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SUPPLEMENTARY MATERIAL TO

Application of magnetite nanoparticle-modified walnut shell as an adsorbent for the removal of the organic dye Coomassie Brilliant Blue R-250

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The percentage removal and the amount of unabsorbed dye on the nanoparticles were calculated using Equations S-1 and S-2.

$$\text{Removal\%} = \frac{C_i - C_f}{C_i} \times 100 \quad \text{(S-1)}$$

$$q_e = \frac{(C_i - C_f) \times V}{W} \quad \text{(S-2)}$$

In the above equations, C_i / mg L^{-1} represents the initial concentration, and C_e / mg L^{-1} represents the unadsorbed or equilibrium concentration. Additionally, q_e / mg g^{-1} represents the adsorption capacity at equilibrium, V / L represents the volume of the solution, and w / g represents the amount of adsorbent.

The equilibrium adsorption isotherms are valuable for determining the distribution of absorbate molecules between the liquid and solid phases at equilibrium during the adsorption process.

$$\frac{C_e}{q_e} = \frac{1}{q_m b} + \frac{C_e}{q_m} \quad \text{(S-3)}$$

$$ln\, q_e = ln\, k_F + \frac{1}{n} ln\, C_e \quad \text{(S-4)}$$

$$q_e = B_T\, ln\, A_T + B_T\, ln\, C_e \quad \text{(S-5)}$$

$$ln\, q_e = ln\, q_m - \beta \varepsilon^2 \quad \text{(S-6)}$$

In the above equations, C_e / mg L^{-1} represents the equilibrium concentration of the solution, q_e / mg g^{-1} denotes the adsorption capacity at equilibrium, q_m / mg g^{-1} represents the maximum adsorption capacity, b / L mg^{-1} stands for the Langmuir constant, k_F / (mg g^{-1}) (L mg^{-1}) $^{(1/n)}$ represents the Freundlich constant where $1/n$ is the heterogeneity factor indicating the nature of the desired adsorption process. B_T / L mol^{-1} and A_T / L g^{-1} are the Temkin constants. β / mol^2 kJ^{-2} represents the useful activity coefficient and ε / kJ mol^{-1} is the Polanyi potential.

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The linear plots (Fig. S-1) for the Langmuir (equation S-3), Freundlich (equation S-4), Temkin (equation S-5), and Dubinin-Radushkevich (equation S-6) equations are obtained by plotting C_e/q_e against C_e, $\ln q_e$ against $\ln C_e$, q_e against $\ln C_e$, and $\ln q_e$ against ε^2, respectively.

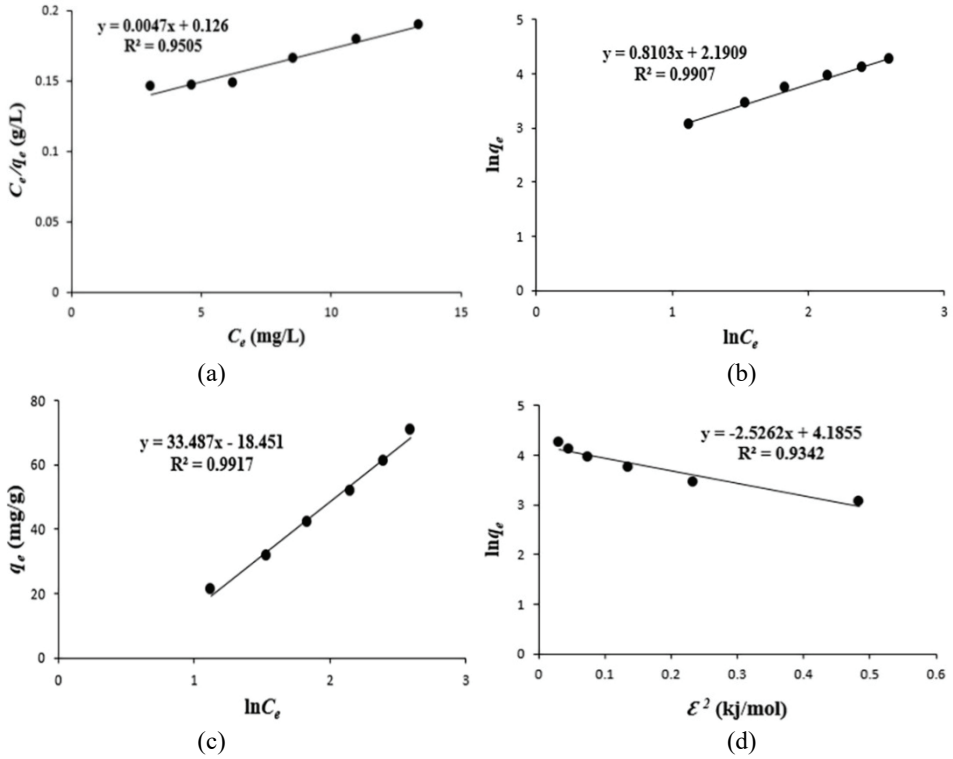


Fig. S-1. Graphs related to equilibrium adsorption isotherms: a) Langmuir, b) Freundlich, c) Temkin, and d) Dubinin-Radushkevich for the adsorption of CBB.

