Electronic Supplementary Information (ESI)

Cellulose Citrate: a Convenient and Reusable Bio-adsorbent for Effective Removal of Methylene Blue Dye from Artificially Contaminated Water

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Adsorption kinetics

Fig. S1 Pseudo first order and Elovich model plots
Adsorption isotherms

Fig. S2 Freundlich and Temkin isotherms plots
Equations

Different equations used in the study:

Pseudo − first order equation: $ln(q_e - q_t) = ln q_e - k_1 t$  \hspace{1cm} (1)

Pseudo − second order equation: $t/q_t = 1/k_2 q_e^2 + (1/q_e)t$  \hspace{1cm} (2)

Elovich equation: $q_t = \frac{1}{\beta} \ln (a\beta) + \frac{1}{\beta} \ln t$  \hspace{1cm} (3)

Where, $q_e$ and $q_t$ are the amounts of dye adsorbed on cellulose-citrate (mg/g) at equilibrium and at time $t$. $k_1$ (min$^{-1}$) and $k_2$ (g/mg/min) are the pseudo-first order rate constant and the pseudo-second-order rate constant. $\alpha$ (mg g$^{-1}$ min$^{-1}$) is the initial adsorption rate and $\beta$ (g mg$^{-1}$) is the relationship between the degree of surface coverage and the activation energy involved in the chemisorption.

van’t Hoff equation: $ln K_c = \frac{\Delta S^o}{R} - \frac{\Delta H^o}{RT}$  \hspace{1cm} (4)

where, $\Delta S^o$, $\Delta H^o$ and $R$ represent entropy change, enthalpy change and the universal gas constant (8.314 J/mol K) respectively. $T$ (K) is the absolute temperature and $K_c$ (L/g) is the standard thermodynamic equilibrium constant, which is expressed by

$$K_c = \frac{q_e}{C_e} \hspace{1cm} (5)$$

where, $q_e$ is the amount of adsorbed MB dye per unit mass of adsorbent at equilibrium (mg/g) and $C_e$ is the equilibrium aqueous concentration of MB.

Further, the value of the Gibbs free energy change $\Delta G^o$ (J/mol) is calculated as:

$$\Delta G^o = -RT \ln K_c \hspace{1cm} (6)$$

The negative value of $\Delta G^o$ indicates the spontaneity of a chemical reaction.

Langmuir isotherm: $$\frac{C_e}{q_e} = \frac{1}{k_L q_m} + \frac{1}{q_m C_e} \hspace{1cm} (7)$$

Freundlich isotherm: $$ln q_e = ln k_F + \frac{1}{n} ln C_e \hspace{1cm} (8)$$

Tempkin isotherm: $q_e = \beta ln k_T + \beta ln C_e$ [where, $\beta = RT/b$] \hspace{1cm} (9)

where the Langmuir constants $q_m$ and $k_L$ represent the maximum adsorption capacity of the adsorbent and the constant energy related to the heat of adsorption, while $C_e$ (mg/L) is the concentration of adsorbate in the liquid phase at equilibrium and $q_e$ (mg/g) is the amount of adsorbate adsorbed on the solid phase at equilibrium. $k_T$ (mg/g) (L/mg)$^{1/n}$ indicates the adsorption capacity, and $n$ reflects the intensity of adsorption according to the Freundlich theory. The constant $\beta$(L/mg) is related to the heat of adsorption, $k_T$(mg/L) is a constant of the Tempkin isotherm, b
(J/mol) is the energy constant of the Tempkin isotherm, R (8.314 J/K mol) is the gas constant and T (K) is the absolute temperature.

One of the essential characteristics of the Langmuir isotherm can be expressed by a dimensionless constant, separation factor, $R_L$, defined as follows:

$$R_L = \frac{1}{1 + k'_L C_0}$$

(12)

The value of $R_L$ indicates the type of the isotherm; which is unfavourable ($R_L > 1$), linear ($R_L = 1$), favourable ($0 < R_L < 1$) or irreversible ($R_L = 0$). ¹

In Table S1 $R_L$ values for each used concentration are reported:

| $C_0$ | $R_L$ |
|-------|-------|
| 10    | 0.31  |
| 20    | 0.18  |
| 30    | 0.13  |
| 40    | 0.10  |
| 50    | 0.08  |
| 70    | 0.06  |
| 100   | 0.04  |
| 120   | 0.04  |
| 150   | 0.03  |

References

¹ Kumari, S., Chauhan, G. S., Ahn, J.-H. Chem. Eng. 2016, 304, 728.