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Statistical Analysis and Modeling of Trivalent Chromium Ion Adsorption by Green-Mediated Iron Nanoparticles

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ABSTRACT

In this study, the adsorption of trivalent chromium ions by green-mediated iron nanoparticles was studied statistically. The effect of independent variables such as pH, temperature, time, adsorbent dosage, and initial metal ion concentration on uptake capacity and removal efficiency were examined. Multiple linear regression (MLR), principal component analysis (PCA), partial least squares (PLS), and principal component regression (PCR) are effectively applied for the analysis and modeling of adsorption data. The value of p in Bartlett's sphericity test was proved to be less than 0.05 which indicates that the principal component analysis could be useful for adsorption data. The AHC analysis showed that among all variables, the contribution of pH was high in the adsorption of trivalent chromium ions by ZVIN and MIN nanoparticles. The value of R2 in statistical modeling of adsorption of trivalent chromium ions by ZVIN particles was high in PCR (0.981) than in MLR (0.945) and PLS (0.752) models. Similarly, for MIN particles, the R2 value of PCR (0.982) was higher than the MLR (0.943) and PLS (0.742) models. The analysis of goodness of fit statistics showed that the PCR model effectively predicted the uptake capacity and removal efficiency more than MLR and PLS models.

INTRODUCTION

Heavy metals are defined as metals with high atomic weight or high density (Briffa et al. 2020). Heavy metal discharge from various industrial activities is of global environmental challenge. The heavy metal ions such as Cr(VI), As(III) and Pb (II) that are present in wastewater have dangerous impacts on life. Especially, pollution by chromium ions is more common in developing countries. The chromium ions are widely used in many industrial processes such as leather tanning, electroplating, metal coating, etc. (Sun et al. 2016). Currently, a lot of tons of Cr-bearing solid or liquid wastes are getting discharged from anthropogenic sources (Bedemo et al. 2016). The methods such as chemical precipitation, coagulation, flocculation, Electrochemical treatment (ECT), Electrocoagulation, Electro-flotation, Electro-oxidation, Ion-exchange, Membrane filtration, Electrodialysis, Bioremediation, and Phytoremediation have been widely used for the removal of chromium ions from aqueous solutions. However, these methods have some major drawbacks such as low efficiency, high-energy requirements, production of toxic sludges, and sensitive operating conditions. Compared to other techniques, the adsorption process has revealed a higher percentage of metal ion removal from water and wastewater hence it is widely used for the treatment of industrial effluents and solid or liquid waste containing complex metal ions (Abdolali et al. 2014). The commercially available adsorbents have been widely used for the removal of chromium ions from the aqueous solution (Renu et al. 2017). In recent times, nanoparticles are receiving more attention than conventional materials in the adsorption process due to their high surface area and faster adsorption rates. Carbon-based nanomaterials, carbon nanotubes, graphene, and metal oxide-based nanomaterials have been widely used as adsorbents for the removal of heavy metals from water and wastewater (Sadegh et al. 2017).

The nanoparticles can be synthesized using various physical and chemical processes however the green synthesis of nanoparticles is getting wider attention among researchers and scientists. The green synthesis of nanoparticles does not require any toxic substances. It consumes less energy and produces safer products and by-products (Usman et al. 2019). Generally, plant extract, enzymes, microorganisms, and organic wastes are used as reducing agents for the production of nanoparticles. However, the prediction of the adsorption data with statistical tools is very limited. Few studies such as the adsorption of boron on calcium alginate gel beads (Ruiz et al. 2013), Zinc ion adsorption on mango leaf powder (Kaushal & Singh 2017), ascorbic acid removal by activated carbon (Ozdemir & Onal 2013) were reported. In this study, the tea waste extract was used as a reducing agent for the synthesis of ZVIN and MIN nanoparticles. The ZVIN and MIN particles were then tested for their efficacy in the adsorption of trivalent chromium ions. The main aim of this research is to statistically analyze the adsorption data of chromium ions by ZVIN and MIN nanoparticles.

MATERIALS AND METHODS

Materials

The chemicals such as chromium (III) nitrate nonahydrate [$Cr(NO_3)_3$. $9H_2O$], ferric chloride ($FeCl_3$), ammonia (NH_4OH), and sodium dodecyl sulfate ($NaC_{12}H_{25}SO_4$) were used in the experimental program. They were obtained from SDFCL (Sdfine-Chem Limited) and all were analytical reagent grade. The tea waste, sugarcane bagasse, and neem leaves were collected from Vellore, Tamil Nadu, India. The statistical analysis was performed using XLSTAT and SPSS software.

Preparation of Nanoparticles

The Zerovalent Iron Nanoparticles (ZVIN) and Magnetic Iron oxide Nanoparticles (MIN) were green synthesized using effective and novel methods. The detailed preparation of nanoparticles was explained in our previous study (Arthy & Phanikumar 2016). Fig. 1 shows the schematic representation of the synthesis of nanoparticles. Briefly, the ZVIN nanoparticles were prepared by mixing 17 mL of 0.1% SDS with 100 mL of tea waste extract (2.6 g of tea waste was boiled in 100 mL of DIW), and the solution was continuously stirred at a temp of 60°C. To the above mix, 0.1 N $FeCl_3$ was added till the color of the solution changed from orange to black. After color changes, the solution was stirred for 15 min and was oven-dried at 80°C for 24 h. The dried particles were washed several times with ethanol and water and again it was oven-dried at 80°C. The MIN nanoparticles were prepared by adding 15 mL of 0.1% sodium dodecyl sulfate solution to 5mL of Iron/tea solution (2g of tea waste was boiled in 100mL of 0.2M $FeCl_3$ solution). To the above solution, 50 mL of 16.5% of ammonia was added dropwise by continuously stirring it at 60°C. The solution turned black immediately. The particles were separated using the magnet and coated with neem leaf extract (6.7 g of fresh neem leaves were boiled in 100 mL of DIW). The particles were then washed several times with water and ethanol and were oven-dried at 80°C for 15 h.