Two kinetic models were employed to determine the better fit: the pseudo-first-order Lagergren model (equation S-8) and the pseudo-second-order Ho model (equation S-9):

$$\frac{dq}{dt} = k_1(q_e - q_t) \tag{S-7}$$

In equation S-7, q_e / mg g^{-1} and q_t / mg g^{-1} represent the adsorption capacities at equilibrium and time t, respectively. k_1 / min^{-1} is the rate constant for surface adsorption in thepseudo-first-order kinetic model. By taking the natural logarithm of both sides of equation 7, another form of the pseudo-first-order kinetic equation is obtained, known as the Lagergren equation:

$$ln(q_e - q_t) = ln\, q_{e1} - k_1 t \tag{S-8}$$

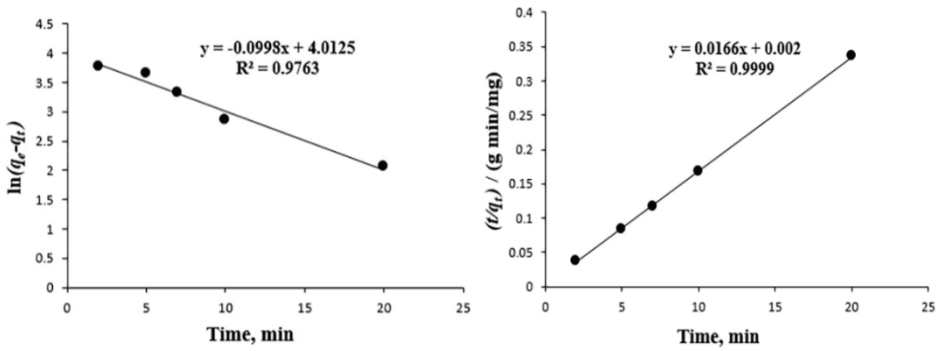
In that equation, q_{e1} represents the adsorption capacity obtained based on the pseudo-first-order kinetic model. By plotting a linear graph of $ln(q_e - q_t)$ against t and analyzing the slope and intercept, the values of k_1 and q_{e1} can be determined. The pseudo-second-order kinetic equation, based on the adsorption capacity, is presented as follows:

$$\frac{dq}{dt} = k_2(q_e - q_t)^2 \quad \text{(S-9)}$$

In this equation, k_2 / g (mg min) $^{-1}$ represents the rate constant for the pseudo-second-order kinetic equation. By integrating and rearranging this equation, an another form of the equation can be obtained, as follows:

$$\frac{t}{q_t} = \frac{1}{k_2 {q_{e2}}^2} + \frac{t}{q_{e2}} \quad \text{(S-10)}$$

In the above equation, q_{e2} / mg g $^{-1}$ represents the adsorption capacity obtained based on the pseudo-second-order kinetic model.



(a) (b)

Fig. S-2. Kinetic graphs of: a) pseudo-first order and b) pseudo-second order for the adsorption of CBB.

In this study, thermodynamic parameters of adsorption such as the changes in Gibbs energy ($\Delta G°$), enthalpy ($\Delta H°$), and entropy ($\Delta S°$) related to the equilibrium constants of adsorption were obtained using equations (S-11) to (S-14). For significant adsorption, the change in Gibbs energy should be negative. The change in Gibbs free energy of adsorption is defined as follows:

$$\Delta G^o = -RT \ ln K_c \quad \text{(S-11)}$$

In that equation, T / K is the temperature, R / 8.314 J mol $^{-1}$K^{-1} is the universal gas constant, and K_c / mg L^{-1} is the equilibrium constant of adsorption. The relationship is expressed as follows:

$$K_c = \frac{q_e}{C_e} \quad \text{(S-12)}$$

In this equation, q_e / mg L^{-1} represents the equilibrium concentration of the adsorbate species on the adsorbent, and C_e / mg L^{-1} represents the equilibrium concentration of the adsorbate species in the solution. Other thermodynamic

variables, such as the change in Gibbs energy, the change in enthalpy, and the standard entropy change of adsorption, can be obtained using the following equation:

$$\Delta G^o = \Delta H^o - T\Delta S^o \quad \text{(S-13)}$$

The thermodynamic parameters such as the changes in enthalpy ($\Delta H°$) and entropy ($\Delta S°$) can also be obtained from the Van't Hoff equation:

$$ln\, K_c = \frac{\Delta S^o}{R} - \frac{\Delta H^o}{RT} \quad \text{(S-14)}$$

Table S-I. Impact of Temperature on the Removal Efficiency of CBB

T / K	q_{exp} / mg g^{-1}	Removal, %
273	10.10	96.16
283	9.19	94.70
298	7.87	92.60
308	6.87	91.00

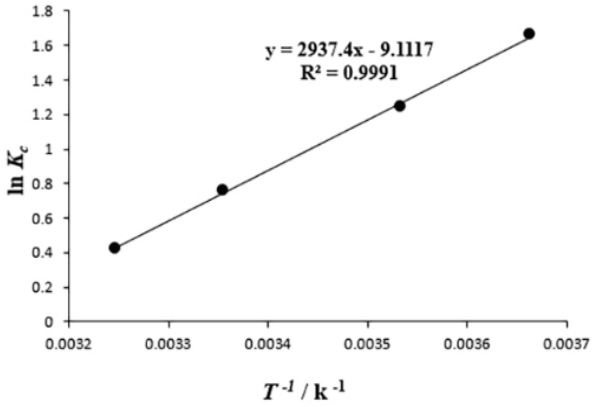


Fig S-3. Thermodynamic graph versus temperature in Kelvin for CBB.