Data Article

Data on efficient removal of acid orange 7 by zeolitic imidazolate framework-8

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A B S T R A C T

A water stable and hybrid nonporous adsorbent, cubic zeolitic imidazolate framework-8 (ZIF-8), was synthesized for Acid orange 7 (AO7) removal from aqueous solutions in batch mode. Central composite design was utilized to explore the individual and interaction effects of pH, AO7 concentration, ZIF-8 dosage and contact time on dye adsorption. A second order polynomial equation ($R^2 = 0.9852$, $LOF = 0.1419$) developed for prediction of the AO7 removal. Sorption model revealed that the adsorbent dosage and the dye concentration are major factors that controlled the AO7 removal efficiency. AO7 removal increased from 55 to 80% by increasing ZIF-8 dosage from 0.2 to 1 g/L. The dye removal, on the other hand, decreased from 84 to 70% with increasing AO7 concentration from 10 to 100 mg/L and increased from 60% to 80% by decreasing pH from 12 to 4. The dye removal followed the pseudo second order kinetic and the Langmuir isotherm model. The maximum monolayer adsorption capacity of 80.47 mg dye/g of ZIF-8 was obtained according to the Langmuir model.

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1. Data

The XRD pattern of the synthesized ZIF-8 is shown in Fig. 1(a). Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscope (SEM) of as-synthesized ZIF-8 are shown in Fig. 1(b) and (c), respectively.

The experimental range and levels of four independent variables are listed in Table 1. Table 2 shows a total of 30 experimental runs that performed based on the experimental design matrix. The removal efficiencies then analyzed using the analysis of variance (ANOVA) to set a prediction model.

To evaluate the efficacy of linear, 2Fl, quadratic and cubic models, the obtained scores from the sequential modeling were compared (Table 3). The relationship between input variables and response was modeled using ANOVA which presented in Table 4. Fig. 2 depict the effect of pH and initial dye concentration on the removal of AO7. Fig. 3 shows the counter plot and response surface plot of pH and adsorbent dose on dye removal.

Fig. 4 compare the removal percentages obtained experimentally for AO7 adsorption with those predicted by the model.

The three well-known isotherm models including Langmuir, Freundlich, Temkin and Dubinin-Radushkevich [1] were fitted with equilibrium data and related constants are listed in Table 5. Fig. 5 shows the fitted experimental data with isotherm models.

Table 6. Adsorption kinetics and their formula for AO7 removal by ZIF-8. Three adsorption kinetic models including pseudo first order, pseudo first order and intra-particle diffusion models [2] were used to describe the kinetic data. The kinetic models and their constants are presented in Table 6 and Table 7 and the plots of these models are shown in Fig. 6.

2. Materials and methods

2.1. Chemicals and reagents

AO7 used in the experiments was obtained from Alvan Sabet Company. All other reagents and chemicals used in the preparation of the adsorbent were purchased from Merck Company.
Fig. 1. Characteristics of the as-synthesized ZIF-8: (a) XRD pattern and (b) FTIR pattern and (c) SEM image of ZIF-8 crystals.
2.2. ZIF-8 synthesis and characterization

Zeolitic imidazolate framework-8 (ZIF-8) is a water stable and porous member of metal organic framework (MOFs). ZIF-8 was prepared at room temperature exactly according to the literature [3]. All of the diffraction patterns in XRD and FTIR tests were in accordance with those in the literature for ZIF-8, indicating that the synthesized adsorbent has pure ZIF-8 phase. The SEM image shows the uniform cubic shapes of the micrometer-sized crystals of ZIF-8. The BET surface area and total pore volume of ZIF-8 are 978 m²/g and 0.51 cm³/g, respectively [3].

2.3. Sorption experiments

Batch mode experiments were employed in this work. All experiments were carried out in duplicate and mean values were reported. The experiments were conducted in incubator shaker at 25 °C and at 200 rpm. After agitating, the residual concentration of AO7 in the solution was determined via spectrophotometer at 484 nm.
2.4. Experimental design and modeling

The AO7 removal was carried out by four chosen independent variables using central composite design (CCD). A second order polynomial equation was applied to explore the influence of variables in terms of linear, quadratic and cross product:

\[ Y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} X_i X_j + \epsilon \]  

(1)
Fig. 3. Counter plot and response surface plots of pH and adsorbent dose on dye adsorption (AO7: 55 mg/L, time: 50 min).

