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Predictive Analysis of the Adsorption of Nickel (II) Ion from Industrial Wastewater using Regression Algorithm

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Abstract - ***The removal of heavy metals from industrial wastewater remains a major environmental challenge, particularly for nickel-contaminated effluents generated by electroplating, mining, and metal-finishing industries. In this study, the dynamic adsorption behaviour of Ni^{2+} ions in a fixed-bed column packed with modified nanocellulosic adsorbents was investigated, and a machine learning-nbased predictive framework was developed to enhance process modelling. Breakthrough data obtained under varying operating conditions namely bed height, influent concentration, and flow rate were analysed using three conventional kinetic models: Thomas, Weibull, and Wolborska. Among these models, the Thomas model provided the best representation of the adsorption process, exhibiting the highest agreement with experimental data ($R^2 > 0.97$), while the Weibull and Wolborska models showed comparatively lower predictive capability. To overcome limitations associated with traditional kinetic modelling, a Support Vector Machine (SVM) regression approach was implemented to predict Ni^{2+} removal efficiency. The Cubic SVM model demonstrated strong predictive performance with a coefficient of determination (R^2) of 0.90 and low prediction errors (RMSE = 4.78, MSE = 22.85, MAE = 3.66). Diagnostic evaluation using predicted–actual plots and residual analysis confirmed the robustness and reliability of the developed model. The results demonstrate that integrating experimental adsorption studies with machine learning algorithms significantly improves the predictive capability and optimization of fixed-bed adsorption systems. This hybrid modelling framework offers a promising strategy for designing efficient and sustainable adsorption processes for heavy metal removal from wastewater.***

Keywords: Dynamic Adsorption; Nickel (II) Removal; Nanocellulose Adsorbent; Regression Analysis; Machine Learning Modelling.

I. INTRODUCTION

The deterioration of global freshwater resources has become one of the most critical environmental challenges of the twenty-first century. Rapid industrialization, urban expansion, and population growth have substantially increased the discharge of untreated or partially treated wastewater into natural water bodies, leading to severe degradation of aquatic ecosystems and potential risks to human health. Industrial wastewater streams frequently contain complex mixtures of contaminants, including dyes, pharmaceuticals, nutrients, and heavy metals, many of which exhibit persistent and toxic characteristics that complicate their removal from water systems (Crini & Lichtfouse, 2019; Fu & Wang, 2011). The increasing demand for clean water coupled with limited freshwater resources has therefore intensified the need for efficient and sustainable water treatment technologies.

Among various water pollutants, heavy metals are considered particularly hazardous due to their non-biodegradable nature, long environmental persistence, and potential for bioaccumulation within biological systems. Once introduced into aquatic environments, heavy metals may accumulate in sediments and living organisms, thereby entering the food chain and posing significant ecological and human health risks (Ali et al., 2019; Li et al., 2019). Exposure to elevated concentrations of heavy metals has been associated with numerous adverse health effects, including neurological disorders, kidney damage, and carcinogenic outcomes depending on the type and concentration of the metal involved (Tchounwou et al., 2012).

Nickel is one of the heavy metals frequently detected in industrial wastewater. It is widely used in numerous industrial processes including electroplating, stainless steel production, catalysts manufacturing, battery fabrication, and pigment synthesis. As a result, large quantities of nickel-containing effluents are discharged from metallurgical, electrochemical, and mining industries (Liu et al., 2020). In aqueous

environments, nickel is predominantly present in the divalent form (Ni^{2+}), which is relatively stable and highly soluble under a wide range of environmental conditions. Although nickel may serve as a trace element in certain biological processes, excessive exposure can lead to severe health complications such as dermatitis, respiratory disorders, kidney damage, and carcinogenic effects (Genchi et al., 2020). Consequently, strict regulatory limits have been established for nickel concentrations in drinking water and industrial discharge to protect both human health and aquatic ecosystems.

Various physicochemical treatment technologies have been developed for the removal of heavy metals from wastewater. Conventional techniques include chemical precipitation, ion exchange, membrane filtration, electrochemical treatment, and coagulation–flocculation. While these methods can effectively reduce heavy metal concentrations under controlled conditions, their practical implementation is often limited by several disadvantages such as high operational costs, generation of secondary sludge, membrane fouling, and complex operational requirements (Bolisetty et al., 2019; Crini & Lichtfouse, 2019). These limitations have stimulated extensive research efforts toward developing more efficient, cost-effective, and environmentally sustainable treatment approaches.

Among the available technologies, adsorption has emerged as one of the most promising techniques for heavy metal removal from aqueous solutions due to its operational simplicity, high removal efficiency, and minimal generation of secondary pollutants. Adsorption processes can utilize a wide variety of natural, synthetic, and waste-derived materials as adsorbents, which enhances their potential for large-scale application in wastewater treatment systems (Foo & Hameed, 2010; Li et al., 2019, Prithirivajan et. Al., 2024.). Conventional adsorbents such as activated carbon, zeolites, and polymeric resins have demonstrated excellent adsorption performance for various pollutants; however, their high production and regeneration costs may limit their widespread industrial use.

Recent advances in materials science have therefore focused on the development of sustainable and renewable adsorbent materials derived from natural resources. Among these materials, nanocellulose has attracted considerable attention due to its high surface area, mechanical stability, biodegradability, and abundance of hydroxyl functional groups that can be chemically modified to enhance adsorption performance. Functionalized nanocellulose-based materials have demonstrated excellent adsorption capacity for heavy metal ions, making them promising candidates for environmentally sustainable water purification technologies (Etuk V. et al., 2018; Klemm et al., 2018; Trache et al., 2020). Furthermore, surface functionalization strategies such as carboxylation, oxidation, and grafting of chelating groups have been shown to significantly improve the metal binding affinity of nanocellulose adsorbents.