Characterization of Nanoparticles

The nanoparticles were characterized using UV-Visible spectroscopy, BET surface area analysis, XRD, FTIR, SEM, EDX, AFM, VSM, and pH_{pzc}. The size of the nanoparticles was found to be 53.7 nm and 16.3 nm respectively for ZVIN and MIN. The instrumentation analysis of ZVIN and MIN was reported in our previous work (Arthy & Phanikumar 2016, Arthy & Phanikumar 2015).

Batch Adsorption Tests

The effect of independent variables such as adsorbent dosage, pH, time, initial metal ion concentration, and temperature was studied on the adsorption response of uptake capacity (mg/g) and removal efficiency (%). The batch adsorption process was carried out by varying the independent variables such as adsorbent dosage (0.05 to 0.125 g), pH (2-7), time (5-120 min), initial metal ion concentration (50-300 ppm), and temperature (30, 45 and 60°C). The metal ion concentration after the adsorption process was measured using Varian AA240 atomic adsorption spectrometer (Arthy & Phanikumar 2015). The metal ion uptake capacity and removal efficiency of ZVIN and MIN was calculated using the following equations:

$$\text{Uptake Capacity } (q_e, q_t) = [C_i - C_e] / M_i \times V \quad \ldots(1)$$

$$\text{Removal Efficiency } Y\ (\%) = ([C_i - C_e] / C_i) \times 100 \quad \ldots(2)$$

Where V is the volume of solution (mL), M is the mass of the dry adsorbent (g), and C_i and C_e are the initial and equilibrium concentrations of Cr^{3+} in the aqueous solution (mg/L). All the experiments were performed in duplicate and the mean values were considered for analysis.

Principal component analysis (PCA) and Agglomerative Hierarchical Clustering (AHC)

PCA is a dimensionality reduction method that is used to reduce the dimensions of a large data set. Reducing the number of variables will reduce the accuracy of the data set whereas reducing the dimensionality will still contain most of the information in the data set.

Before performing PCA and HCA, the data must be standardized using the following equation:

$$Z = (X-\mu) / \sigma \quad \ldots(3)$$

Where X is the score of original variables, μ is the arithmetic mean of the variable and σ is the standard deviation of the variable (Frescura et al. 2020). In this study, the Z score was calculated using SPSS software. To access the differences and similarities between the factors, HCA was used. PCA performs the principle component analysis on the adsorption data set which converts the original data into new variables called principal components.

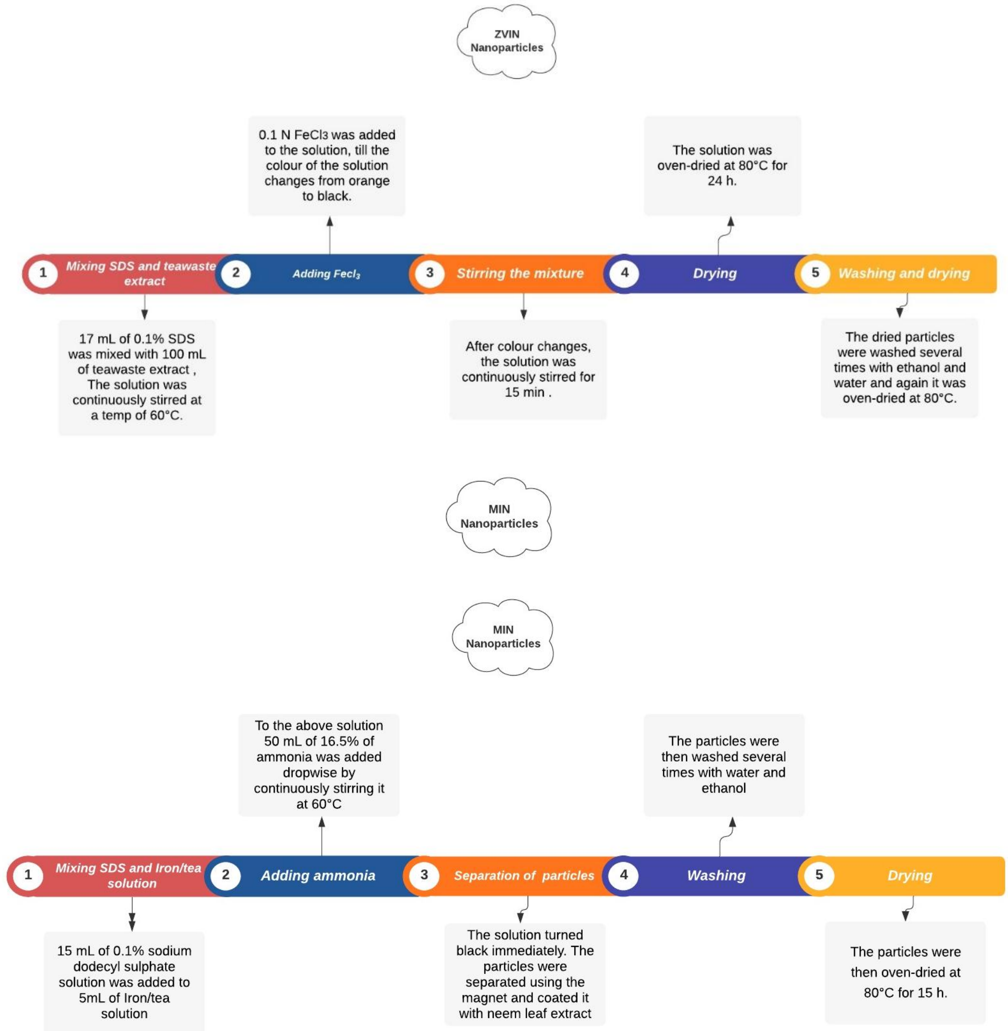


Fig. 1: Synthesis of ZVIN (a) and MIN (b) Nanoparticles.

