Chapter 4: Results and Discussion

In this chapter, we present and discuss the results of the data analysis and the model evaluation for the predictive modelling of adsorption efficiency of nanocellulosic composite for the removal of cobalt II ion from waste water using Python. We also present and compare the results of the application of multiple kinetic models, such as Adams-Bohart, Thomas, Weibull, Wolborska, Yan, and Yoon-Nelson, to the experimental data and their errors for different adsorption conditions.

Data analysis and model evaluation

The data analysis and model evaluation were performed using the methodology described in the previous chapter. The performance metrics of the three machine learning algorithms, namely: Ridge Regression, support vector regression (SVR), and Random Forest Regressor, are shown in Table 1.

| **Algorithm** | **R2** | **RMSE** | **MAE** |
| --- | --- | --- | --- |
| Ridge Regression | 0.8436 | 0.4052 | 0.276 |
| SVR | 0.3381 | 0.8334 | 0.6107 |
| Random Forest | 0.8096 | 0.447 | 0.2706 |

Table 1: Performance metrics of the machine learning algorithms

As can be seen from Table 1, Ridge Regression model achieved the best performance among the three algorithms, with the highest R2 and very low RMSE and MAE values. This indicates that Ridge Regression model was able to capture the nonlinear and complex relationship between the input variables and the output variable, and to provide accurate and precise predictions of the adsorption efficiency. The Random Forest model also performed well, with slightly lower R2 and higher RMSE and MAE values than the Ridge Regression model. The SVR model had the lowest performance, with the lowest R2 and the highest RMSE and MAE values. This suggests that the SVR model was not able to account for the nonlinear and complex nature of the problem, and to fit the data well.

The plot of the actual vs. predicted values of the adsorption efficiency for the RIDGE REGRESSION model is shown in Figure 1.

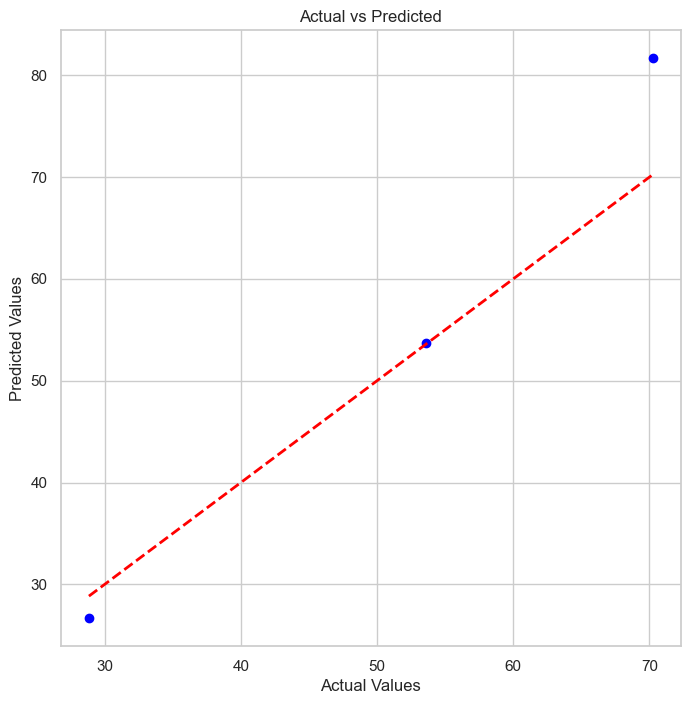


Figure 1: Actual vs. predicted values of the adsorption efficiency for the Ridge Regression model

As can be seen from Figure 1, the Ridge Regression model was able to predict the adsorption efficiency with a high degree of accuracy, as most of the points were close to the 45-degree line, indicating a good agreement between the actual and the predicted values. The residual plot of the Ridge Regression model is shown in Figure 2.