In industrial wastewater treatment applications, adsorption processes are often implemented using fixed-bed column systems because they enable continuous operation and provide valuable design information for large-scale implementation (Bandar et al., 2023; Banza et al., 2022; Chen et al., 2024). Fixed-bed columns allow efficient contact between the adsorbent and the contaminated solution while facilitating the evaluation of important operational parameters such as bed height, flow rate, and influent concentration. The dynamic performance of a fixed-bed adsorption system is commonly described using breakthrough curves, which represent the variation of effluent concentration as a function of time or treated volume (Bohart & Adams, 1920; Worch, 2012). Breakthrough curve analysis provides essential information for understanding mass transfer mechanisms and predicting column performance under different operating conditions.

To describe the dynamic behavior of adsorption columns, several mathematical models have been developed. Among the most widely applied models are the Thomas, Wolborska, and Weibull models, which are frequently used to analyze breakthrough curves and estimate key parameters such as adsorption capacity and kinetic constants (Han et al., 2009; Yan et al., 2017). Although these classical models provide valuable insights into adsorption mechanisms, they

often rely on simplifying assumptions that may not fully capture the complex nonlinear interactions occurring in real wastewater treatment systems.

In recent years, data-driven modeling approaches have gained significant attention for analyzing complex environmental processes. Machine learning (ML), a rapidly evolving branch of artificial intelligence, offers powerful computational tools capable of identifying hidden patterns within large datasets and generating predictive models without requiring explicit mechanistic equations (Jordan & Mitchell, 2015). Machine learning techniques have been successfully applied in numerous environmental engineering applications, including pollutant prediction, wastewater treatment optimization, and process control (Chen et al., 2020; Mosavi et al., 2019). These methods are particularly effective for modeling nonlinear relationships between operational variables and system performance.

Regression-based machine learning algorithms represent one of the most commonly used approaches for predictive modeling in chemical and environmental engineering. Algorithms such as linear regression, support vector regression, decision tree regression, Gaussian process regression, and artificial neural networks have been widely applied to model adsorption processes and predict pollutant removal efficiencies (Hastie et al., 2009; Pirbazari et al., 2021). These approaches enable the development of predictive models capable of estimating adsorption performance under varying operational conditions, thereby reducing experimental costs and improving process optimization.

Despite the growing number of studies on adsorption-based removal of heavy metals, most investigations rely primarily on conventional deterministic models for describing adsorption dynamics in fixed-bed systems. Such models may not adequately capture the complex nonlinear interactions among operational variables that influence adsorption performance in real wastewater systems. Furthermore, the integration of machine learning techniques with experimental adsorption data for predicting nickel removal efficiency in fixed-bed systems remains relatively limited.

Therefore, the present study aims to develop a predictive framework that integrates classical adsorption modeling with machine learning regression techniques to analyze the dynamic removal of Ni^{2+} ions in a fixed-bed adsorption system. Experimental adsorption data are combined with regression algorithms implemented in MATLAB to construct predictive models capable of estimating adsorption efficiency under different operating conditions. In addition, the study evaluates the performance of classical breakthrough models, including the Thomas, Wolborska, and Weibull models, alongside machine learning-based regression approaches. This integrated approach provides a comprehensive comparison between mechanistic adsorption models and data-driven predictive techniques for improving the design and optimization of adsorption-based wastewater treatment systems.

II. MATERIALS AND METHODS

The predictive modelling framework developed in this study was based on an experimentally generated adsorption dataset previously submitted to the Department of Chemical Engineering (Etuk, 2022). The dataset was derived from fixed-bed column experiments investigating the adsorption behaviour of Ni^{2+} ions from aqueous solution using magnetic nanocellulosic adsorbents (Etuk et al. 2021; Etuk et al., 2022). Experimental adsorption datasets of this nature are widely used for the development of predictive adsorption models because they contain information on process variables that strongly influence adsorption performance in dynamic column systems. The dataset comprised several independent process variables that are known to influence fixed-bed adsorption performance, including influent metal ion concentration, hydraulic residence time, influent flow rate, and bed height. These parameters were selected because they directly affect mass transfer dynamics, residence time, and breakthrough behaviour in fixed-bed adsorption systems (Yanyan et al., 2018). The dependent variable used for model development was adsorption efficiency, expressed as the percentage removal of Ni^{2+} ions from the influent stream.

2.1 Development of the regression-based predictive model

A regression-based machine learning framework was implemented to establish a predictive relationship between the operating parameters of the adsorption system and the resulting adsorption efficiency. The predictive model was developed using the Regression Learner Toolbox embedded in MATLAB (MathWorks Inc., USA). MATLAB has become a widely adopted computational platform in chemical engineering and environmental modelling due to its extensive machine learning libraries and capability for rapid algorithm implementation (MathWorks, 2022; Wang et al., 2020).

2.1.2 Preprocessing and variable selection

Prior to model development, the dataset was imported into the MATLAB computational environment either through the graphical user interface or through MATLAB script commands. This is an essential step in machine learning model development which ensures that the dataset is appropriately structured for algorithm training and evaluation. The variables in the dataset were categorized into predictor variables and response variables. The predictor variables were initial adsorbate concentration (C_0), breakthrough or contact time (t_β), Influent flow rate (Q) and Adsorbent bed height (H). These variables were selected because they are well-established operating parameters that influence adsorption kinetics, residence time distribution, and mass transfer behaviour in fixed-bed adsorption systems. The response variable used in the modelling framework was adsorption efficiency, representing the percentage removal of Ni^{2+} ions from the wastewater stream.

Dataset partitioning: - To ensure unbiased model training and performance evaluation, the dataset was partitioned into training and testing subsets. Approximately 50% of the dataset was allocated for model training, while the remaining 50% was reserved for independent testing and prediction.

