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Determination of optimum isotherm and kinetic models for phosphate sorption onto iron oxide nanoparticles: nonlinear regression with various error functions

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ABSTRACT

The aim of this study was to determine optimum kinetic and isotherm models for phosphate (P) sorption onto iron oxide nanoparticles through nonlinear regression analysis. Equilibrium batch experiments were conducted at the experimental conditions of initial P concentration = 0.5–20 mg/L, adsorbent doses = 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6 g/L, and shaking time = 24 h. Kinetic batch experiments were also performed at the experimental conditions of initial P concentrations = 1, 2, 4, 6, 8, and 10 mg/L, adsorbent dose = 0.6 g/L, and shaking time = 10 min–24 h. Six isotherm models (Langmuir, Freundlich, Temkin, Redlich–Peterson, Khan, and Sips) were used to analyze the equilibrium data through nonlinear regression analysis. Three kinetic models (pseudo-first-order, pseudo-second-order, and Elovich) were used to analyze the kinetic data through nonlinear regression. Error functions including the sum of the squared errors, hybrid fractional error function (HYBRID), average relative error, Marquardt's percent standard deviation, and sum of the absolute errors (EABS) were used to minimize the error distribution between experimental data and predicted model fits in the optimization process. To compare the five error values, the results of each set were normalized and summed. Considering both coefficient of determination (R^2) and Chi-square (χ^2), the Redlich–Peterson (Freundlich) model was found to provide the best fit to the experimental data in the equilibrium model analyses, and the optimum parameter values were obtained by the HYBRID error function with the parameter values of $K_R/a_R = 3.59$–4.15 mg/g and g = 0.69–0.89 from the Redlich–Peterson model. Considering both R^2 and χ^2, the Elovich (or pseudo-second-order) model was found to provide the best fit to the kinetic data in the kinetic model analyses, and the optimum parameter values produced by the EABS error function with the parameter values of $\alpha = (3.60 \times 10^5)$–$(4.80 \times 10^6)$ mg/g/h and $\beta = 4.43$–13.07 g/mg from the Elovich model.

Keywords: Error function; Isotherm model; Iron oxide nanoparticle; Kinetic model; Nonlinear regression; Phosphate sorption

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