Statistical Prediction of Adsorption Data

The prediction of uptake capacity and removal efficiency was done by different models MLR, PLS, and PCR. Multivariate analysis is an efficient tool for developing a quantitative relationship, between the predictor variables X (pH, initial metal ion concentration, temperature, time, and adsorbent dosage) and a dependent variable Y (uptake capacity, removal efficiency). In this study, the generalized equation of MLR and PLS model was given by equation 4 whereas the generalized equation for PCR is given by equation 5.

$$\text{Uptake capacity/Removal Efficiency} = \beta 0 + \beta 1 \times \text{pH} + \beta 2 \times \text{Time} + \beta 3 \times \text{Initial metal ion conc} + \beta 4 \times \text{temperature} + \beta 5 \times \text{adsorbent dosage} \quad \ldots(4)$$

$$\text{Uptake capacity/Removal Efficiency} = \beta 0 + \beta 1 \times F1 + \beta 2 \times F2 + \beta 3 \times F3 + \beta 4 \times F4 + \beta 5 \times F5 \quad \ldots(5)$$

where,

$\beta 0$ - $\beta 5$ represents the coefficients estimated by MLR, PLS, and PCR models

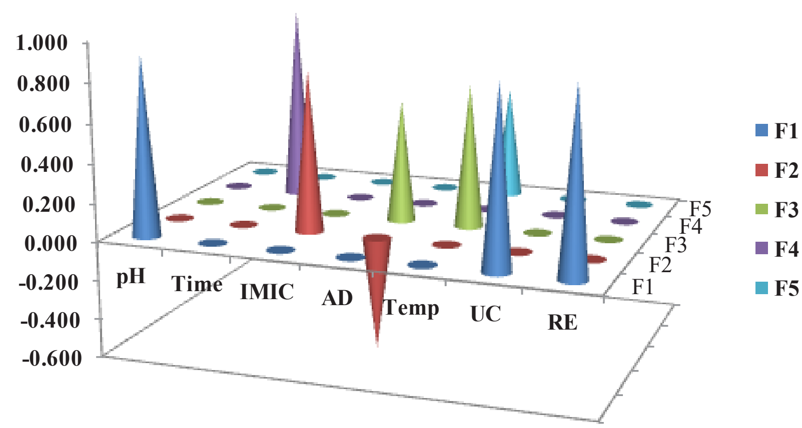
RESULTS AND DISCUSSION

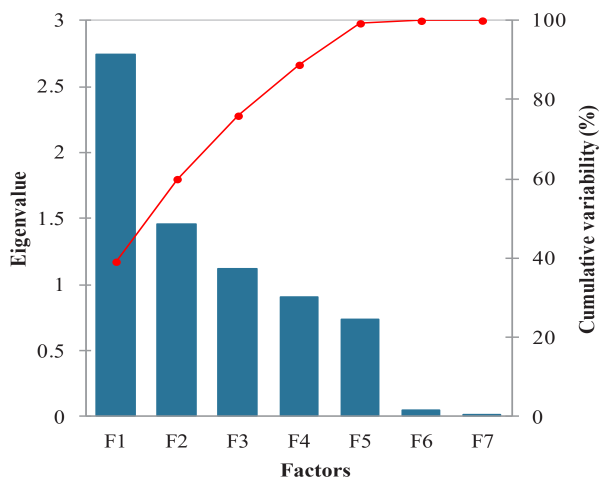
The maximum experimental uptake capacity of ZVIN and MIN were found to be 231.19 and 232.59 mg/g respectively. The removal efficiency of ZVIN and MIN were found to be 92.6% and 93% respectively (Arthy & Phanikumar 2016).

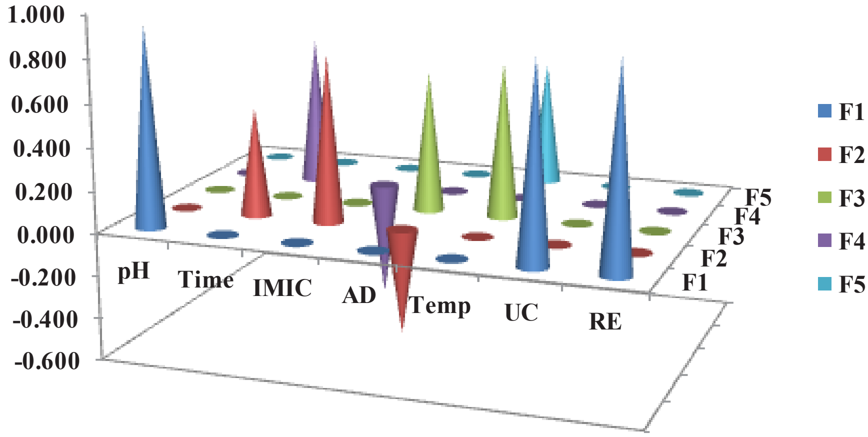
Analysis of Data

Principal Component Analysis (PCA)

