## Removal of perfluorooctanoic acid using graphene oxide nanocomposites: Optimization, isotherm, and kinetics

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Perfluorooctanoic acid (PFOA) is an enduring and recalcitrant emerging contaminant from per- and polyfluoroalkyl substances (PFAS) family that poses significant environmental concerns. Its widespread presence and significant bioaccumulation have garnered increasing global attention, highlighting the urgent need for its effective removal. Adsorption is considered as an effective method for removing PFOA, and there is still an ongoing urge to develop more efficient adsorbents for this purpose. Thus, to address PFOA contamination in the global aquatic system, this study prepared a simple and promising ultrasonically-accelerated cetyltrimethylammonium bromide-functionalized graphene oxide nanocomposites and used for the PFOA removal. The surface functionality of the nanocomposites is adjusted by changing the amounts of CTAB to achieve satisfactory performance in adsorbing PFOA. The physicochemical attributes of the adsorbents were characterized by XRD, FTIR, BET, FESEM, and XPS. Results revealed the successful grafting and intercalation of CTAB molecules onto GO sheets, facilitated by ionic interactions between the positively charged  $-N^+R_3$  moieties and the oxygenated functional groups on GO sheets, contributing to the effective removal of PFOA. In the batch experiments, central composite design (CCD) of response surface methodology (RSM) was utilized to evaluate the interaction effects and impact of process parameters. The optimized conditions: adsorbent dose: 200 mg/L, pH: 3.5, and time: 50 min, revealed a PFOA removal of ~98.5%. Non-linear regression analysis revealed that the adsorption process was most accurately represented by pseudo-second-order kinetics and Freundlich isotherm, with a maximum experimental uptake capacity of ~710 mg/g. The adsorption of PFOA exhibited a rapid increase in the initial 20 min, followed by a slower adsorption process, eventually reaching equilibrium. The electrostatic, hydrophobic, and hydrogen bonding interactions are the responsible mechanisms for PFOA adsorption, as confirmed by spectroscopic and zeta potential analyses. Overall, this study offers fundamental insights into PFOA adsorption behavior and proposes that modifying GO with CTAB could enhance the adsorption potential for practical implications.