Dataset partitioning is a standard practice in machine learning because it allows the predictive capability of a trained model to be evaluated on previously unseen data (Pirbazari et al., 2021). This approach minimizes the risk of model overfitting, and improves the generalization capability of the predictive model. Following dataset partitioning, the training subset was used to develop regression models capable of predicting adsorption efficiency from the selected process variables. The Regression Learner application in MATLAB allows multiple regression algorithms to be evaluated simultaneously, enabling the identification of the model with the best predictive performance.

Regression-based machine learning algorithms are particularly suitable for adsorption modelling because they can approximate complex nonlinear relationships between adsorption variables and system performance (Jawad et al., 2020; Semero et al., 2018). During the training stage, the algorithm iteratively adjusts model parameters to minimize the difference between predicted and observed values of adsorption efficiency.

Several regression model families frequently applied in environmental and process modelling were evaluated, including linear regression models, regression tree–based models, support vector machine (SVM) regression, Gaussian process regression (GPR), ensemble learning approaches, and artificial neural network (ANN) regression. These algorithms differ significantly in their capability to capture nonlinear relationships, computational complexity, generalization ability, and robustness to noise present in experimental datasets. For example, linear regression models are computationally efficient but often limited in representing complex nonlinear systems, whereas machine learning approaches such as SVMs, ensemble methods, and neural networks are capable of modelling highly nonlinear interactions among process variables and have demonstrated improved predictive performance in environmental and adsorption modelling applications (Hastie et al., 2009; Bishop, 2006; Chen et al., 2020; Li et al., 2022). The comparative evaluation of these algorithms allows the identification of the most appropriate model for predicting adsorption performance.

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2.2 Model validation and performance evaluation

The predictive accuracy of the trained models was evaluated using widely accepted statistical performance metrics. Model validation is essential for assessing the reliability of predictive tools used in environmental process modelling (Wang et al., 2020). The following statistical indicators were used to evaluate model performance: -

Root Mean Square Error (RMSE); RMSE measures the standard deviation of the residuals and indicates how closely predicted values match the observed values. It is given by;

$$\text{RMSE} = \sqrt{\frac{1}{n}} \sum_{i=1}^{n} (q_{e,exp} - q_{e,calc})^2$$

Where, $q_{e,exp}$ = observed (experimental) value, $q_{e,calc}$ = predicted value from the model, and n = number of observations.

Mean Absolute Error (MAE) MAE quantifies the average magnitude of prediction errors without considering their direction.

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} (q_{e,exp} - \hat{q}_{e,calc})$$

Coefficient of Determination (R^2) R^2 represents the proportion of variance in the response variable that is explained by the predictive model.

$$R^2 = \frac{(q_{e,exp} - q_{e,calc})^2}{\sum_{i=1}^{n} (q_{isotherm} - q_{e,calc})^2 - (q_{isotherm} - q_{e,calc})^2}$$

These statistical indicators are widely used in adsorption modelling and machine learning applications for environmental systems because they provide complementary information about prediction accuracy and model robustness (Hastie et al., 2009; Semero et al., 2018).

Models exhibiting lower RMSE and MAE values combined with higher R^2 values were considered to have superior predictive capability

2.2.1 Model deployment and prediction

After the performance evaluation stage, the regression algorithm that demonstrated the best predictive performance was selected as the final predictive model. The selected model was subsequently exported from the MATLAB Regression Learner environment to generate an executable MATLAB script. The exported model was then applied to the testing dataset, which had not been used during the training stage. This step enabled the generation of predictions for adsorption efficiency under varying operational conditions. Testing the model on unseen data provides a realistic evaluation of the model's predictive capability and ensures that the developed regression model can be applied for forecasting adsorption performance in practical wastewater treatment wastewater scenarios (Jawad et al., 2020; Wang et al., 2020).

III. RESULTS AND DISCUSSION

The three widely applied kinetic models, namely: - Weibull, Thomas, and Wolborska were evaluated to describe the dynamic adsorption behaviour of Ni^{2+} ions onto magnetic nanocellulosic adsorbent. The model parameters were obtained from nonlinear regression analysis under different operating conditions of different bed height (4cm, 8cm, and 12cm), different flow rate (4ml/min, 8ml/min and 12ml/min) and different initial solute concentration (50mg/L, 100mg/L and 150mg/L). The performance of each model was assessed using the coefficient of determination (R^2), which quantifies the degree of agreement between predicted and experimental breakthrough data.

Across all experimental conditions, the Thomas model consistently exhibited the highest R^2 values, generally exceeding 0.97. This indicated that the Thomas model provided the most reliable representation of the dynamic adsorption behavior of Ni^{2+} ions in the investigated fixed-bed system with the magnetic nanocellusic adsorbents. Similar observations have been reported in adsorption studies involving heavy metals in continuous column systems (Yan et al., 2017; Banza et al. 2022: Bandar et al., 2023; Prithivirajan et al., 2024).

3.1.1 Effect of bed height on adsorption performance

Increasing the bed height from 4 to 12 cm significantly influenced adsorption behaviour. The equilibrium adsorption capacity predicted by the Thomas model decreased from approximately 21534 mg g^{-1} to 12509 mg g^{-1} as bed height increased. This behaviour can be attributed to enhanced mass transfer resistance and longer diffusion pathways within deeper adsorbent beds (Worch, 2012, Rahman et al., 2024; Chen et al., 2024).

Despite this decline in calculated adsorption capacity, the coefficient of determination improved with increasing bed height, reaching values as high as 0.9946. This indicates that higher bed heights improve model predictability by stabilizing the mass transfer zone (MTZ) and creating more uniform adsorption conditions along the column. In contrast, the Weibull model exhibited declining R^2 values with increasing bed height, suggesting limited ability to capture the dynamic adsorption behaviour under these conditions.

