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Computational Analysis of Cu^{2+} Adsorption on Synthetic NaX Zeolite

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Keywords

Adsorption,
NaX zeolite,
Cu^{2+},
Composite surface design.

Abstract

The effect of several experimental conditions (mass, concentration and temperature) on the adsorption capacity of copper on synthetic NaX zeolite was investigated. The adsorbent was characterized by scanning electron microscopy. The effect of these conditions on the performance of the adsorbent was studied using composite surface design methodology. It was found that all the studied parameters have a statistically significant influence on the working adsorption capacity.

1. Introduction

Industrial evolution has been responsible for environmental pollution since many industrial effluents have been directly discharged in natural water sources [1-2]. Heavy metals are considered one of the most dangerous inorganic contaminants since they are not biodegradable and can accumulate in living organisms, causing various diseases [3]. Lead, mercury, copper, cadmium, nickel and chromium are among the most common pollutants found in discharged industrial effluents [4]. Zeolites are microporous crystalline aluminosilicates containing large amounts of framework cations. Also, they have valuable exchange properties and are applied in water and wastewater treatment [5-6]. Synthetic zeolites have very reproducible and tunable physico-chemical properties that make them very attracting for heavy metals adsorption [7-8].

The main objective of this paper is to study the behavior of NaX zeolite for Cu^{2+} removal from water using the composite surface design methodology. Different factors that affect the adsorption process were studied in batch conditions. These include mass effect, temperature and the initial metal ions concentrations.

2. Materials and Methods

2.1. Materials

The synthetic NaX Faujasite (Na88Al88Si104O384) samples were provided by IFP Energie Nouvelle. These samples were used as received without any further chemical modification. copper nitrate (Cu(NO3)2.3H2O), was purchased from Sigma Aldrich, and used as received. Ultrapure water was used throughout.

2.2. Characterization

Scanning electron microscopy (SEM) is used to study the surface topography and morphology of solid materials on a scale down to about 10 nm. The analysis was performed using SEM, JEOL 7001 FEG. SEM utilizes electrons to show an enlarged image of a specimen by detecting secondary electrons to form an image for observation. The SEM's resolution is 0.5 to 4nm.

2.3. Batch Adsorption Experiments

Copper ion solutions were prepared from their corresponding nitrate salts in ultrapure water to obtain solutions of different concentrations. In typical batch studies, a weighed amount (10, 20 and 30 mg) of the solid powder was placed in a flask containing 100 mL of a metal solution of desired concentration. The flask was continuously stirred at 25 °C, 35°C and 45°C at 300 rpm. At the end of each step the solution was filtered and the metal ion concentration was determined using Atomic Adsorption Spectrophotometer (AAS, Perkin Elmer AA200). The same procedure was repeated for the three divalent metals used. The removal efficiency was calculated by Eq. (1) as

$$R = \frac{C_0 - C_t}{C_0} \times 100 \quad (1)$$

where C_0 and C_t are the heavy metal initial concentration and at time t concentrations.

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3. Results and Discussion

3.1. Structure Characterization

Scanning electronic micrographs show the crystallites of NaX forming fine cubic particles with an average size 3 µm (Figure 1).

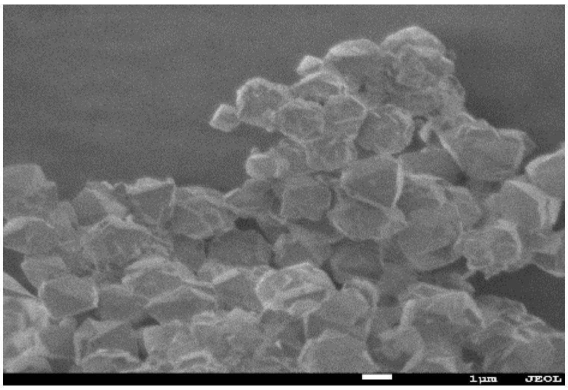

Figure 1. Scanning electron microscopy

3.2. Composite Surface Design Modeling

Solution concentration (C), temperature (T), and adsorbent mass (m) were chosen asthe independent variables with their levels and ranges: 30,100, 300 ppm for (C), 25 °C, 35°C, 45°C for (T) and 10, 20, 30 mg for (m). we obtained the final equation in terms of coded values (Eq. (2))

$$\% Adsorption = 21.19 - 36.17\,A - 2.36\,B + 4.45\,C + 0.34\,AB - 0.58\,AC + 0.61\,BC + 31.13\,AA - 0.81\,BB - 1.15\,CC \quad (2)$$

and in terms of actual factors (Eq. (3))

$$\% Adsorption = 101.01 - 0.83C + 0.16\,T + 0.76\,m + 2.49E - 004\,CT - 4.28E - 004\,Cm + 6.08E - 003\,Tm + 1.71E - 003\,CC - 8.12E - 003\,TT - 0.01\,mm \quad (3)$$

3.3. Analysis of Variance (ANOVA)

The ANOVA was performed using the Design-Expert software and the results are presented in Table 1. The Model F-value of 91.13 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise. The solution concentration has the greatest effect on adsorption with the highest F-value of 794.81.

Table 1. Estimated ANOVA for response surface model

Source	F value	p-value
Model	91.13	< 0.0001
A-Concentration	794.81	< 0.0001
B-Temperature	3.28	0.0880
C-mass	11.59	0.0034
AB	0.049	0.8269
AC	0.15	0.7072
BC	0.15	0.7035
A^2	107.52	< 0.0001
B^2	0.13	0.7192
C^2	0.27	0.6108

3.4. Residuals and Model Adequacy

To know whether the selected model gives adequate approximation of the real system or not, the normal probability plots of the Studentized residuals and the predicted versus actual value plots were applied. Figure 2 shows the normal probability plots of the Studentized residuals for adsorption. It is clear from the figure that the residuals follow a normal distribution, as the data points follow a straight line.