A principal component consists of a score vector and a loading vector. The score vector contains information on how the adsorbents are related to each PC. Loading vectors define the reduced dimension space and contain information on how the variables relate to each PC (Alvarez-Uriarte et al. 2011). The influence of variables such as pH, initial metal ion concentration, temperature, time, adsorbent dosage, uptake capacity, and removal efficiency on factors is given by factor loadings. It helps in the identification of the most important variables which has a significant influence (positive or negative) on the factors. The factor loading higher than 0.5 was assumed to be significant (Alvarez-Uriarte et al. 2011). Hence, the factor loading of less than 0.5 was not reported in this study. Fig. 2(a) illustrates the factor loading of ZVIN particles on the adsorption of trivalent chromium ions. Factor 1 has high positive loading for pH (0.921), uptake capacity (0.911) and removal efficiency (0.929). Factor 2 has high positive loading for initial metal ion concentration (0.826) and high negative loading for adsorbent dosage (-0.578). Factor 3 has high positive loading for adsorbent dosage (0.624) and temperature (0.735). Factors 4 and 5 have high positive loading for time (0.998) and temperature (0.577) respectively. Fig. 2(b) shows the scree plot of ZVIN particles, totally of seven factors were extracted for the adsorption of trivalent chromium ions using ZVIN particles. The Eigenvalue of the factors were found to be 2.743, 1.380, 1.098, 1.001, 0.733, 0.042 and 0.004 respectively for factor 1, factor 2, factor 3, factor 4, factor 5, factor 6 and factor 7. The percentage of variability was found to be 39.188%, 19.717%, 15.682%, 14.293%, 10.47%, 0.593% and 0.057% respectively for factor 1, factor 2, factor 3, factor 4, factor 5, factor 6 and factor 7. Fig. 2(c) illustrates the factor loading of MIN-particles on the adsorption of trivalent chromium ions. Factor 1 has high positive loading for pH (0.934), uptake capacity (0.907), and removal Efficiency (0.934). Factor 2 has high positive loading







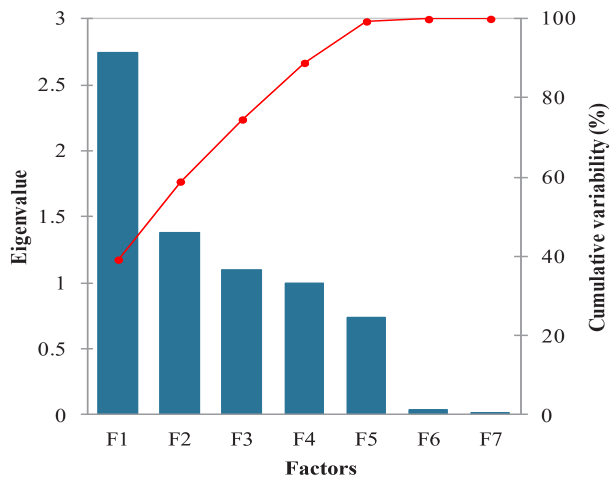


Fig. 2: Loading plot of ZVIN (a) and MIN (c) and Scree plot of ZVIN (b) and MIN (d).

for time (0.508) Initial metal ion concentration (0.785) and negative loading for adsorbent dosage (-0.5). Factor 3 has high positive loading for adsorbent dosage (0.661) and temperature (0.724). Factor 4 has high positive loading on time (0.701) and negative loading on initial metal ion concentration (-0.552). Factor 5 has high factor loading on temperature (0.584). Fig. 2(d) shows the scree plot of MIN- particles which resulted in seven factors, the Eigenvalues of the factors were found to be 2.738, 1.460, 1.120, 0.899, 0.734, 0.045, and 0.004 respectively for factor 1, factor 2, factor 3, factor 4, factor 5, factor 6 and factor 7. The percentage of variability was found to be 39.117%, 20.859%, 15.999%, 12.847%, 10.481%, 0.647% and 0.050% respectively for factor 1, factor 2, factor 3, factor 4, factor 5, factor 6 and factor 7.

Eigenvalues indicate the importance of the factors. Thus, the factors with an Eigen value greater than one were assumed to be significant. Similarly, the percentage of variability should also be greater than 10 (Alvarez-Uriarte et al. 2011). Hence, the number of factors retained for ZVIN and MIN was found to be 4 and 3 respectively. For ZVIN and MIN particles, Factor 3 showed high positive loading for temperature when compared with Factor 5 hence it is not considered. The cumulative variance of ZVIN and MIN were found to be 88.88% (four factors) and 75.97% (three factors), while the minimum decisive factor of the satisfactory analysis is 70% (Cvejanov & Skrbic 2017, Sciutto et al. 2017).

Agglomerative Hierarchial Clustering (AHC)

Agglomerative hierarchical clustering is an iterative classification method, which clusters the dissimilarities between objects together. The type of dissimilarity depends on the nature of the data and the subject studied. The result of AHC is shown in the dendrogram which shows the progressive

Table 1: AHC Result analysis by class of ZVIN.

Class	1	2
Objects	14	4
Sum of weights	14	4
Within-class variance	6.074	1.466
Minimum distance to the centroid	0.698	0.319
Average distance to the centroid	2.141	0.918
Maximum distance to the centroid	3.695	1.518

Table 2: AHC Result analysis by class of MIN.

