



Methylene Blue Dye Adsorption from Wastewater Using Hydroxyapatite/Gold Nanoparticles Composites: Kinetic and Thermodynamics Studies

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Supplementary information

Adsorption Kinetics

Lagergren pseudo-first-order equation shows that the rate of change of solute uptake with time is directly associated to the variation in the quantity of solute uptake at equilibrium and the volume of solute uptake with time is given by Eq (1):

$$\frac{dq_t}{dt} = k_1 (q_e - q_t), \quad (1)$$

On integrating equation (1) within the limits $q_t=0$ at $t=0$ to $q_t=q_e$ at $t=t$ and converting it into linear form, the equation become

$$\log (q_e - q_t) = \log q_e - \frac{k_1}{2.303} t, \quad (2)$$

where q_e and q_t are the adsorption capacity at equilibrium and at time t (min), respectively. k_1 is the rate constant of pseudo-first-order adsorption (min^{-1}). The values of k_1 and q_e can be estimated from the graph of $\log (q_e - q_t)$ vs t .

Pseudo-second-order equation is written as:

$$\frac{dq_t}{dt} = k_2 (q_e - q_t)^2, \quad (3)$$

On integrating the above equation within the limits and changing into linear form, we got an equation (4):

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t, \quad (4)$$

Where k_2 is pseudo-second-order rate constant ($\text{g mg}^{-1} \text{min}^{-1}$). The values of k_1 , k_2 , q_e and regression coefficients are listed in Table 1 for different concentrations ranging from 10-60 ppm.

Adsorption Isotherm

The linear form of Langmuir and Freundlich is represented in Eqs. (5) and (6), respectively.

$$\frac{C_e}{q_e} = \frac{1}{Q_m b} + \frac{1}{Q_m} C_e, \quad (5)$$

$$\ln q_e = \ln K + (1/n) \ln C_e, \quad (6)$$

Where, Q_m (mg/g) and b (L/mg) are Langmuir constants representing monolayer adsorption capacity and heat of adsorption respectively. K (mg/g) and n are Freundlich constants denoting adsorption capacity and adsorption intensity respectively. q_e is the adsorption capacity (mg/g) of dye and C_e is the equilibrium concentration (mg/L) of dye solution.

Antibacterial studies

The antibacterial activities of the AuNPs solution, HA/Au nanocomposite and dye adsorbed waste HA/Au nanocomposite samples were studied by agar well diffusion assay according the standard rules and recently reported procedure (Sharma et al. 2020). The overnight bacterial culture was diluted (1:100) to get 10^5 CFU/ml for each bacteria to be studied (*Pseudomonas aeruginosa*, *Staphylococcus aureus* and *Micrococcus luteus*) and was dispersed employing sterile swab comprising a bacterial suspension on Muller Hinton Agar plates. Thereafter, wells having sizes of 6 mm diameter were punched into the agar plates involving a bacterial suspension and loaded with 50 mg/ml of AuNPs and synthesized nanocomposite samples and held at room temperature for 2 hours for dispersion. The plates were then incubated at 37 °C for 24 hours. The diameters around the inhibition zones were measured in mm after the incubation of 24 h against all the bacterial strains.