costly, and resource-consuming. Therefore, the adoption of a machine learning-based technique offers an alternative solution with the potential to accelerate the optimization process, enhance prediction accuracy, and identify the most relevant variables without having to conduct all the trials directly [12, 13].

Several research have proved the efficiency of machine learning in the field of water treatment and chemical process prediction, including by constructing predictive models based on algorithms such as Random Forest, Support Vector Machine (SVM), Gradient Boosting, and k-Nearest Neighbors (kNN) [14-18]. These models are not only capable of delivering accurate predictions but can also be used to quantify the influence of each parameter

on process outcomes using feature importance. However, at this point, there is little research fully comparing the effectiveness of several machine learning models for the specific example of Cr (VI) adsorption utilizing KOH-activated wood charcoal. Furthermore, there are few research that focus on establishing the primary parameters controlling adsorption efficiency using this data-driven approach. This represents a research gap which requires to be solved.

Based on this foundational information, the present investigation tries to examine the performance of multiple machine learning algorithms in predicting the adsorption efficiency of Cr (VI) using KOH-activated wood charcoal. The techniques studied include linear regression, random forest, support vector machine, gradient boosting, k-nearest neighbors, and decision tree. In addition to analyzing the level of prediction accuracy of each model based on evaluation metrics such as correlation coefficient (R^2), root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE), and mean square error (MSE). The current research also aims to investigate the variables that most influence the adsorption efficiency through the feature importance approach. Thus, the results of the present research have the potential to contribute to the development of data-based optimization methods in the field of heavy metal waste processing, as well as increase the integration of the idea of Industry 4.0 in the field of environmental technological development.

2. MATERIALS AND METHODS

2.1 Experiment Data

The adsorbent preparation methodology and adsorption procedures were used and have been discussed in detail based on our past research [19]. The variable data used in this investigation were concentration variables, adsorption time, and adsorbent quantity. Several of these characteristics were examined using the percentage of performance result in Cr(VI) removal. The efficiency value was derived using equation (1) with C_0 is the initial concentration of Cr(VI) (mg/L), while C_e is the equilibrium concentration of Cr(VI) (mg/L). The Cr(VI) concentration level after the adsorption process was evaluated using visible spectrophotometry according to the procedures (SNI 6989.71:2009). The parameter variables used in the optimization procedure can be observed in Table 1.

Table 1. Optimization parameter for Cr(VI) removal by KOH-activated wood charcoal

Variable	Lower	Middle	Higher
Initial Cr(VI) concentration (mg/L)	10	30	50
Time (min)	40	80	120
Adsorbent mass (g)	0.5	1	1.5

$$\text{Cr(VI) removal (\%)} = \frac{(C_0 - C_e)}{C_0} \times 100\% \quad (1)$$

2.2 Process Optimization

The optimization process of Cr(VI) adsorption by KOH-Activated Wood Charcoal has been investigated using Orange Data Mining software version 3.38. Model evaluation in the present research was conducted to evaluate the performance of Cr(VI) adsorption efficiency prediction by various machine learning algorithms such as: Linear Regression (LR), Random Forest (RF), Support Vector Machine (SVM), Gradient Boosting (GB), k-Nearest Neighbors (kNN), and Decision Tree (DT). Every model had been developed using a dataset of adsorption experiment results, with input variables in the form of initial Cr(VI) concentration, contact time, and adsorbent amount, while the output target was the percentage of adsorption efficiency. To assure the accuracy of the evaluation, a cross-validation approach (k-fold cross-validation) was utilized with a k value set at 10. Model performance evaluation was carried out by computing many primary metrics, including the correlation coefficient (R^2), root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE) and mean square error (MSE). The R^2 value is used to measure the proportion of target variation that can be explained by the model, whereas RMSE, MAE, MAPE and MSE represent the level of model prediction error in the same units as the original data.

Feature importance analysis was performed to identify the process parameters with the highest impact on Cr(VI) adsorption efficiency. Two techniques were utilized in this study: univariate regression and RReliefF. In univariate regression, each input variable is examined individually against the desired output to quantify its relative contribution to differences in adsorption efficiency. Meanwhile, the RReliefF approach is utilized to account for the relevance and dependency of features by weighting each feature based on its ability to discriminate target values between similar samples. By combining these two methodologies, the results are expected to provide a more thorough view of which variables are most crucial in improving the adsorption process.