Fig. 4. Normal probability plot of the predicted values of AO7 uptake efficiency versus actual values (a), predicted response versus actual response (b).

Table 5
Adsorption isotherms and related constants for AO7 adsorption.

| Isotherm               | Formula                      | Plot                      | Parameter     | Value  |
|------------------------|------------------------------|---------------------------|---------------|--------|
| Langmuir               | \( q_e = \frac{q_m b c_e}{1 + b c_e} \) | \( \frac{1}{q_e} \) vs. \( \frac{1}{c_e} \) | \( q_{max} \) (mg/g) | 80.47  |
|                        |                              |                           | \( K_L \) (L/mg) | 1      |
|                        |                              |                           | \( R^2 \)       | 0.96   |
| Freundlich             | \( q_e = k_F c_e^\alpha \)  | \( \log q_e \) vs. \( \log C \) | \( K_F \) (mg/g (L/mg)^{1/n}) | 29.99  |
|                        |                              |                           | \( n \)         | 2.71   |
|                        |                              |                           | \( R^2 \)       | 0.86   |
| Temkin                 | \( q_e = \frac{RT \ln(k_T c_e)}{b} \) | \( q_e \) vs. \( \ln C_e \) | \( k_t \) (L/mg) | 7.94   |
|                        |                              |                           | \( B_1 \)       | 18.39  |
|                        |                              |                           | \( R^2 \)       | 0.69   |
| Dubinin-Radushkevich   | \( q_e = q_m \exp (-\beta \varepsilon^2) \) | \( q_e \) vs. \( \varepsilon^2 \) | \( q_{max} \) (mg/g) | 76.74  |
|                        |                              |                           | \( \beta \)      | 1.01E-07|
|                        |                              |                           | \( R^2 \)       | 0.76   |
Fig. 5. Fitting the experimental data with (a) Langmuir, (b) Freundlich, (c) Temkin and (d) Dubinin-Radushkevich models (ZIF-8: 0.6 g/L, pH: 6, time 12 h.).
In the above equation, Y is the predicted response (AO7 uptake), Xi and Xj are the independent variables, β0 is a constant value, βi, βii, and βij are the regression coefficients for linear, second order, and interaction effects, respectively and ε is the error of the model. The higher F-value (59.32) and smaller p-value (<0.0001) in Table 3, illustrates that the quadratic model gives the best fit to experimental data. The amount of lack of fit was non-significant (0.1419), and the values of R², adjusted R² and predicted R² were found to be 0.9852, 0.9713 and 0.9245 respectively, which represents the experimental data predicted well by the model. The uniform distribution of predicted data near to regression line indicated the adequacy of the developed model. The empirical relationship between the independent variables and the response based on the experimental data, after modifying the model, was explained as:

\[ Y = 69.71 - 2.83 X_1 - 4.75 X_2 + 10.58 X_3 + 1.25 X_1 X_2 + 1.75 X_1 X_3 + 1.41 X_1^2 + 4.66 X_2^2 - 3.34 X_3^2 \]  

(Eq. 2)

The above equation explains how AO7 uptake by ZIF-8 and influenced by the individual variables. The positive sign for each term represents that AO7 adsorption increased with increasing the variable value and vice versa.

2.5. Effect of various process variables

As Fig. 2 illustrates, by increasing the pH from 4 to 12, the dye removal efficiency was decreased. The AO7 uptake also decreased by increasing initial AO7 concentration from 10 to 100 mg/L. The degree of AO7 uptake, on the other hand, increased with increasing adsorption dosage from 0.2 to 1 g/L.

2.6. Adsorption isotherms

In order to improve the adsorption mechanism pathways and effective design of adsorption systems, it is necessary to understand and interpret the adsorption isotherms. Sorption experiments for isotherm modeling were done by applying 0.6 g ZIF-8/L to solutions containing 10, 25, 50, 75 and 100 mg AO7/L at pH of 6 and 25 °C for 12 h. As mentioned in Fig. 5 and Table 5, the adsorption data fitted well by the Langmuir model and the maximum monolayer adsorption capacity of ZIF-8 for AO7 was obtained 80.47 mg/g.
2.7. Adsorption kinetics

Kinetic studies evaluate the mechanism and rate of adsorption process [13–17]. By comparing the obtained regression coefficient ($R^2$) values for each model, it can be stated that adsorption of AO7 by ZIF-8 obeyed pseudo second order model.
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Transparency document

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