Green synthesis, characterization, and application of Fe3O4 nanoparticles for methylene blue removal: RSM optimization, kinetic, isothermal studies, and molecular simulation

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Abstract

Methylene Blue (MB) is a cationic dye causing various health problems such as asthma, heartbeat, eye and skin irritation, nausea, and distress during prolonged exposure. In this regard, the green magnetite nanoparticle was synthesized using the extract of Prosopis farcta. The synthesized Fe_3O_4nanoparticle was characterized by X-ray powder diffraction (XRD), Field emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM), Fourier transforms Infrared spectroscopy (FTIR), vibrating sample magnetometer (VSM), and Brunauer-Emmett-Teller (BET). The corresponding parameters, including the primary concentration of MB (5–65 mg/L), the dose of synthesized nanoparticle (0.025–0.925 g/L), solution pH (3–11), and contact time (20–60 min), were considered. Also, central composite design (CCD), as one of the response surface methodologies (RSM), was used for the related modelling and optimization. The particle size of the adsorbent was between 5 and 70 nm, and the nanoparticle has 206.75 m^2/g of a specific surface, 6.1 nm of average pore size, and 0.3188 cm^3/g of the total pore volume. The optimal conditions for MB removal by the nanoparticle were found to follow an initial MB concentration of 20 mg/L, 0.7 g/L of the nanoparticle dose, pH = 9, and a contact time of 50 min. The pseudo-second-order (PSO) and Freundlich models were the best kinetic and isothermal models for MB removal by the synthesized nanoparticle. Molecular modelling was used to optimize the MB molecular configuration and compute HOMO-LUMO energies, quantum-chemical descriptors, and molecular electrostatic potential to evaluate the nature reactivity of the MB molecule.

Keywords: *Adsorption, Green synthesis, Iron oxide, Methylene blue, Nanoparticle, Prosopis farcta*