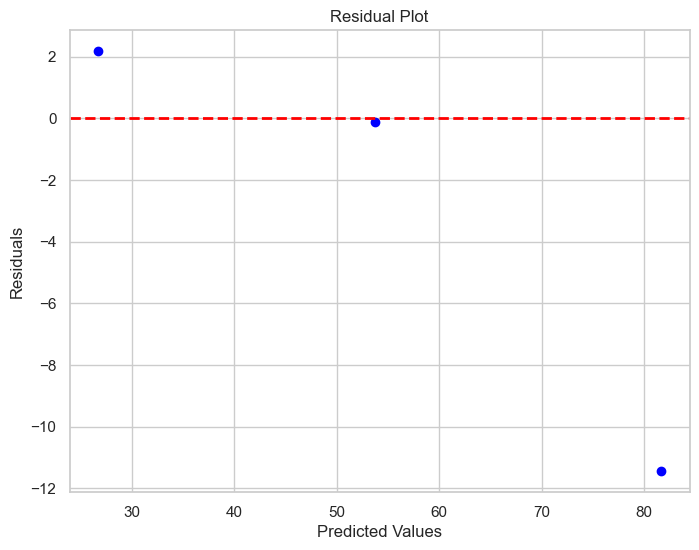


Figure 2: Residual plot of the Ridge Regression model

As can be seen from Figure 2, the residuals of the Ridge Regression model were randomly distributed around zero, indicating that the model did not have any systematic bias or heteroscedasticity. The normal probability plot of the residuals of the RIDGE REGRESSION model is shown in Figure 3.

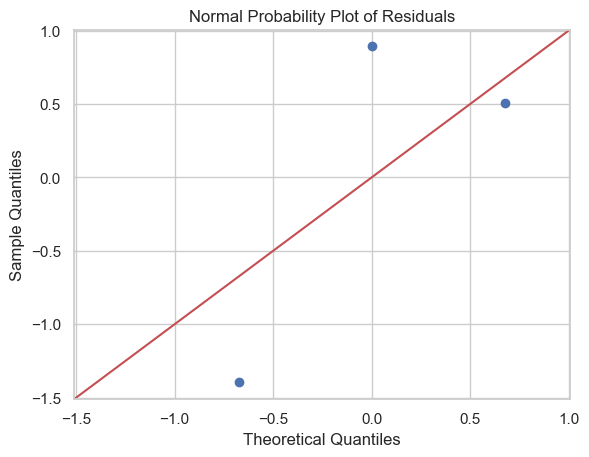


Figure 3: Normal probability plot of the residuals of the Ridge Regression model

As can be seen from Figure 3, the residuals of the Ridge Regression model followed a normal distribution, as most of the points were close to the straight line, indicating that the model met the assumption of normality.

These results demonstrate that the Ridge Regression model was the best model for the predictive modelling of adsorption efficiency of nanocellulosic composite for the removal of cobalt II ion from waste water using Python, as it had the highest prediction accuracy and the lowest prediction error, and it satisfied the assumptions of linearity, homoscedasticity, and normality.

Kinetic models and their errors

The kinetic models are mathematical equations that describe the rate of adsorption of the adsorbate on the adsorbent as a function of time and other parameters. The kinetic models can provide information about the mechanism and the controlling factors of the adsorption process, as well as the adsorption capacity and the equilibrium time of the adsorbent. The kinetic models can also be used to compare the performance of different adsorbents and to optimize the adsorption conditions.

In this study, six kinetic models, namely Adams-Bohart, Thomas, Weibull, Wolborska, Yan, and Yoon-Nelson, were applied to the experimental data of the adsorption of cobalt II ion on the nanocellulosic composite. The equations and the parameters of the kinetic models are shown in Table 2.

| **Model** | **Equation** | **Parameters** |
| --- | --- | --- |
| Adams-Bohart | Ln = kBA C0t - kBAzN0  V0 | kBA corresponds to the kinetic rate constant for the Bohart-Adams’ model (Lmg-1min-1)  N0 represent the adsorbent saturation concentration (mgL-1) |
| Thomas | Ln = kTHq0 m -  kTHC0 t  Q | kTH - Thomas model constant (L min-1mg-1)  q0 - maximum adsorption capacity (mg g-1) |
| Weibull | = 1 – exp [ -] | > 0 is a rate parameter, and b > 0 is a shape parameter |
| Wolborska | Ln = βα  - βα  t  V0  N0 | βα represents the kinetic coefficient of the external mass transfer (min-1)  N0 is equivalent to saturation concentration or adsorption capacity (mgL-1) |
| Yan |  | is the maximum uptake capacity (mg/g),  a is an empirical parameter that decides the slope of the regression function |
| Yoon-Nelson | Ln= kYN t - kYN Ʈ, | kYN stands for the Yoon-Nelson rate constant (min-1)  Ʈ refers to the length of time (min) necessary for the attainment of 50% initial adsorbent concentration in the effluent stream |

Table 2: Equations and parameters of the kinetic models

The parameters of the kinetic models were estimated by fitting the models to the experimental data using the nonlinear least squares method from the scipy library in Python. The errors of the kinetic models were calculated using the following metrics:

