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Prediction of Ion Adsorption by Minerals Using Machine Learning Model

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The migration, distribution, and final fate of ions in the aqueous environment are largely controlled by the adsorption of iron minerals (e.g., goethite). Previous studies have carried out laboratory adsorption experiments on the adsorption of anions and cations by goethite under different reaction conditions, and a large amount of adsorption data has been obtained. The SCM (Surface Complexation Model), based on thermodynamic equilibrium theory, is an effective tool to investigate the partition of ions at the mineral-water interface. Unfortunately, the weak robustness of the model parameters may limit the predictive ability of the SCM for unseen adsorption data. Therefore, we propose another machine learning-based modeling approach that successfully achieves high accuracy predictions for six cations (Cd^{2+}, Co^{2+}, Cu^{2+}, Ni^{2+}, Pb^{2+}, Zn^{2+}) and five anions (SeO_4^{2-}, SO_4^{2-}, CrO_4^{2-}, AsO_4^{3-}, PO_4^{3-}). The first hydrolysis constants of the ions can be used as distinctive descriptors to distinguish the adsorption behavior of various ions, according to the results of pH_{50}-based feature engineering. After comparing 288 model scores and residual analyses for various input-output combinations, equilibrium concentration and fractional removal were determined to be the optimum input unit and output predicted target, respectively. Our research findings demonstrated the successful modelling of the absorption of metal ions on minerals using machine learning techniques, providing an alternative approach for predicting the migration and fate of elements in aquatic systems with wide application range and fast calculation speed.