Class	1	2
Objects	16	4
Sum of weights	16	4
Within-class variance	3.646	1.436
Minimum distance to centroid	0.176	0.308
Average distance to centroid	1.480	0.914
Maximum distance to centroid	3.636	1.520

grouping of data. From the dendrogram, the appropriate number of classes into which the data can be grouped can be identified. In this study, the ward's agglomeration method and Euclidean distance of dissimilarity were chosen.

Fig. 3(a) and 3(b) show the dendrogram of ZVIN and MIN particles respectively. The dendrogram has been majorly classified into two clusters C1 and C2 for both ZVIN and MIN particles. The AHC was used to examine the different operating conditions of adsorbents in the removal of trivalent chromium ions. The elements belonging to the same group are similar to each other and the elements in different groups are heterogeneous in relation to the same variables (Vandeginste 1998). In this study, cluster C2 belongs to the observations on pH for both ZVIN and MIN particles. The cluster C1 belongs to the observations of other input variables like time, temperature, initial metal ion concentration, and adsorbent dosage. The result indicates that, when compared with other independent variables, the pH influences more the removal of trivalent chromium ions by ZVIN and MIN nanoparticles. Table 1 and Table 2 show the AHC result by class respectively for ZVIN and MIN particles. The C2 is more homogeneous than the C1. This is validated by the result of the Within-class variance shown in Table 1 and Table 2 of ZVIN and MIN. The within-class variance of C1 is found to be 6.074 and 3.646 respectively for ZVIN and MIN which is higher than C2.

Modeling of Adsorption Data

Multiple Linear Regression Analysis

The purpose of multiple linear regression is used to learn the relationship between the predictor variable and the dependent variable. In linear regression, models of the unknown parameters are estimated from the data using linear models. Linear regression has many practical applications such as prediction, forecasting…etc. It can be used to fit a predictive model to an observed set of input x and output y values. The generalized equation of MLR is given by equation 6.

$$Y_i = \beta 0 + \beta_1 X_1 + \ldots\ldots. + \beta_n X_n \qquad \ldots(6)$$

Where, β_i (i = 0,.,n) are the parameters generally estimated by least squares and X_i (i =1,.,n) are the explanatory variables (predictors) (Sousa et al. 2007). Multiple linear regression analysis (MLR) is one of the most widely used methodologies for expressing the dependence of a response variable on several independent variables. Despite its success in many applications, the regression approach can face serious difficulties when the independent variables are correlated with each other (McAdams et al. 2000). Multicollinearity, or high correlation among the independent variables in a regression equation, can make it difficult to correctly identify the most important contributors to a physical process. In this study, the linear regression was calculated using the 'Forward' model. Eq. 7 and 9 show the MLR model for uptake capacity of ZVIN and MIN respectively whereas Eq. 8 and 10 show the MLR model for removal efficiency of ZVIN and MIN respectively.

Uptake capacity of ZVIN - 0.789 pH + 0.525 IMIC - 0.351 Adsorbent dosage …(7)

Removal Efficiency of ZVIN - 0.949 pH …(8)

Uptake capacity of MIN - 0.792pH + 0.510 IMIC - 0.346 Adsorbent dosage …(9)

Removal Efficiency of MIN - 0.95 pH …(10)

Principal Component Regression

Principal component regression (PCR) combines principal component analysis (PCA) and multiple linear regression (MLR). In PCR, instead of directly using dependent variables on the explanatory variables, the principal components of explanatory variables are used as regressors. The principal components with higher variances are selected as regressors. The PCR is used to overcome the multicollinearity problem. Eq. 11 shows the generalized equation of PCR.

$$Y_i = \beta 0 + \beta_1 F_1 + \ldots. + \beta_n F_n \ldots(11)$$

Where, β_i (i = 0,., n) are the parameters generally estimated by least squares and F_i (i =1,.,n) are the factors calculated by principal component analysis. Eq. 12 and 14 show the PCR model for uptake capacity of ZVIN and MIN respectively whereas Eq. 13 and 15 show the PCR model for removal efficiency of ZVIN and MIN respectively. In

Table 3: Statistical analysis of uptake capacity by ZVIN and MIN nanoparticles.

Uptake Capacity	ZVIN			MIN		
	MLR	PCR	PLS	MLR	PCR	PLS
Observations	18	18	18	20	20	20
Sum of weights	18	18	18	20	20	20
DF	14	15	16	16	16	18
R^2	0.945	0.981	0.752	0.943	0.982	0.742
Adjusted R^2	0.934	0.978	0.513	0.932	0.978	0.521
MSE	0.066	0.022	0.234	0.068	0.022	0.245
RMSE	0.257	0.148	0.484	0.261	0.148	0.495
MAPE	29.328	27.011		41.409	39.142	
DW	0.985	0.631		1.015	0.649	
Cp	3.482	4.737		3.265	4.000	
AIC	-45.398	-66.078		-50.183	-72.865	
SBC	-41.836	-63.407		-46.200	-68.882	
PC	0.086	0.027		0.086	0.028	

this study, the linear regression of principal components was calculated using the 'Forward' model.

