Augmentation of neodymium ions removal from water using two lanthanide-based MOF: ameliorated efficiency by synergistic interaction of two lanthanides

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Kinetic of Adsorption

The data obtained in this study were fitted with five common kinetic models described below.

Pseudo-first order:

$$\ln \left( q_e - q_t \right) / q_e = -k_1 t$$  \hspace{1cm} (1)

Pseudo-second order:

$$\frac{t}{q_t} = \frac{1}{h} + \frac{t}{q_e}, \ h = k_2 q_e^2$$ \hspace{1cm} (2)

Elovich:

$$q_t = \frac{1}{\beta} \ln (\alpha \beta) + \frac{1}{\beta} \ln (t)$$ \hspace{1cm} (3)

Inert Particle Diffusion:

$$q_t = C + K_D t^{0.5}$$ \hspace{1cm} (4)

Modified Freundlich:

$$q_t = K C_0 t^\alpha$$ \hspace{1cm} (5)

Where \( q_e \) (mg/g) is the equilibrium adsorption capacity of the MOF, \( q_t \) (mg/g) is the adsorption capacity at time \( t \) (min), \( k_1 \) (1/min-1) is the rate constant of pseudo-first-order model, \( k_2 \) (g/min.mg) is the rate constant of the pseudo-second-order model, \( K_D \) is the intraparticle diffusion rate constant (mg/g.min^{0.5}), \( K \) is the apparent adsorption rate constant (L/g.min), \( C_0 \) is the initial concentration of Nd ions, \( \alpha \) is the initial rate (mg/g.min), and \( \beta \) is a chemisorption constant (g/mg).

The mentioned kinetic models have been applied for evaluation of kinetic study of the process and the plots of fitted models with experimental data are presented in Figure S1-5.

**Figure S1.** The plot of Pseudo first-order kinetic model
Supporting information

Figure S2. The plot of Pseudo-second order kinetic model

Figure S3. The plot of Intra particle Diffusion kinetic model

Figure S4. The plot of Elovich kinetic model

Figure S5. The plot of modified Freundlich kinetic model


**Isotherm of Adsorption**

The experimental data were plotted with Langmuir, Freundlich, and Tempkin isotherm models.\(^2\)

**Langmuir model:**

\[
\frac{C_e}{q_e} = \frac{1}{q_m C_e} - \frac{1}{K_L q_m}
\]  \hspace{1cm} (6)

**Freundlich model:**

\[
\ln q_e = \ln K_F + \left(\frac{1}{n}\right) \ln C_e
\]  \hspace{1cm} (7)

**Tempkin model:**

\[
q = \frac{R T}{b T} \ln K_T C_e
\]  \hspace{1cm} (8)

Where \(q_e\) is the equilibrium adsorption capacity of the MOF, \(C_e\) is the concentration of Nd solution at equilibrium, \(q_m\) is the maximum sorption capacity of the MOF, \(K_L\) is the Langmuir constant (L/mg), \(K_F\) (L/g) is the Freundlich constant, \(1/n\) is the heterogeneity factor, \(R\) is the ideal gas constant (8.314 J/mol·K), \(T\) is the absolute temperature (K), and \(b_T\) (J/mol) is heat of adsorption (J/mol).

Figure S6-8 depict the linear plots of three isotherm models with experimental data.

![Langmuir isotherm](image)

**Figure S6.** Linear plot of Langmuir isotherm
Supporting information

Figure S7. Linear plot of Freundlich isotherm

Figure S8. Linear plot of Temkin isotherm

Thermodynamic of Adsorption

For calculating the thermodynamic parameters, the following equations have been considered.\textsuperscript{3}
where \( C_0 \) (mg/l) is the initial concentration of Nd ions, \( C_e \) (mg/l) is the equilibrium concentration of Nd ions, \( \Delta H^\circ \) is the average change in standard enthalpy, \( \Delta S^\circ \) is the average change in standard entropy, \( \Delta G^\circ \) is the average of change in standard free energy of sorption, \( R \) is the universal gas constant and \( K \) is the equilibrium constant.

The linear plot of Vant Hoff equation based on the experimental data is shown in Figure S9.

**Figure S9.** Linear plot of Vant-Hoff equation

**REFERENCES:**

1. Onal, Y. Kinetics of adsorption of dyes from aqueous solution using activated carbon
Supporting information

