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Modeling and Optimization by RSM-BBD Design for Acid Dye Removal from Aqueous Solution using Water-Dispersible Superparamagnetic Iron Oxide Nanoparticles

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ABSTRACT

This work presents the synthesis of Water-dispersible superparamagnetic iron oxide nanoparticles (SPIONS) Fe_3O_4 with different average sizes, obtained by different methods: co-precipitation with surface modification and polyol method. The obtained SPIONs, which were coated with (PEG /EG) with hydrophilic properties, showed excellent dispersion capacity in water and colloidal stability. The nanoparticles were analyzed by X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). The nanoparticles were used as adsorbents for the adsorption of Naphthol green B (NGB) dye in aqueous solutions, by optimizing adsorption parameters such as initial dye concentration, solution pH and adsorbent dose, using the Box- Behnken (BBD) response surface method. The results show that the BBD method is an effective approach to optimize the adsorption process and maximize the adsorption capacity of the dye. The Langmuir and Freundlich isotherm models were used to study the adsorption equilibrium, and the first- and second-order kinetic equations were used to model the adsorption kinetics.

Keywords: SPIONS, co-precipitation, polyol, Box- Behnken design.

1 Introduction

Fe_3O_4 nanoparticles (NPs) are magnetic nanomaterials that have attracted the attention of researchers due to their exceptional magnetic properties, and high specific surface area [1]. They have been widely studied for water decontamination as they can effectively adsorb organic and inorganic pollutants present in wastewater. However, Fe_3O_4NPs have hydrophobic properties and a strong tendency to agglomerate due to their high surface energy, which limits their dispersion and reactivity in aqueous environments. To improve functionality and achieve stable dispersion of Fe_3O_4 NPs, it is common to coat and functionalize them with surface agents [2]. In this study, superparamagnetic iron oxide nanoparticles (Fe_3O_4) were synthesized using three different approaches, which are intended to serve as effective adsorbents in the removal of anionic dyes from aqueous solutions. The impact of key parameters, such as initial pH, adsorbent dosage, initial dye concentration, and contact time, on the adsorption capacity was evaluated. The optimal operational conditions for the adsorption process were determined using the box Behnken design method within the response surface methodology (RSM-BBD).

2 Experimental

2.1. Synthesis of magnetic Fe_3O_4 nanoparticles by polyol method

Magnetic Fe_3O_4 nanoparticles were prepared using the polyol method by dissolving the mixture of 3.96 g of ($FeCl_3$ .6H2O) and 2.04 g of ($FeSO_4.7H_2O$) in 100 mL of (PEG/EG 1:1 v/v) .16 mmol of NaOH was added to the solution of metal chlorides with stirring at room temperature, causing an immediate color change to deep black-brown. After 1/2 h, the temperature of solution was raised during 1 h to 190 °C and then kept constant for 1 h30 min in the temperature range 240-250 °C. The solid product was isolated by cooling the reaction mixture to room temperature and centrifuging. A black solid was obtained and washed

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with ethanol twice and with a mixture of ethanol and ethyl acetate(1:1, v/v) three times to remove the excess (PEG/EG) and was dried.

2.2. Batch adsorption procedure

The adsorption process was carried out at room temperature with varying initial pH values, initial concentration of the NGB dye, contact time, and adsorbent mass. After reaching equilibrium, the suspension was filtered and subsequently analyzed using a UV/visible spectrometer. To determine the adsorption capacity, the amount adsorbed per unit mass of NPs (mg/g) was calculated using the following expressions:

$$qe = \frac{(c_0 - c_e)V}{m} qe = \frac{(c_0 - c_e)V}{m} \quad (1)$$

3 Results & Discussions

3.1 Effect of pH, mass and initial dye concentration:

The results shown in Figure 1A demonstrate that the adsorption of NGB increases as the pH decreases. However, optimal adsorption occurred at acidic solution due to the strong attraction between NGB and the adsorbent. Figure 1B shows that the amount of adsorbed dye increases with the addition of the adsorbent, beyond which the decolorization efficiency does not improve further. This behavior is attributed to the increasing number of adsorption sites with the mass of the adsorbent, which consequently depletes the GNB solution with a fixed initial concentration. Figure 1C demonstrates that the amount of adsorbate fixed on the material increases with an increase in the dye solution's concentration. In fact, the increase in concentration induces a higher driving force of the concentration gradient, thereby enhancing the diffusion of dye molecules in solution through the surface of the adsorbent.

(A) (B) (C)

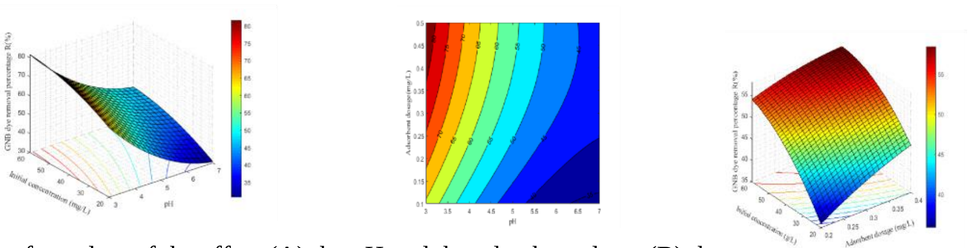

Figure 1. Surface plots of the effect (A) the pH and the adsorbent dose; (B) the pH and the initial concentration; (C) the adsorbent dose and initial concentration on GNB dye removal efficiency.

4 Conclusions

Based on the conducted experiment, it can be concluded that Water-dispersible Fe_3O_4 SPIONs synthesized by polyol method, can be effectively used to adsorb the NGB dye from the solution, and the optimal conditions are as follows: 0.43 g of adsorbent at an agitation speed of 350 ppm for 60 minutes. The optimal pH was found to be 3 with an initial NGB dye concentration of 51 ppm.

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