Uptake capacity of ZVIN - $0.534 \times F1 + 0.321 \times F2$ …(12)

Removal Efficiency of ZIVN - $0.545 \times F1 - 0.270 \times F2$ …(13)

Uptake capacity of MIN - $0.534 \times F1 + 0.303 \times F2 - 0.124 \times F3$ …(14)

Removal Efficiency of MIN - $0.549 \times F1 - 0.224 \times F2 + 0.117 \times F3$ …(15)

Partial Least Square

Partial least square is a rapid, well-organized, and best regression method based on covariance. It is a technique that decreases the predictors to a lesser set of uncorrelated components and achieves least square regression on these components, instead of on the original data. PLS is used to find a relationship between explanatory variables (X) and independent variables (y). The generalized equation for PLS is given by the following equation

$$Y=Xb \qquad \text{…(16)}$$

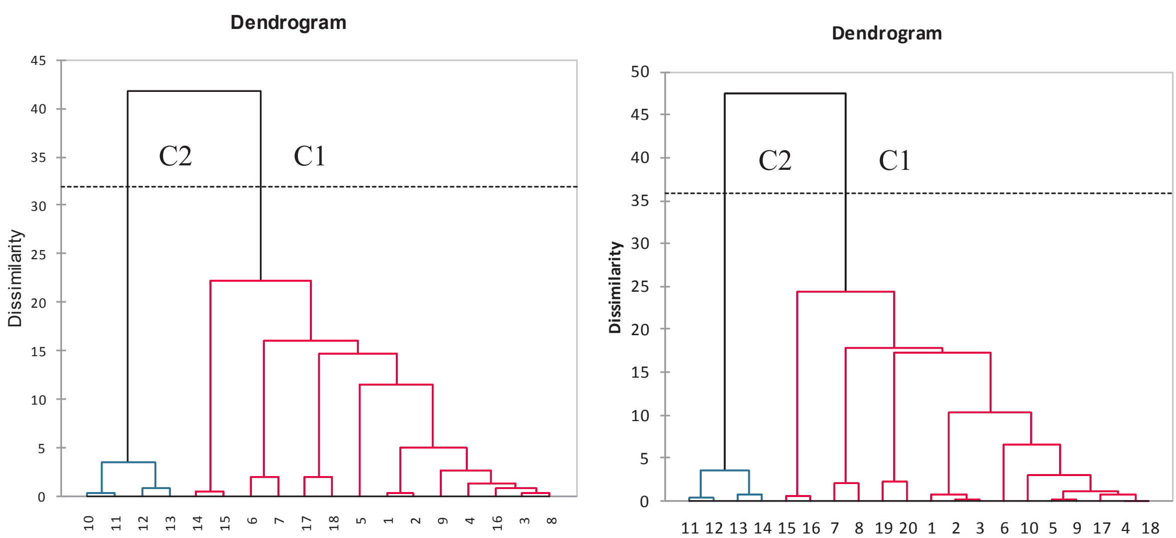


Fig. 3: Dendrogram obtained from AHC of ZVIN (a) and MIN (b) particles.

Table 4: Statistical analysis of Cr^{3+} ion removal by ZVIN and MIN nanoparticles.

Removal Efficiency	ZVIN			MIN		
	MLR	PCR	PLS	MLR	PCR	PLS
Observations	18	18	18	20	20	20
Sum of weights	18	18	18	20	20	20
DF	16	15	16	18	16	18
R²	0.901	0.970	0.790	0.902	0.965	0.794
Adjusted R²	0.895	0.966	0.473	0.897	0.958	0.466
MSE	0.105	0.034	0.199	0.103	0.042	0.195
RMSE	0.325	0.184	0.446	0.321	0.204	0.442
MAPE	148.729	110.638		53.343	33.135	
DW	0.990	1.069		1.152	1.245	
Cp	3.070	2.403		2.195	4.000	
AIC	-38.635	-58.233		-43.553	-60.098	
SBC	-36.854	-55.562		-41.562	-56.115	
PC	0.124	0.042		0.119	0.052	

Where b is the calibration vector. Eq. 17 and 19 show the PLS model for uptake capacity of ZVIN and MIN respectively whereas Eq. 18 and 20 illustrate the PLS model for removal efficiency of ZVIN and MIN respectively.

Uptake capacity of ZVIN - 0.766 × pH + 0.038 × Time + 0.121 × IMIC - 0.199Adsorbent dosage + 0.232 Temperature …(17)

Removal Efficiency of ZVIN - 0.785 × pH + 0.039 × Time + 0.124 × IMIC - 0.204 × Adsorbent dosage + 0.238 × Temperature …(18)

Uptake capacity of MIN - 0.773 × pH - 0.058 × Time + 0.116 × IMIC - 0.186 × Adsorbent dosage + 0.206 × Temperature …(19)

Removal Efficiency of MIN - 0.8 × pH - 0.06 × Time + 0.120 × IMIC - 0.192 × Adsorbent dosage + 0.213 × Temperature …(20)

Comparison of MLR, PCR and PLS Models

Goodness of Fit

Tables 3 and 4 show the statistical analysis of the adsorption data by ZVIN and MIN respectively. The DF represents the number of degrees of freedom, which indicate that the number of independent values, can vary in a study without breaking any constraint. The DF of MLR, PCR, and PLS was given in Tables 3 and 4. The values indicated that the PCR and PLS model has high degrees of freedom when compared with MLR for both uptake capacity and removal efficiency of ZVIN and MIN nanoparticles. The R^2 is interpreted as the amount of the variability of the dependent variable explained by the model. The better fit of the model should have the value of R^2 close to 1. In this study, the R^2 value of PCR was found to be greater than in other models. Similarly, the adjusted R^2 value is also greater for the PCR model (Tables 3 and 4). The mean of the squares of the error (MSE) is the average squared difference between the predicted values and the actual values. The Root Mean Square Error (RMSE) is the standard deviation of the residuals. The values closer to zero are better hence, the MSE and RMSE values of the PCR model were found to be less when compared with MLR and PLS models. The mean absolute percentage error (MAPE) is a measure of the prediction accuracy of forecasting methods. The result shows that the PCR model has less MAPE value than MLR (Tables 3 and 4).

