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Title: Mechanistic insight into CBB-G removal by NiO@chitosan beads using molecular docking, fixed-bed analysis, and life cycle assessment

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Abstract: Introduction – In this study, the present work describes a work that analyzed the synthesis/performance of NiO@chitosan composite beads for the removal of Coomassie Brilliant Blue G (CBB-G) from aqueous systems successfully under both batch and fixed-bed conditions. Methods – NiO nanoparticles were prepared by co-precipitation and homogenized in a chitosan matrix to generate stable, spherical beads with improved adsorption performance. XRD, FTIR, FE-SEM/EDS, BET, zeta potential, and pH_{pzc} characterization suggested NiO incorporation and adsorption sites existed. The batch analyses have shown that the adsorption efficiency was strongly dependent on stirring speed, dosage of the adsorbent, dye concentration, pH and temperature of the sample to attain an optimum condition at 150 r/min (revolutions per minute), 54 g/L, 30 mg/L, pH 7 °C and 30 °C. For linear kinetic analysis, a pseudo second order model ($R^2 = 0.9993$) was used, while the equilibrium data supported Langmuir isotherm ($R^2 \approx 0.99$), confirming the dependence of monolayer adsorption on physical interactions. Results and Discussion – In fixed-bed adsorptive investigations, breakthrough profiles were majorly dependent on bed height, inlet concentration, and feed flow velocity. The Thomas and Yoon–Nelson models with high $R^2 \approx 0.99$ corroborated significantly with experimental outcome where predictive accuracy was validated with Clark model. Thermodynamic results ($\Delta H^\circ = 39.58$ kJ/mol) suggested spontaneous, endothermic, and physisorption-powered adsorption. Molecular docking verified electrostatic, hydrogen bonding, and van der Waals interactions between dye and bead surface. The beads had good reusability with only minimal effect upon losses in efficiency. Life cycle analysis indicated bead synthesis exerts largest environmental burden (105 kg CO₂-eq/kg), with 6.94 kg required per m³ treatment, leading to 852 kg CO₂-eq/m³. Overall, the developed NiO@chitosan beads exhibited excellent adsorption performance and reusability; however, further optimization of the synthesis process is necessary before they can be considered a fully sustainable adsorbent for large-scale wastewater treatment.

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