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Effect of magnetic nanoparticle on the morphology and interaction mechanisms between herbicide and nanocomposite hydrogels

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The excessive application of water-soluble pesticides to enhance field productivity can have severe impacts on human health and the environment. Due to their versatility and ability to absorb molecules within their structure, magnetic hydrogels are extensively studied by researchers as a rapid and safe option for decontaminating aquatic environments. This work aims to investigate the influence of magnetic nanoparticles of magnetite (Fe3O4) and magnetite functionalized with aminopropyltriethoxysilane (APTES) (Fe3O4@NH2) on the morphology and interaction mechanisms between herbicide molecules and the chains of novel magnetic hydrogels composed of carboxymethylcellulose and zeolite supported on networks of poly(methacrylic acid)-co-polyacrylamide (PMAA-co-PAAm). Scanning electron microscopy (SEM) analyses and adsorption isotherm studies were employed respectively. Using ImageJ software, the diameters of nanoparticles and hydrogel pores were measured for pure hydrogel and magnetic hydrogels containing 2.0% w/v of Fe3O4 or 2.0% w/v of Fe3O4@NH2. The magnetic nanoparticles exhibited varied diameters, with a minimum of 68 nm and a maximum of 302 nm. The pore diameters of the pure hydrogel and magnetic hydrogels also showed heterogeneous dimensions, ranging from 0.20 to 5.50 µm. Regarding morphological properties, it was observed that the presence of magnetic nanoparticles did not induce changes in the structure and shape of the pores. For the adsorption isotherm studies of the herbicide paraquat, six different mathematical isotherm models were employed to determine which model best described each system's behavior. The results indicated that the pure hydrogel and the hydrogel with 2.0% w/v of Fe3O4 followed models describing heterogeneous interactions (Harkins-Jura and Temkin, respectively), involving interactions with active sites of varying energy levels and multilayer adsorption with interactions between adsorbate molecules. Conversely, the hydrogel with 2.0% w/v of Fe3O4@NH2 fitted the Langmuir model, which describes a behavior where the interaction energy between the adsorbate and interaction sites leads to monolayer adsorption. In conclusion, despite the nanoparticles not significantly affecting the morphology, the incorporation of magnetite nanoparticles did impact the mechanisms involving the material's interaction with pollutant molecules. Therefore, the data obtained in this study can assist researchers in choosing the most suitable material for applications in water body decontamination systems.