Figure 3 shows that the predicted values of copper adsorption efficiency obtained from the model and the actual experimental data were in good agreement, providing evidence for the validity of the regression model.

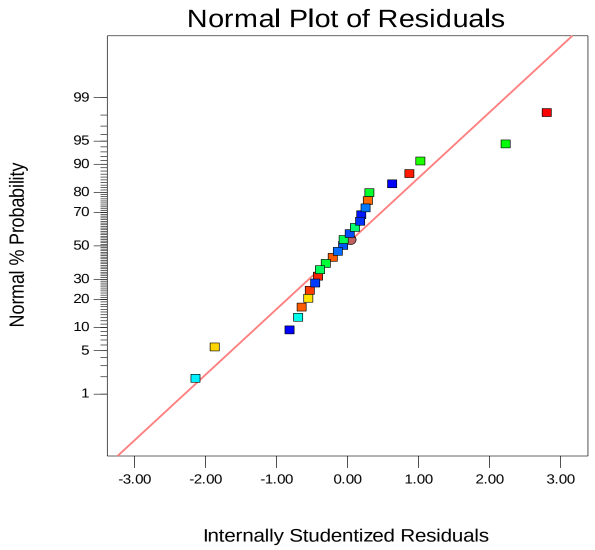

Figure 2. Normal % probability versus internally studentized residuals

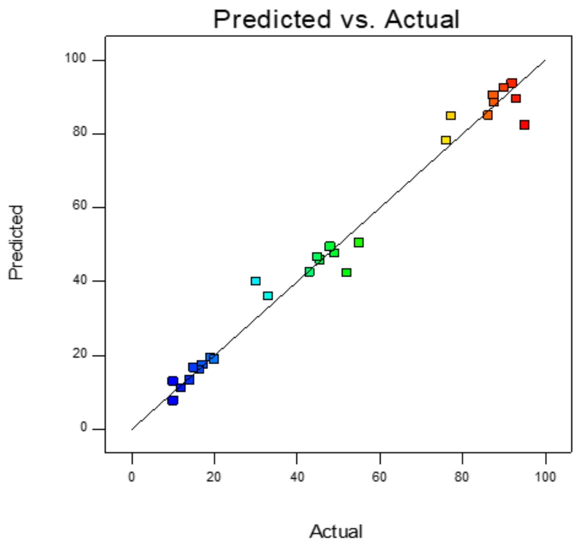

Figure 3. Comparison of model predictions of % adsorption with the experimental data

4. Effect of Concentration and Adsorbent Mass on the Adsorption Performance

The 2D surface response plots of the quadratic model were utilized to investigate the interactive relationships between independent variables and the removal efficiency of copper om NaX zeolite. As shown in Figures 4 and 5, in each plot, one variable was kept constant, while the other two were varied within the experimental ranges. It is clear from these plots that under the conditions used in this study that the % adsorption is more significant when working at low level of C and higher m.

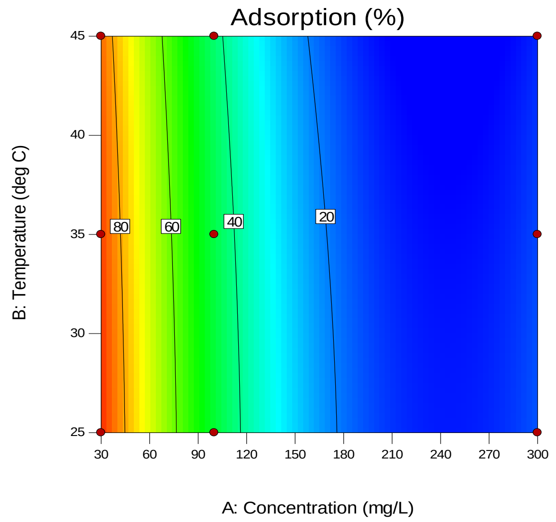

Figure 4. 2D surface response plots of the quadratic model for % adsorption (T vs C)

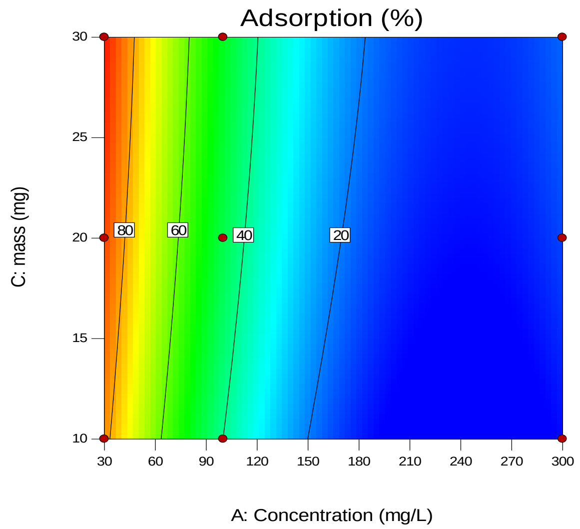

Figure 5. 2D surface response plots of the quadratic model for % adsorption (m vs C).

5. Conclusions

The performance of synthetic NaX zeolite for copper adsorption was investigated under different experimental conditions including concentration, mass and temperature. Statistical surface design analysis indicated that all the studied parameters have significant effect on the adsorption capacity with concentration the most significant one.

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