Data visualization was made to clarify the interpretation of the model findings and feature importance analysis. The relationship between expected and real values for each model was represented using a predicted vs. actual scatter plot, which indicates how well the model predictions correspond with the actual experimental data. This graphic is furnished with a 45-degree reference line to allow examination of the level of forecast error. In addition, a bar chart is utilized to illustrate the results of the feature importance analysis, where each characteristic (concentration, duration, adsorbent mass) is ordered based on its importance score for efficiency prediction. This representation helps communicate the results intuitively and facilitates analytical interpretation of the performance of each model and the function of input factors in the Cr (VI) adsorption process.

3. RESULTS AND DISCUSSION

3.1 Machine Learning Optimization

The present research evaluated the performance of six machine learning models, namely Linear Regression (LR), Random Forest (RF), Support Vector Machine (SVM), Gradient Boosting (GB), k-Nearest Neighbors (kNN), and Decision Tree (DT), in predicting the adsorption efficiency of Cr(VI) by KOH-activated wood charcoal. The evaluation was carried out based on the R^2 , RMSE, MAE, MAPE, and MSE values using a 10-fold cross-validation approach. Table 2 displays the R^2 , RMSE, MAE, MAPE, and MSE for each model. Based on the data collected, the Gradient Boosting model exhibited the best performance with a R^2 value of 0.896, followed by the Decision Tree model with a R^2 value of 0.881, the Random Forest model with a R^2 value of 0.801, and the Linear Regression model with a R^2 value of 0.798. While the SVM and kNN models showed low R^2 values, so the predictions of the two models regarding adsorption efficiency were still less accurate. In addition, the accuracy level of the Gradient Boosting model may be confirmed using the RMSE, MAE, MAPE, and MSE values that represent the minimal prediction error. Thus, it can be stated that the Gradient Boosting model is more successful in optimizing and forecasting the results of Cr(VI) adsorption by KOH-activated wood charcoal compared to numerous other models.

Table 2. Performance of Several Machine learning Model Optimization

Model	R^2	RMSE	MAE	MAPE	MSE	Actual Removal (%)	Prediction Removal (%)
Linear Regression	0.798	4.029	3.212	0.043	16.233	96.996	97.072
Random Forest	0.804	3.969	2.882	0.038	15.756	96.996	92.994
SVM	0.270	7.658	4.757	0.065	58.652	96.996	84.041
Gradient Boosting	0.896	2.888	1.754	0.023	8.340	96.996	95.745
kNN	0.549	6.022	4.095	0.057	36.261	96.996	91.751
Decision-Tree	0.881	3.092	2.025	0.026	9.563	96.996	93.797

The results presented suggest that the relationship between process parameters (initial concentration, contact time, and adsorbent mass) and adsorption efficiency is complex and nonlinear and involves interactions between variables that are not simple, thus requiring a predictive model that is able to capture this complexity. Gradient boosting, as a boosting-based ensemble model, works by developing a decision tree gradually to rectify errors from prior forecasts, thereby being able to capture more subtle and accurate relationship patterns. Through feature importance analysis, it is known that the initial Cr(VI) concentration parameter has the biggest impact to the prediction of adsorption efficiency, followed by contact time, and then adsorbent mass. These results suggest that the efficacy of the adsorption process in lowering Cr(VI) levels is more sensitive to fluctuations in the initial concentration of the metal ions in the solution. In reality, this means that to optimize adsorption performance, the main attention should be directed to controlling the concentration of heavy metal sources.

Furthermore, gradient boosting successfully identified the possible existence of nonlinear interaction phenomena between process parameters. As an example, the model shows that enhancing the adsorbent mass is effective in increasing efficiency only within a specific concentration range. At extremely high Cr(VI) amounts, even when the adsorbent amount is increased, the efficiency does not increase proportionally due to the limited number of available active sites, indicating saturation of the adsorbent surface. It demonstrates the significance of optimizing operational parameters to avoid unnecessary waste of adsorbent material. The model also reveals the kinetic characteristics of Cr(VI) adsorption, including a significant increase in efficiency at the initial contact time, which then slows down until it reaches a state close to equilibrium. This phenomenon is in accordance with the general physicochemical adsorption mechanism, where active sites on the adsorbent surface are abundant in the initial stage but decrease over time due to being occupied by metal ions. Thus, gradient boosting not only provides accurate predictions but also enriches the understanding of the adsorption dynamics that occur in this system.