3.1.2 Effect of influent flow rate

Increasing the influent flow rate from 4 to 12 mL min^{-1} resulted in an increase in the Thomas rate constant (K_{th}) from approximately 3.22×10^{-4} to 1.80×10^{-3} L mg^{-1} min^{-1}. The increase in rate constant suggests enhanced mass transfer kinetics at higher flow rates due to improved convective transport of solute molecules. However, the adsorption capacity (q_e) decreased significantly from 15235 mg g^{-1} to 6463 mg g^{-1}. This reduction is attributed to reduced residence time within the adsorption column, which limits the opportunity for Ni^{2+} ions to interact with active adsorption sites (Shafeeyan et al., 2014). Although the Wolborska model captured some aspects of early breakthrough behaviour, its predictive accuracy remained lower than that of the Thomas model.

3.1.3 Effect of initial Ni^{2+} concentration

Increasing influent Ni^{2+} concentration from 50 mg L^{-1} to 150 mg L^{-1} significantly influenced adsorption kinetics. Higher influent concentrations increased the driving force for mass transfer, resulting in higher adsorption capacities. However, the Thomas rate constant decreased with increasing concentration. This trend indicates that although adsorption capacity increases, the overall adsorption kinetics become slower due to saturation of available adsorption sites (Foo and Hameed, 2017; Sheikhi et al., 2023). The results confirm that Ni^{2+} adsorption in the present system is governed primarily by external film diffusion and intraparticle diffusion mechanisms, consistent with findings reported for other heavy metal adsorption systems (Albadarin et al., 2017).

3.3 Machine Learning–Based Predictive Regression Model

Machine learning techniques have recently emerged as powerful tools for predicting adsorption performance in complex environmental systems due to their ability to capture nonlinear interactions between process variables (Hastie et al., 2009; Madhukumar et al., 2022, Chen et al., 2024).

In this study, a predictive regression model was developed to estimate nickel (II) removal efficiency (%R) under different operating conditions using experimental adsorption data on the basis of the following parameters: adsorbent mass (m, g), bed height (H, cm), influent flow rate (Q, mL min^{-1}), nitial Ni^{2+} concentration (C_o, mg L^{-1}), breakthrough time (t_b, min). The complete dataset was divided into training and testing subsets, each representing approximately 50% of the available data. A 3-fold cross-validation procedure was applied during model training to minimize overfitting and improve generalization capability.

The trained regression model was applied to this dataset to predict Ni^{2+} removal efficiency under previously unseen operating conditions.

The training dataset contains both predictor variables and the response variable (%R). These data were used to train several regression algorithms and identify the model with the highest predictive accuracy. The training dataset used for regression model development is presented in Table 3.1

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Table 3.1 Training dataset used for model development

Adsorbent	M (g)	H (cm)	Q (mL min^{-1})	C_0 (mg L^{-1})	t_b (min)	Removal Efficiency (%R)
C-NFC	4	4	8	100	60	37.37
C-NFC	8	8	8	100	100	43.62
C-NFC	12	12	8	100	130	62.62
C-NFC	4	4	4	100	80	40.54
C-NFC	4	4	12	100	15	30.00

Also, an independent testing dataset was used to evaluate the predictive capability of the developed model. The dataset is shown in Table 4.6.

Table 3.2 Test dataset used for model validation

Adsorbent	M (g)	H (cm)	Q (mL min^{-1})	C_0 (mg L^{-1})	t_b (min)
C-NFC	4	4	8	150	100
C-NFC	4	4	8	50	90
MF-NFC	4	4	4	100	75
MNFC	4	4	12	100	60
MF/MNFC	4	4	12	100	140

3.4 Model selection and performance evaluation

Several regression algorithms were evaluated to determine the most suitable predictive model. Among them, the Support Vector Machine (SVM) algorithm demonstrated the highest predictive accuracy. The Cubic Support Vector Machine regression model was therefore selected as the optimal predictive model. The performance of the developed model was evaluated using standard statistical indicators including: Root Mean Square Error (RMSE), Mean Squared Error (MSE), Mean Absolute Error (MAE)Coefficient of determination (R^2).

Table 3.3 Performance metrics of the regression model

Metric	Value
RMSE	4.7804
MSE	22.852
MAE	3.655
R^2	0.90
Prediction speed	540 observations s^{-1}
Training time	15.05 s
Algorithm	Support Vector Machine
Selected model	Cubic SVM

The coefficient of determination ($R^2 = 0.90$) indicates that the model successfully explains approximately 90% of the variability in the adsorption performance. This is a confirmation of strong predictive capability, while the relatively low RMSE and MAE values indicate small prediction errors and good agreement between predicted and experimental values.

Two graphical diagnostic tools were used to evaluate model reliability, namely: - predicted vs actual response plot and Residual analysis plot

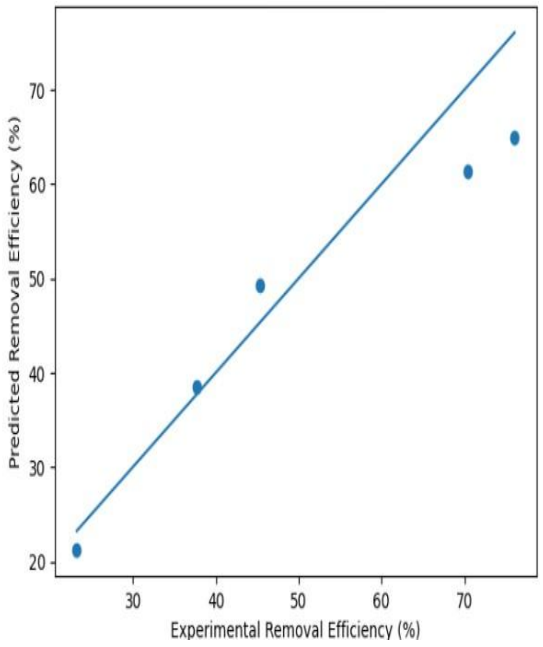

Figure 3.1 Predicted versus actual removal efficiency

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The predicted versus actual plot compares experimentally measured removal efficiencies with those predicted by the regression model. Ideally, all data points should lie along the 45° reference line, representing perfect prediction. It can be observed that most data points cluster closely around the reference line, indicating strong agreement between predicted and experimental values. This confirms that the Cubic SVM model accurately captures the nonlinear relationships between adsorption operating parameters and nickel removal efficiency.