Durbin-Watson (DW) is a test for autocorrelation in the residuals from a statistical regression analysis. DW statistic value always lies between 0 and 4. If the result lies between 0 and <2 there is a positive autocorrelation. If the value is 2 there is no autocorrelation detected in the sample. If the value lies between >2 and 4 it is negative autocorrelation. In this study, the value suggests a positive correlation for both ZVIN and MIN nanoparticles (Tables 3 and 4). Mallows Cp coefficient evaluates the accuracy and bias of the full model to the models with a subset of the predictors. The Mallows Cp value should be close to the number of predictors plus the constant. The nearer the Cp coefficient to the predictor variable, the less the model is biased. The value of Cp of ZVIN and MIN on uptake capacity and removal efficiency

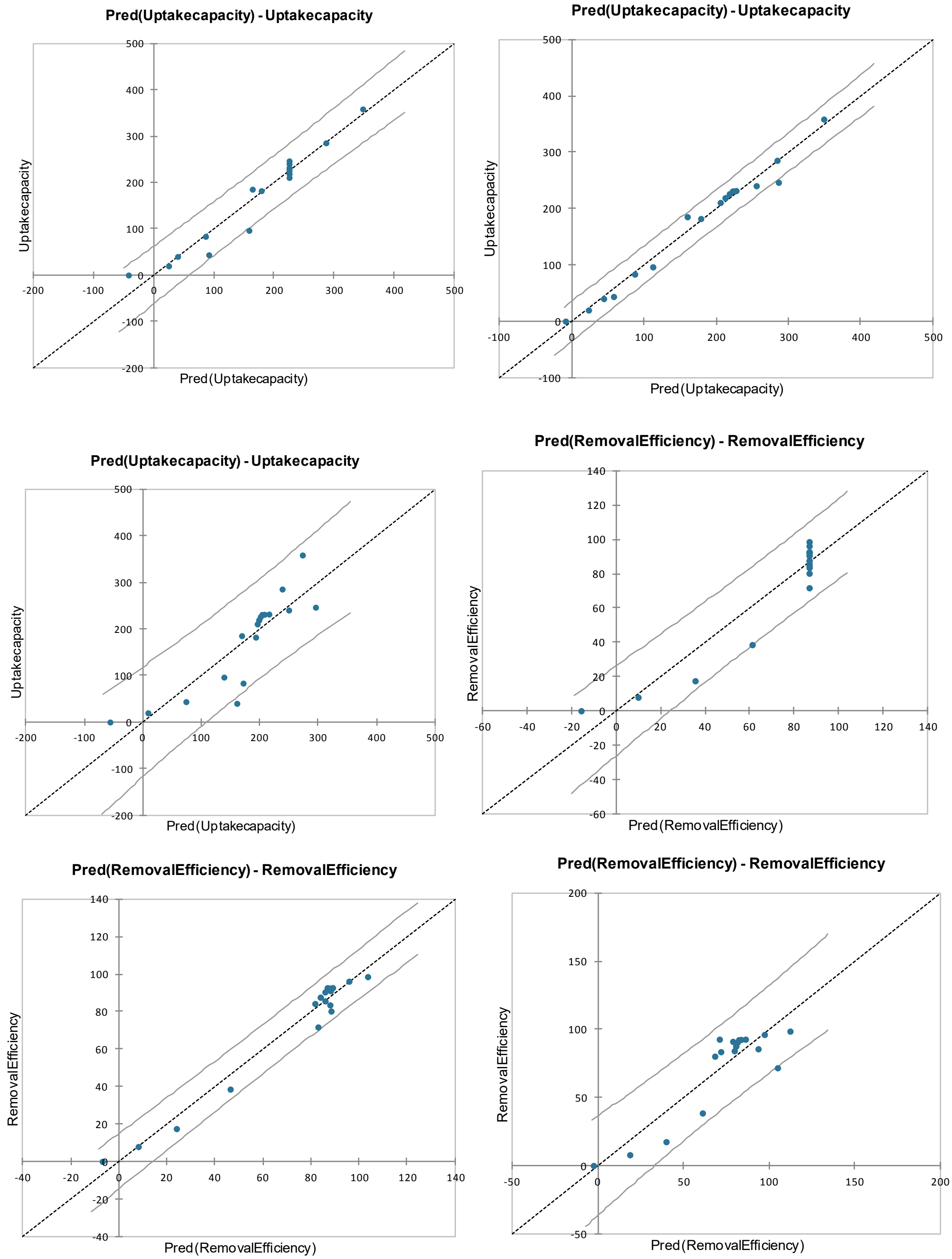


Fig. 4: Variation of predicted values on uptake capacity (a, b, c) and removal efficiency (d, e, f) of ZVIN nanoparticles by MLR (a, d), PCR (b, e) and PLS(c, f) models.