Another key element shown by the model results is its capacity to recognize extreme settings when adsorption efficiency diminishes, such as extremely lengthy contact durations or very high metal concentrations. These conditions may be connected to secondary reaction events, changes in the physical properties of the adsorbent (such as pore blockage), or the creation of a passive layer on the adsorbent surface. By being able to predict the effects of these parameters, gradient boosting can assist design adsorption systems that are more effective and efficient in terms of energy, time, and material utilization.

Despite its predictive character, a sensitivity analysis of the gradient boosting model suggests that the initial Cr(VI) concentration is the important variable that needs to be managed most in the design and operation of adsorption units. To improve process efficiency in industry, design improvements should involve reducing the initial concentration by pretreatment or increasing the availability of active adsorbent sites through material modification. This finding accords with modern wastewater treatment concepts that prioritize efficacy, energy efficiency, and material sustainability. The deployment of the gradient boosting model in this study illustrates the integration of Industry 4.0-based machine learning technologies into environmental management. This approach not only improves forecast accuracy but also accelerates data analysis, process optimization, and data-driven decision-making for the treatment of hazardous waste such as Cr(VI) ions. Thus, the application of gradient boosting in forecasting Cr(VI) adsorption effectiveness offers a new paradigm in the design and optimization of water treatment systems, ultimately contributing to global efforts in maintaining environmental sustainability.