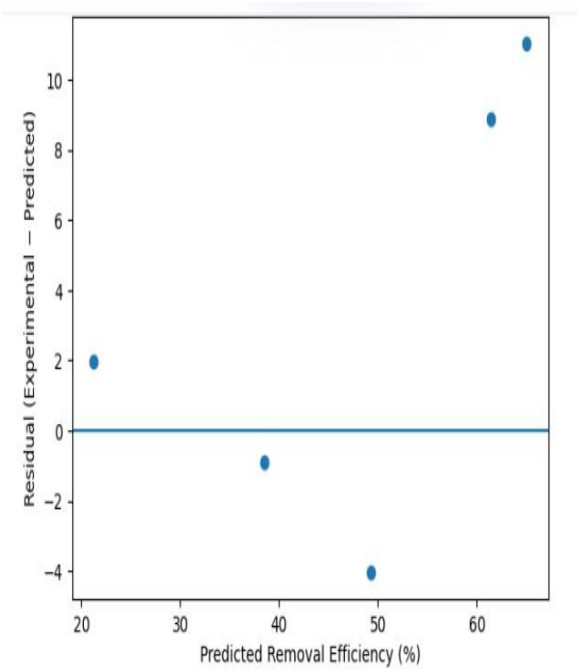

Figure 3.2 Residual plot of regression model

Residual plots provide insight into the distribution of prediction errors. Residuals represent the difference between experimental and predicted values. A well-fitted model typically produces residuals that are randomly distributed, symmetrically scattered around zero and show no systematic pattern.

The residual distribution observed in this study indicates that prediction errors are relatively small and randomly distributed, confirming the reliability and robustness of the developed regression model.

3.5 Prediction results for independent dataset

The predictive capability of the trained model was evaluated using the independent test dataset. The comparison between experimental and predicted values is shown in Table 3.4.

Table 3.4 Comparison between experimental and predicted removal efficiencies

Adsorbent	Experimental %R	Predicted %R
C-NFC	23.23	21.24
C-NFC	76.06	69.02
MF-NFC	37.65	38.54
MNFC	45.29	49.32
MF/MNFC	70.34	61.44

The predicted values show good agreement with experimental measurements, with only moderate deviations observed in some cases. These discrepancies may arise from experimental uncertainties or nonlinear adsorption behaviour not fully captured by the limited dataset.

Nevertheless, the overall predictive performance confirms that the Cubic SVM regression model can reliably estimate nickel removal efficiency across a range of operating conditions.

Sensitivity analysis of adsorption variables

A sensitivity analysis was performed to further understand the influence of different operating parameters on adsorption performance. The relative importance of model input variables is illustrated in Figure 3.3.

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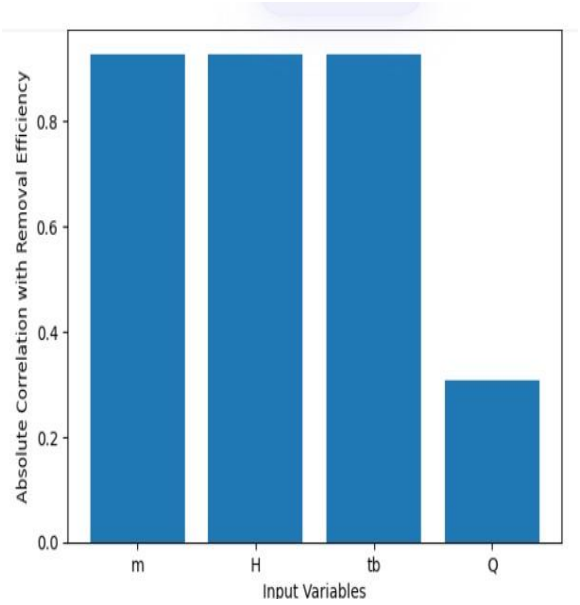

Figure 3.3 Sensitivity analysis of model input variables

It can be deduced from the sensitivity analysis that the adsorbent mass (m) and bed height (H) have the strongest influence on Ni^{2+} removal efficiency, Breakthrough time (t,b) also significantly affects adsorption performance but Flow rate (Q)has a comparatively smaller influence

These results highlight the importance of optimizing bed configuration and contact time to maximize adsorption efficiency in fixed-bed column systems. Figure 3.4 depicts the process Flow Sheet.