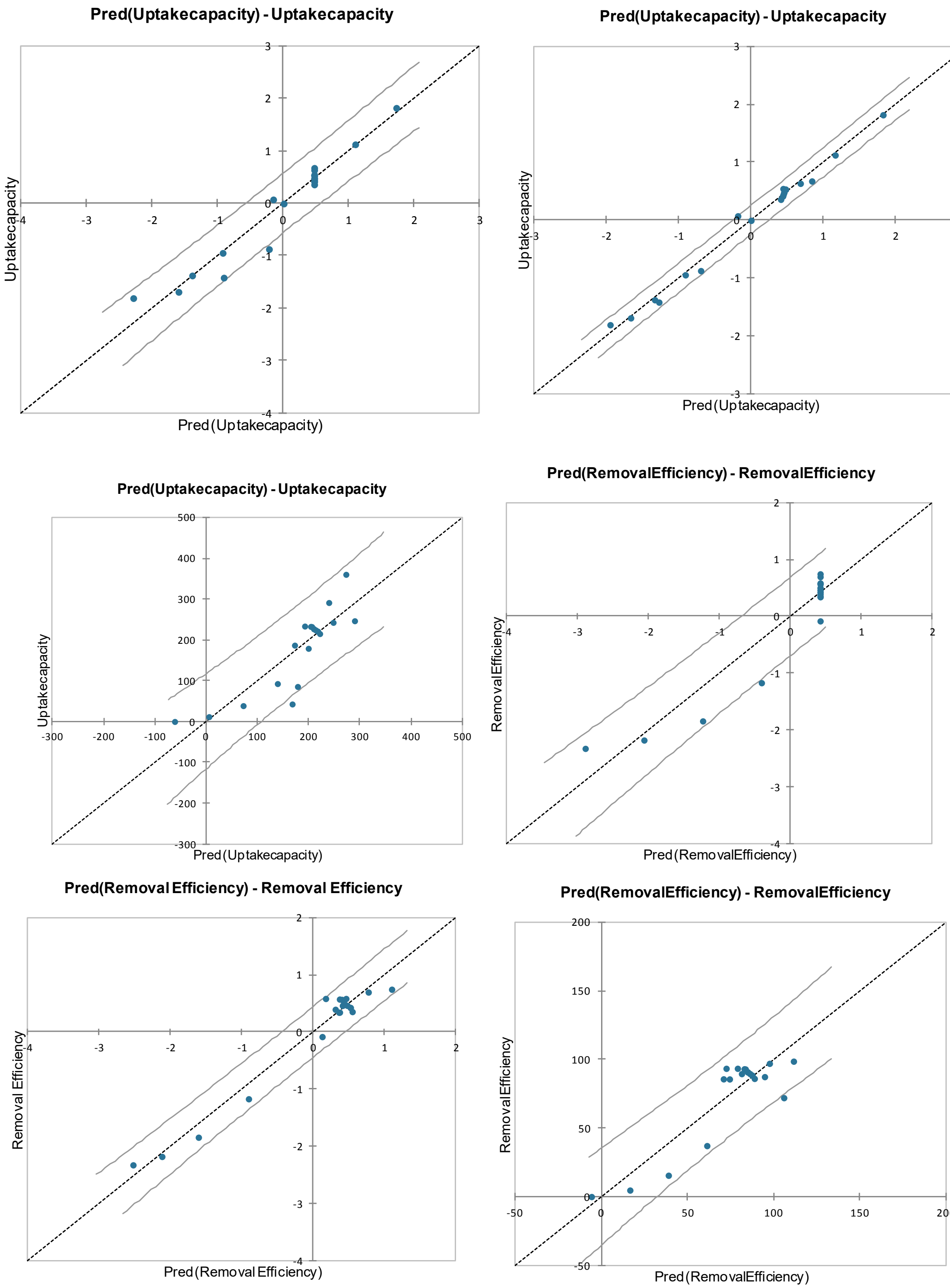


Fig. 5: Variation of predicted values on uptake capacity (a, b, c) and removal efficiency (d, e, f) of MIN nanoparticles by MLR (a, d), PCR (b, e) and PLS(c, f) models.

indicated that both MLR and PCR models are less biased. Akaike's information criterion (AIC) is an estimator of prediction error. AIC estimates the amount of information lost by the model. It is used to compare the quality of the model. Schwarz's Bayesian Criterion (SBC) is a decisive factor for model selection, the model with the lowest BIC is chosen. Table 3 and 4 shows the PCR model has fewer AIC and SBC values than the MLR model for both uptake capacity and removal efficiency of ZVIN and MIN nanoparticles. Amemiya's prediction criterion (PC) is similar to adjusted R^2, where, it penalizes more heavily than adjusted R-square. The value of PC is less for the PCR model when compared to the MLR model for both ZVIN and MIN nanoparticles on the removal of Cr^{3+} ions.

Thus the analysis of goodness of fit indicates that the PCR model is best suited for the prediction of uptake capacity and removal efficiency for MLR, PCR, and PLS models.

Prediction of Uptake Capacity and Removal Efficiency

Fig. 4 and 5 show the variation of predicted values on uptake capacity and removal efficiency of ZVIN and MIN nanoparticles by MLR, PCR, and PLS models. The figures show that the PCR model has effectively predicted the uptake capacity and removal efficiency of ZVIN and MIN nanoparticles.

CONCLUSION

In this paper, two statistical analysis techniques (PCA and HCA) and three statistical modeling techniques (PCR, MCR, and PLS) were applied to the adsorption data. These data analysis tools enhance the understanding of the adsorption process. PCA and HCA were applied to identify the chief contribution of independent variables in the removal of Cr^{3+} ions from an aqueous solution. The results indicated that among all variables, the contribution of pH in the removal of Cr^{3+} ions from an aqueous solution was found to be high. PCR, MLR, and PLS were used for the prediction of adsorption data. The analysis of goodness of fit for MLR, PCR, and PLS models indicates that the PCR model is best suited for the prediction of uptake capacity and removal efficiency.

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