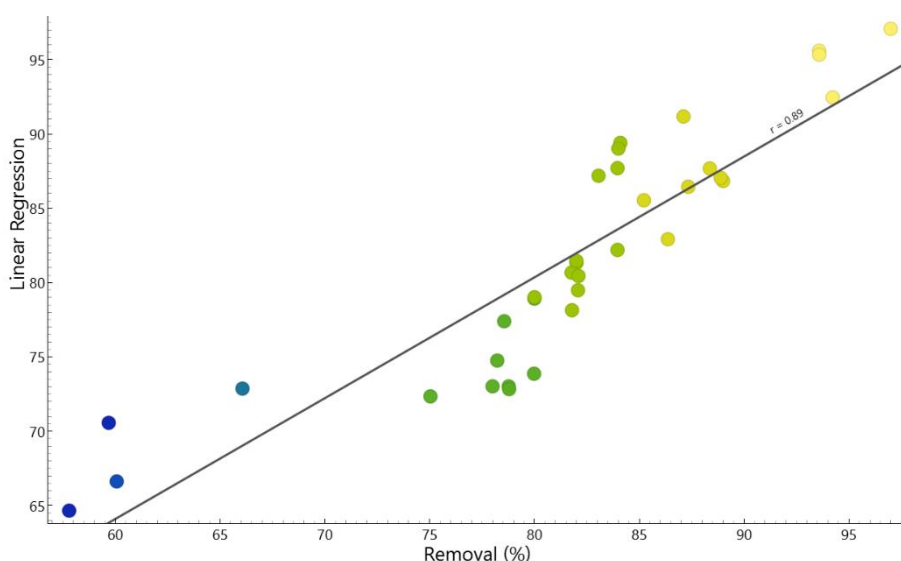


Figure 1. Linear Regression

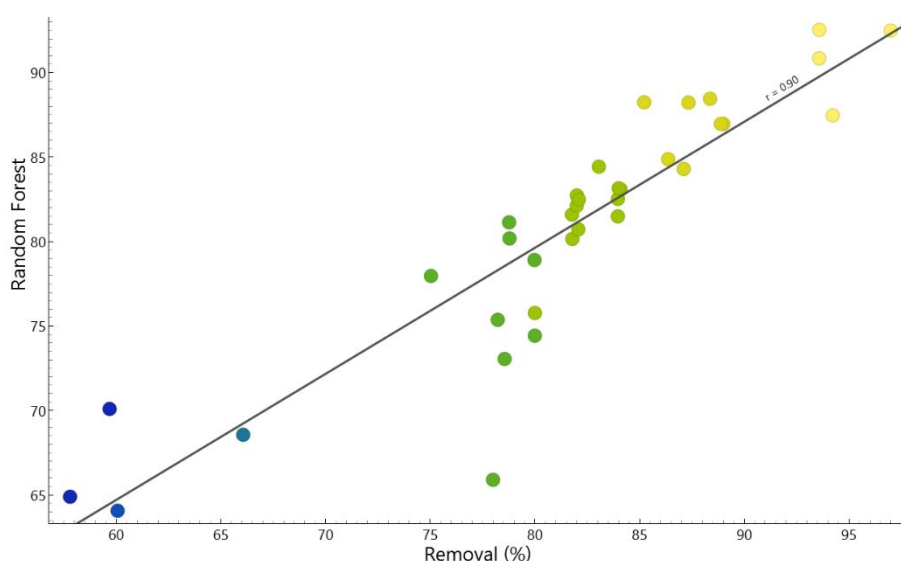


Figure 2. Random Forest

For additional verification and analyze the accuracy and generalization capabilities of each machine learning model utilized, a scatter plot was visualized comparing the model's projected adsorption efficiency values with the actual experimental values. This scatter plot serves as a visual help to examine the extent to which the model's

predictions approximate the actual findings. The closer the model is to the diagonal line ($y = x$), the more accurate the model's predictions are. Figures 1 to 6, respectively, exhibit visualizations of the projected vs actual values for each model: linear regression, decision tree, random forest, support vector machine (SVM), gradient boosting, and k-nearest neighbors (kNN). The y-axis displays the predicted number calculated from the machine learning model, whilst the x-axis indicates the removal percentages achieved through laboratory experiments. In each scatter plot, points distributed close to the diagonal line indicate a good fit between the prediction and the actual data, while points scattered far from the diagonal line indicate a deviation from the predictions. This representation provides a straightforward overview of each model's predicted performance and allows for the identification of potential overfitting or underfitting.