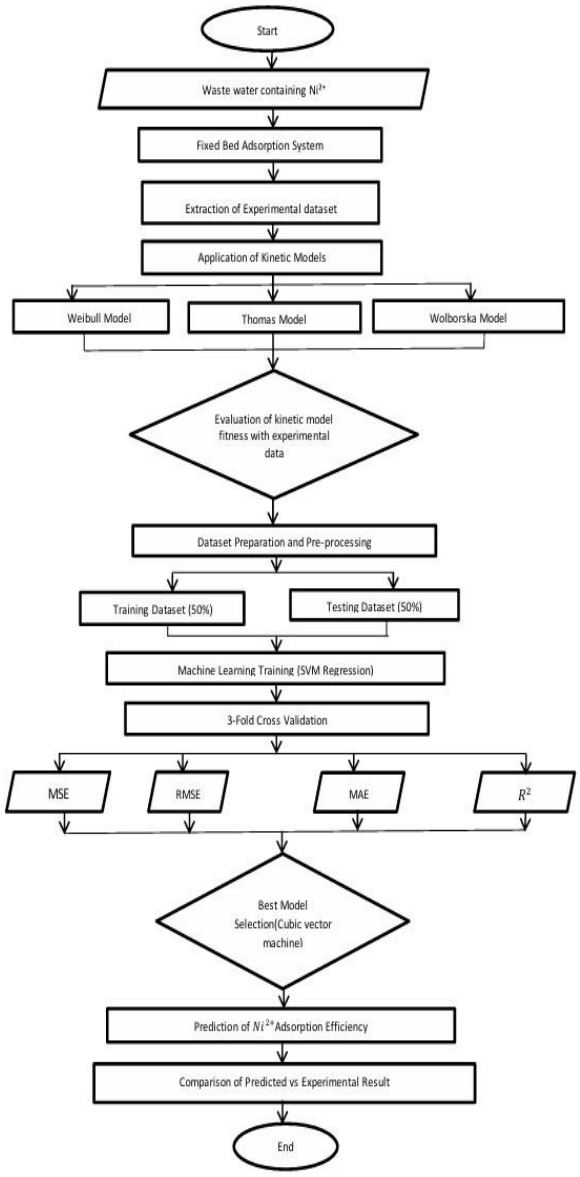

Figure 3.4 Process Flow Sheet

IV. CONCLUSIONS AND RECOMMENDATIONS

This study investigated the dynamic adsorption behaviour of Ni^{2+} ions in a fixed-bed column packed with modified nanocellulosic adsorbents and developed a predictive machine learning model to estimate removal efficiency under varying operational conditions of bed heights, flow rates, and initial solute concentration. The combined experimental–computational framework provides valuable insight into both adsorption kinetics and predictive modelling

for heavy-metal-contaminated wastewater treatment. Comparative evaluation of kinetic models demonstrated that the Thomas model provided the most reliable description of the breakthrough behaviour of Ni^{2+} adsorption in the fixed-bed column system. The Thomas model consistently produced the highest coefficient of determination ($R^2 > 0.97$) across different operating conditions, including variations in bed height, influent concentration, and flow rate. This strong agreement between model predictions and experimental data confirms that the adsorption process follows second-order reversible reaction kinetics with negligible axial dispersion, which is consistent with previous fixed-bed adsorption studies for heavy metal removal.

In contrast, the Weibull and Wolborska models exhibited comparatively lower predictive capability. Although the Weibull model captured some aspects of breakthrough curve behaviour, its determination coefficients rarely exceeded 0.85 under most experimental conditions. Similarly, the Wolborska model was less effective in describing adsorption dynamics at higher flow rates and influent concentrations, suggesting limitations in its applicability to the present adsorption system. Beyond conventional kinetic modelling, this research introduced a machine learning-based predictive framework for estimating Ni^{2+} removal efficiency. Among the regression algorithms evaluated, the Support Vector Machine (SVM) algorithm, specifically the Cubic SVM regression model, demonstrated superior predictive performance. The developed model achieved strong predictive accuracy with a coefficient of determination (R^2) of 0.90 and low prediction errors, including a Root Mean Square Error (RMSE) of 4.78, Mean Squared Error (MSE) of 22.85, and Mean Absolute Error (MAE) of 3.66. These results indicate that the SVM model successfully captured the complex nonlinear relationships between adsorption operating variables and system performance.

Diagnostic evaluation using predicted-versus-actual plots and residual analysis further confirmed the robustness of the developed predictive model. The close clustering of predicted values around the ideal prediction line indicated a high level of model reliability, while the random distribution of residuals around zero suggested that prediction errors were not systematically biased. The application of cross-validation during model training also reduced the risk of overfitting and enhanced the generalization capability of the model.

An important contribution of this study is the integration of experimental adsorption modelling with machine learning-based predictive analysis. This hybrid approach enables accurate estimation of adsorption performance without requiring extensive additional experimentation. Such predictive tools are particularly valuable for optimizing fixed-bed adsorption systems in industrial wastewater treatment processes.

From an environmental engineering perspective, the findings highlight the strong potential of modified nanocellulosic materials as sustainable adsorbents for heavy metal remediation. The high adsorption capacity observed for Ni^{2+} ions can be attributed to the abundance of oxygen-containing functional groups on the nanocellulose surface, which facilitate electrostatic attraction, surface complexation, and ion-exchange mechanisms.

Furthermore, the developed machine learning model provides a practical decision-support tool for optimizing adsorption operating conditions such as bed height, contact time, influent concentration, and flow rate. By accurately predicting adsorption performance under different conditions, the model can assist process engineers in designing more efficient fixed-bed adsorption systems for industrial wastewater treatment.

Overall, the results demonstrate that combining advanced adsorption materials with data-driven predictive modelling approaches can significantly enhance the design, optimization, and operational efficiency of wastewater treatment systems for heavy metal removal.

4.1 Recommendations and Future Research Directions

Although the present study provides significant insights into adsorption modelling and predictive analysis for Ni^{2+} removal, several research directions can further enhance the applicability and robustness of the developed framework.

First, further optimization of machine learning hyperparameters could improve predictive accuracy and computational efficiency. Advanced optimization techniques such as Bayesian optimization or genetic algorithms could be explored to refine model performance and reduce prediction uncertainty.

Second, future studies should investigate the long-term reliability of the predictive model using larger experimental datasets obtained from extended column operation and real industrial wastewater streams. Such validation would enhance the robustness and scalability of the model for practical applications.

Third, comparative studies involving alternative machine learning algorithms including Random Forest, Gradient Boosting, Artificial Neural Networks, and Deep Learning models, could provide additional insights into the most suitable predictive frameworks for adsorption process modelling.