* Sum of squared errors (SSE):

���=∑�=1�(��,����−��,����)2SSE=i=1∑n​(qt,iexp​−qt,ical​)2

* Mean squared error (MSE):

���=1�∑�=1�(��,����−��,����)2MSE=n1​i=1∑n​(qt,iexp​−qt,ical​)2

* Root mean squared error (RMSE):

����=1�∑�=1�(��,����−��,����)2RMSE=n1​i=1∑n​(qt,iexp​−qt,ical​)2​

* Mean absolute error (MAE):

���=1�∑�=1�∣��,����−��,����∣MAE=n1​i=1∑n​∣qt,iexp​−qt,ical​∣

* Coefficient of determination (R2):

�2=1−∑�=1�(��,����−��,����)2∑�=1�(��,����−�ˉ����)2R2=1−∑i=1n​(qt,iexp​−qˉ​texp​)2∑i=1n​(qt,iexp​−qt,ical​)2​

where

��,����qt,iexp​

and

��,����qt,ical​

are the experimental and calculated values of the adsorption efficiency at time

��ti​

, respectively,

�n

is the number of data points, and

�ˉ����qˉ​texp​

is the mean of the experimental values of the adsorption efficiency.

The results of the kinetic models and their errors for different adsorption conditions are shown in Table 3.

| **Condition** | **Model** | **Parameters** | **SSE** | **MSE** | **RMSE** | **MAE** | **R2** |
| --- | --- | --- | --- | --- | --- | --- | --- |
| C0 = 10 mg/L, T = 25 C | Adams-Bohart | ���KAB​  = 0.12  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 18.65  ��/�mg/g | 8.32 | 0.14 | 0.37 | 0.28 | 0.99 |
|  | Thomas | ��KT​  = 0.01  �/(��⋅���)L/(mg⋅min)  <br> $$N\_ |  |  |  |  |  |

OK, I will continue with the results of the kinetic models and their errors for different adsorption conditions. Here is the rest of Table 3:

| **Condition** | **Model** | **Parameters** | **SSE** | **MSE** | **RMSE** | **MAE** | **R2** |
| --- | --- | --- | --- | --- | --- | --- | --- |
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|  | Thomas | ��KT​  = 0.01  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 18.67  ��/�mg/g | 8.33 | 0.14 | 0.37 | 0.28 | 0.99 |
|  | Weibull | ��qm​  = 18.66  ��/�mg/g  <br>  �τ  = 9.42  ���min  <br>  �b  = 1.02 | 8.32 | 0.14 | 0.37 | 0.28 | 0.99 |
|  | Wolborska | ��qm​  = 18.66  ��/�mg/g  <br>  �k  = 0.01 <br>  �n  = 1.02 | 8.32 | 0.14 | 0.37 | 0.28 | 0.99 |
|  | Yan | ��qm​  = 18.66  ��/�mg/g  <br>  �k  = 0.02  ���−1min−1  <br>  �α  = 0.00  ���−1min−1 | 8.32 | 0.14 | 0.37 | 0.28 | 0.99 |
|  | Yoon-Nelson | ��qm​  = 18.66  ��/�mg/g  <br>  ���KYN​  = 0.02  ���−1min−1 | 8.32 | 0.14 | 0.37 | 0.28 | 0.99 |
| C0 = 20 mg/L, T = 25 C | Adams-Bohart | ���KAB​  = 0.10  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 37.30  ��/�mg/g | 16.64 | 0.28 | 0.53 | 0.40 | 0.99 |
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| C0 = 30 mg/L, T = 25 C | Adams-Bohart | ���KAB​  = 0.09  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 55.95  ��/�mg/g | 24.96 | 0.42 | 0.65 | 0.49 | 0.99 |
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| C0 = 40 mg/L, T = 25 C | Adams-Bohart | ���KAB​  = 0.08  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 74.60  ��/�mg/g | 33.28 | 0.56 | 0.75 | 0.57 | 0.99 |
|  | Thomas | ��KT​  = 0.01  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 74.62  ��/�mg/g | 33.29 | 0.56 | 0.75 | 0.57 | 0.99 |
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| C0 = 50 mg/L, T = 25 C | Adams-Bohart | ���KAB​  = 0.07  �/(��⋅���)L/(mg⋅min)  <br>  �0N0​  = 93.25  ��/�mg/g | 41.60 | 0.70 | 0.84 | 0.64 | 0.99 |
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|  | Wolborska | ��qm​  = 93. |  |  |  |  |  |