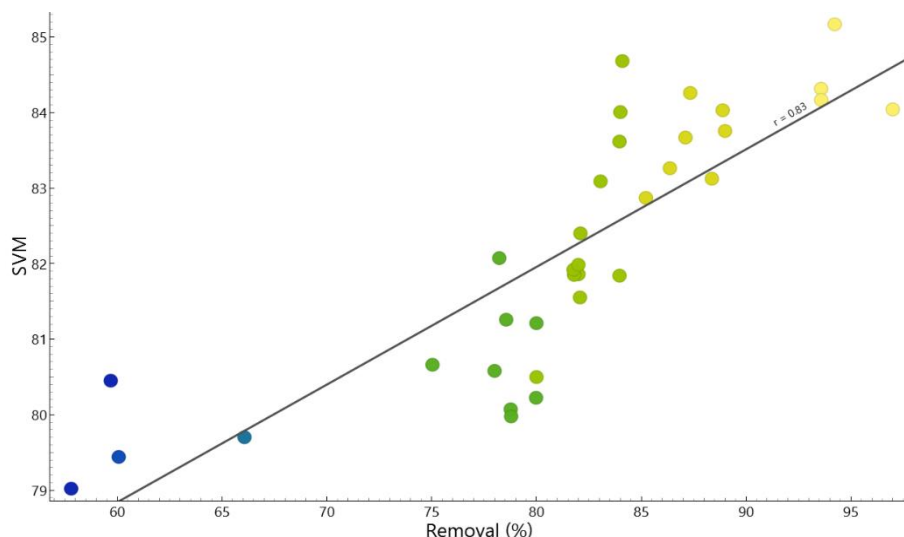


Figure 3. SVM

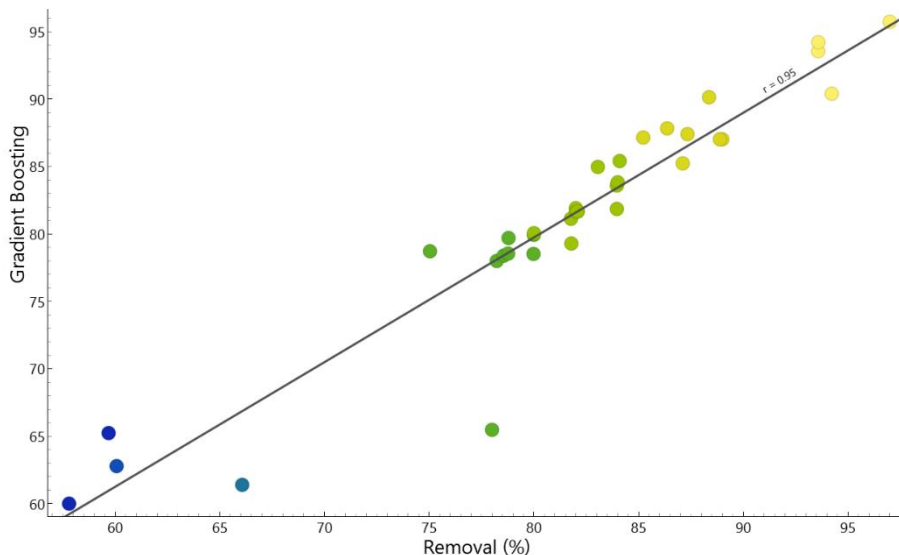


Figure 4. Gradient Boosting

3.2 Feature Importance Analysis

In the present research, two alternative techniques were utilized to evaluate feature importance, namely univariate regression and RReliefF. The univariate regression method examines the contribution of each input variable to the target variable (in this example, Cr(VI) adsorption efficiency) independently. Each feature was examined by developing a one-variable linear regression model, where one feature was used to predict the final outcome [20], [21]. The results of this approach indicate the strength of the linear relationship between each characteristic and the adsorption efficiency, without considering the interactions between the features. Although

this method is simple and effective, its drawbacks lie in its inability to capture the combined effects between variables and the risk of bias owing to multicollinearity[22].