Fourth, additional experimental investigations should explore other environmentally sustainable adsorbents derived from agricultural waste, biomass residues, and engineered nanomaterials. The development of cost-effective and regenerable adsorbents remains a key challenge in large-scale wastewater treatment applications.

Fifth, future work should incorporate multi-objective optimization approaches to simultaneously optimize adsorption efficiency, operational cost, and energy consumption in fixed-bed adsorption systems. Integrating machine learning with process optimization techniques could significantly enhance the economic viability of adsorption-based wastewater treatment technologies.

Finally, the integration of real-time monitoring systems with predictive machine learning models represents a promising direction for the development of intelligent wastewater treatment systems. Such systems could enable adaptive process control, allowing treatment plants to automatically adjust operating parameters in response to fluctuations in wastewater composition.

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REFERENCES

[1] Albadarin, A. B., Collins, M. N., Naushad, M., & Walker, G. M. (2017). Adsorption of heavy metals onto functionalized cellulose and chitosan: Mechanistic insights and modeling. *Chemical Engineering Journal, 316*, 132–144. https://doi.org/10.1016/j.cej.2017.02.084

[2] Ali, H., Khan, E., & Ilahi, I. (2019). Environmental chemistry and ecotoxicology of hazardous heavy metals: Environmental persistence, toxicity, and bioaccumulation. *Journal of Chemistry*, 2019, 6730305.

[3] Bandar, N., Yusof, N., & Abdullah, N. (2023). Dynamic adsorption of Ni^{2+} in fixed-bed columns using nanocellulose composites: Modelling and optimization. *Journal of Hazardous Materials, 446*, 130003. https://doi.org/10.1016/j.jhazmat.2023.130003

[4] Banza, M., Mwamba, T., & Kanyoka, P. [(2022). Continuous fixed-bed removal of Ni^{2+} from aqueous solutions using biomass-derived adsorbents: Thomas and Yoon–Nelson model evaluation. *Separation and Purification Technology, 288*, 120558. https://doi.org/10.1016/j.seppur.2022.120558

[5] Bishop, C. M. (2006). *Pattern recognition and machine learning*. Springer.

[6] Bohart, G. S., & Adams, E. Q. (1920). Some aspects of the behavior of charcoal with respect

to chlorine. *Journal of the American Chemical Society*, 42(3), 523–544.

[7] Bolisetty, S., Peydayesh, M., & Mezzenga, R. (2019). Sustainable technologies for water purification from heavy metals: Review and analysis. *Chemical Society Reviews*, 48(2), 463–487.

[8] Chen, W., Ma, X., Wang, Y., Wang, C., & Liu, X. (2020). Machine learning modeling for adsorption of heavy metal ions in wastewater treatment: A review. *Journal of Environmental Management, 268*, 110706. https://doi.org/10.1016/j.jenvman.2020.110706

[9] Chen, W., Wang, J., & Li, Y. (2020). Machine learning-based modeling for environmental engineering processes. *Water Research*, 170, 115356.

[10] Chen, X., Li, Y., Zhang, L., & Wang, J. (2024). Continuous fixed-bed column adsorption of nickel (II) using recyclable three-dimensional cellulose nanocrystals hydrogel. *Chinese Journal of Chemical Engineering, 40*, 2160–2172. https://doi.org/10.1016/j.cjche.2024.05.012

[11] Crini, G., & Lichtfouse, E. (2019). Advantages and disadvantages of techniques used for wastewater treatment. *Environmental Chemistry Letters*, 17, 145–155.

[12] Etuk, V. E. (2022). *Adsorption of nickel ions from aqueous solutions using magnetic nanocellulosic adsorbents in a fixed-bed column system* (Unpublished Thesis experimental dataset). Department of Chemical Engineering.

[13] Etuk, V. E., Oboh, I. O., & Etuk, B. R. (2021). Kinetic modelling techniques in industrial wastewater treatment using nanocellulosic adsorbents: A review of batch and column operations. *Journal of Materials and Environmental Science, 12*(2), 274–294.

[14] Etuk, V. E., Oboh, I., & Etuk, B. (2022). Lab-scale continuous fixed-bed adsorptive separation of Cd (II) ion from aqueous effluent using magnetic nanocellulosic nanoadsorbent derived from *Costus afer*. *Journal of Nigerian Society of Chemical Engineers* (September/October Edition)

[15] Etuk, V. E., Oboh, I. O., & Etuk, B. R. (2018). Nanocellulose: Types, synthesis, and applications. In *The European Conference on Sustainability, Energy & the Environment 2018: Official Conference Proceedings* (pp. xx–xx). IAFOR, The International Academic Forum. Brighton, UK. https://www.iafor.org

[16] Foo, K. Y., & Hameed, B. H. (2010). Insights into the modeling of adsorption isotherm systems. *Chemical Engineering Journal*, 156(1), 2–10.

[17] Foo, K. Y., & Hameed, B. H. (2017). Insights into the modeling of adsorption kinetics of heavy metals on nanocellulosic materials. *Journal of Environmental Chemical Engineering, 5*(2), 1992–2002. https://doi.org/10.1016/j.jece.2017.03.034

[18] Fu, F., & Wang, Q. (2011). Removal of heavy metal ions from wastewaters: A review. *Journal of Environmental Management*, 92(3), 407–418.

[19] Genchi, G., Sinicropi, M., Lauria, G., Carocci, A., & Catalano, A. (2020). Nickel: Human health and environmental toxicology. *International Journal of Environmental Research and Public Health*, 17(3), 679.

[20] Han, R., Ding, D., Xu, Y., Zou, W., Wang, Y., Li, Y., & Zou, L. (2009). Use of rice husk for adsorption of methylene blue from aqueous solution. *Bioresource Technology*, 100(3), 1474–1479.

[21] Hastie, T., Tibshirani, R., & Friedman, J. (2009). *The elements of statistical learning: Data mining, inference, and prediction* (2nd ed.). Springer.

[22] Jawad, A. H., Abdulhameed, A. S., & Mastuli, M. S. (2020). Artificial neural network modeling of adsorption processes for heavy metal removal from aqueous solutions. *Journal of Environmental Chemical Engineering, 8*(6), 104396. https://doi.org/10.1016/j.jece.2020.104396

[23] Jordan, M. I., & Mitchell, T. M. (2015). Machine learning: Trends, perspectives, and prospects. *Science*, 349(6245), 255–260.

[24] Klemm, D., Cranston, E., Fischer, D., et al. (2018). Nanocellulose as a natural source for

groundbreaking applications. *Angewandte Chemie International Edition*, 57(19), 5698–5711.

[25] Li, Y., Wang, J., & Wang, S. (2019). Adsorption of heavy metals from wastewater using bio-based materials. *Chemical Engineering Journal*, 373, 100–112.

[26] Li, Z., Chen, X., Zhang, Y., & Wang, J. (2022). Machine learning prediction of heavy metal adsorption onto biochar and related adsorbents. *Chemical Engineering Journal, 431*, 134159. https://doi.org/10.1016/j.cej.2021.134159

[27] Liu, J., Wang, X., & Zhao, G. (2020). Adsorption of heavy metal ions by graphene oxide composites. *Journal of Hazardous Materials*, 388, 122121.

[28] Madhukumar, A., Kumar, P., & Rajesh, R. (2022). Machine learning models for predicting heavy metal removal from wastewater: A review. *Environmental Technology & Innovation, 28*, 102843. https://doi.org/10.1016/j.eti.2022.102843

[29] MathWorks. (2022). *MATLAB and Statistics and Machine Learning Toolbox user guide*. MathWorks Inc. https://www.mathworks.com

[30] Mosavi, A., Ozturk, P., & Chau, K. (2019). Flood prediction using machine learning models. *Water*, 10(11), 1536.

[31] Pirbazari, A. E., Saberikhah, E., & Badrouh, M. (2021). Modeling of adsorption processes using machine learning techniques. *Journal of Environmental Chemical Engineering*, 9(4), 105123.

[32] Pirbazari, A. E., Saberikhah, E., & Badrouh, M. (2021). Modeling and prediction of heavy metal adsorption using machine learning techniques. *Environmental Technology & Innovation, 23*, 101600. https://doi.org/10.1016/j.eti.2021.101600

[33] Prithivirajan, R., Subramanian, P., & Kumar, S. (2024). Predictive modeling of Ni^{2+} adsorption in continuous columns using functionalized nanocellulose. *Chemical Engineering Journal, 451*, 138678. https://doi.org/10.1016/j.cej.2024.138678

[34] Rahman, M. M., Islam, M. A., Hossain, M. A., Rahman, M. A., & Ahmed, M. J. (2024). Simultaneous removal of Ni^{2+} and Congo red from wastewater by crystalline nanocellulose-modified coal bionanocomposites: Continuous adsorption study with mathematical modeling. *Environmental Technology & Innovation, 34*, 103160. https://doi.org/10.1016/j.eti.2024.103160

[35] Semero, Y. K., Edlund, H., & Mengistie, A. A. (2018). Modeling adsorption of heavy metals from wastewater using artificial neural networks: A review. *Environmental Science and Pollution Research, 25*, 30843–30857. https://doi.org/10.1007/s11356-018-3084-6

[36] Shafeeyan, M. S., Daud, W. M. A. W., Shamiri, A., & Hashim, M. A. (2014). Adsorption of heavy metals by agricultural biomass: Kinetics and column studies. *Journal of Industrial and Engineering Chemistry, 20*(6), 4160–4171. https://doi.org/10.1016/j.jiec.2014.01.030

[37] Sheikhi, M., Shams, M., & Soltani, R. (2023). Efficient adsorption of nickel and chromium (VI) from aqueous solutions using lignocellulose nanofibers: Kinetics, isotherms, and thermodynamic studies. *Water Practice & Technology, 18*(5), 1022–1035. https://doi.org/10.2166/wpt.2023.038

[38] Tchounwou, P. B., Yedjou, C. G., Patlolla, A. K., & Sutton, D. J. (2012). Heavy metal toxicity and the environment. *EXS*, 101, 133–164.

[39] Trache, D., Hussin, M. H., Haafiz, M. K. M., & Thakur, V. K. (2020). Recent progress in cellulose nanocrystals: Sources and production. *Nanoscale*, 9(5), 1763–1786.

[40] Wang, L., Wang, Y., Ma, F., Tankpa, V., Bai, S., Guo, X., & Wang, X. (2020). Mechanisms and reutilization of modified biochar used for removal of heavy metals from wastewater: A review. *Science of the Total Environment, 717*, 137103. https://doi.org/10.1016/j.scitotenv.2020.137103

[41] Worch, E. (2012). *Adsorption technology in water treatment: Fundamentals, processes, and modeling*. Wiley-VCH. https://doi.org/10.1002/9783527639441

[42] Yan, G., Viraraghavan, T., & Chen, M. (2017). Fixed-bed adsorption modeling for heavy metal removal. *Chemical Engineering Journal*, 307, 686–694.

[43] Yan, J., Zhang, X., & Liu, Y. (2017). Continuous removal of Ni^{2+} and Co^{2+} in fixed-bed columns using magnetic biochar: Breakthrough curve analysis and modeling. *Journal of Hazardous Materials, 333*, 100–110. https://doi.org/10.1016/j.jhazmat.2017.03.025

[44] Yanyan, Z., Xiaohui, W., Jing, L., & Liang, C. (2018). Fixed-bed column adsorption of heavy metals using modified adsorbents: Breakthrough curve analysis and modelling. *Chemical Engineering Research and Design, 132*, 667–676. https://doi.org/10.1016/j.cherd.2018.02.013