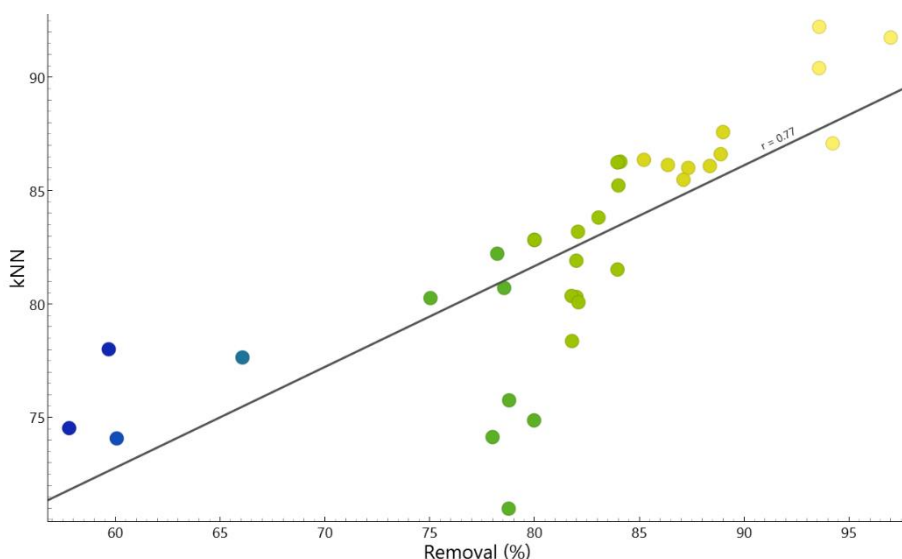


Figure 5. kNN

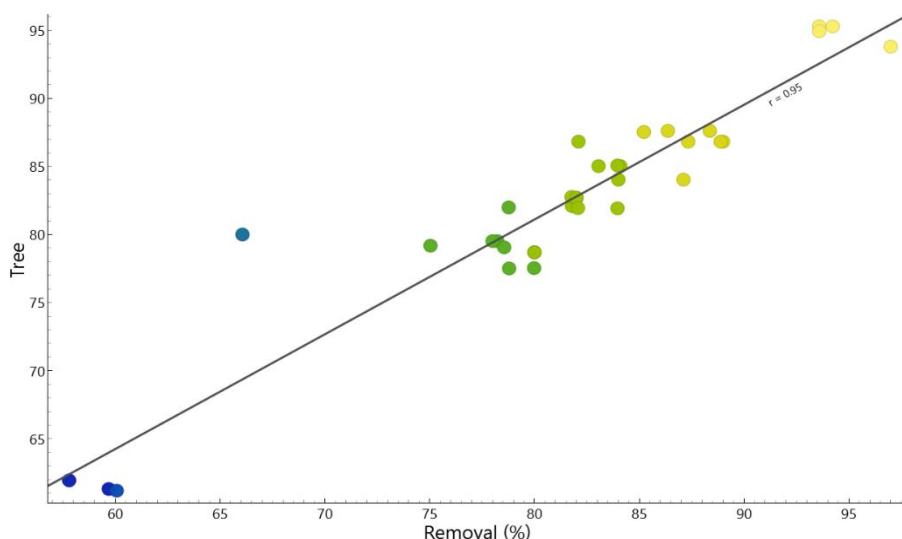


Figure 6. Decision Tree

In contrast, the RReliefF (Regression Relief F) technique is a model-agnostic method that evaluates feature relevance based on how well a feature distinguishes across samples with various target values [23], [24]. This algorithm operates by comparing each data instance with its nearest neighbor and analyzing if the difference in feature values correlates with the difference in target values [25], [26]. Features that reliably discriminate across instances with different goal values will obtain higher significance scores. RReliefF has the advantage of capturing non-linear correlations and interactions between features, making it more adaptable for usage with complex experimental data. By comparing the findings of these two methodologies, a more holistic picture of the variables that most influence the effectiveness of the adsorption process is obtained.

The analytical results based on these two methodologies are shown in Tables 3 and 4. The univariate regression analysis produced similar feature scores across all machine learning models, as this method evaluates the direct statistical correlation between each operational parameter and adsorption efficiency irrespective of the learning techniques. This consistency suggests that the impact of each variable is determined by its intrinsic connection with the response, rather than by model-specific characteristics. The initial concentration demonstrated the highest univariate score among the assessed parameters, underscoring its pivotal influence on the adsorption

process, succeeded by the contact time and the quantity of adsorbent. The significant impact of initial concentration is due to the enhanced mass transfer driving force resulting from steeper concentration gradients, whereas the influence of contact time relates to adsorption kinetics and the achievement of equilibrium. The comparatively diminished impact of adsorbent dosage is likely attributable to the saturation of active sites at elevated dosages.

Table 3. Results of analysis of influential factors based on univariate regression values

Model	Variable		
	Initial concentration	Time	Adsorbent mass
Linear Regression	27.471	9.853	0.074
Random Forest	27.471	9.853	0.074
SVM	27.471	9.853	0.074
Gradient Boosting	27.471	9.853	0.074
kNN	27.471	9.853	0.074
Decision-Tree	27.471	9.853	0.074

The data collected suggests the initial concentration of Cr(VI) is the most significant aspect controlling adsorption performance, followed by contact time, while the adsorbent mass gives the lowest contribution in all models studied. The substantial effect of the initial concentration can be explained by the adsorption mechanism itself, where higher the concentration of the heavy metal solution leads to an enhanced concentration gradient between the liquid phase and the adsorbent surface. This state boosts the driving force for the diffusion of Cr(VI) ions to the active sites of the adsorbent, hence increasing the amount of ions successfully collected in a given unit of time.

Table 4. Results of analysis of influential factors based on RReliefF values

Model	Variable		
	Initial concentration	Time	Adsorbent mass
Linear Regression	0.521	0.420	0.297
Random Forest	0.510	0.424	0.307
SVM	0.504	0.416	0.313
Gradient Boosting	0.465	0.393	0.264
kNN	0.483	0.405	0.292
Decision-Tree	0.489	0.395	0.291

The Gradient Boosting model, for example, assigns the highest priority score to the concentration variable, with a contribution proportion above 50% to the efficiency variation in the training data. This conclusion is consistent with prior literature reports conducted by Kumar et al. al, 2019 [27] and Dermawan et al, 2025 [28], It suggests that at low concentrations, adsorption performance can be limited by the small number of dissolved ions available to interact with the adsorbent surface. The contact time variable ranks second in terms of its influence on adsorption efficiency. This highlights the essential time dynamics in the mass transport process and surface equilibrium. Although not as powerful as concentration, the contact time between the Cr(VI) solution and the adsorbent surface permits ions to be more broadly disseminated to the active sites. Increasing the contact time till the system finds equilibrium[29]. This is represented in the Support Vector Machine model, which yields a medium feature importance score for the time variable, with a contribution ranging from 25% to 35% to the model output.

Meanwhile, adsorbent mass contributed the least to the variation in adsorption efficiency, with its significance score consistently below 20% across all models. This anomaly can be explained by the probability that within the studied adsorbent mass range (0.5–1.5 grams), the available active surface area is sufficient for the adsorption process, such that increasing the mass does not considerably improve the efficiency. In this setting, the system has reached a saturation point when future increases in the amount of adsorbent have a negligible influence on the overall performance. This analysis decision-making in experimental design and the creation of more efficient adsorption systems. By focusing on the most relevant variables, such as concentration and contact time, the optimization process can be carried out in a more targeted and resource-efficient manner. Furthermore, these results further illustrate the usefulness of machine learning methodologies in providing a more thorough and data-driven knowledge of the adsorption process.

The results of this research reveal that selecting an appropriate machine learning model greatly improves the prediction accuracy in optimizing the Cr(VI) adsorption process. The Gradient Boosting model successfully captures the non-linear relationship between input and output variables, which cannot be properly handled by the Linear Regression model. This validates observations in the literature that heavy metal adsorption systems are generally complex due to multi-parameter interactions such as diffusion, surface reactions, and adsorbate competition. Another notable discovery is the dominance of the initial Cr(VI) concentration parameter on adsorption efficiency. This is in line with the physicochemical adsorption mechanism, where increasing the concentration raises the potential difference between the adsorbate in solution and the adsorbent surface, hence accelerating mass transfer. The effects of duration and adsorbent mass were also observed but were relatively smaller compared to concentration. This is understandable, considering that extended contact times normally only increase efficiency until equilibrium conditions are reached, while fluctuations in adsorbent mass within the utilized range tend to have a saturation effect.

The advantages of employing Orange Data Mining in this study lay in the ease of exploring multiple models, analyzing feature importance, and visualizing results, all of which support the notion of integrating Industry 4.0 technology into environmental research. The adoption of a machine learning approach accelerates the optimization process, lowers the need for further tests, and enhances the behavior of the adsorption system. However, many limitations should be recognized. The dataset employed in this study was rather short (50 data combinations), which may limit the generalizability of the model to industrial-scale adsorption systems. Therefore, further research is required utilizing a larger dataset, including more additional factors such as pH, temperature, and particle size.

4. CONCLUSION

The present study examined the performance of multiple machine learning models including Linear Regression, Random Forest, Support Vector Machine, Gradient Boosting, k-Nearest Neighbors, and Decision Tree in modeling and optimizing the adsorption efficiency of Cr(VI) by KOH-activated wood charcoal. The evaluation findings showed that the Gradient Boosting model gave the best prediction performance, with a R^2 value approaching 0.90, showing a high competence in expressing the non-linear relationship between operational parameters. Through feature importance analysis, it was found that the initial Cr(VI) concentration was the most impactful variable on the adsorption efficiency. boosting the concentration enhanced the driving force of metal ion diffusion to the adsorbent surface, thus speeding and boosting the adsorption capacity. Contact time ranked second, highlighting the crucial role of temporal dynamics in establishing adsorption equilibrium. In contrast, the adsorbent mass showed a smaller contribution, showing that increasing the mass within the investigated range did not significantly improve the efficiency, probably due to the saturation of active sites. The results of the present research demonstrate that the machine learning approach is not only beneficial in enhancing the accuracy of adsorption efficiency estimates but also provides in-depth insights into the sensitivity of each process parameter. This understanding is vital for designing efficient and cost-effective wastewater treatment systems and supporting the use of data-driven technology to assist the development of more sustainable environmental processes.

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