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A Component Additivity Approach for Surface Complexation Modeling of PFOS and PFOA Adsorption in Quartz-Dominated Glacial Aquifers

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Per- and polyfluoroalkyl substances (PFAS) are persistent, mobile contaminants widely detected in soils and groundwater systems worldwide, raising significant concern due to their environmental longevity and potential human health impacts (Sunderland et al., 2018). PFAS sorption in fate and transport models is commonly represented using empirical distribution coefficients (Kd), which limits their predictive capability under variable geochemical conditions. This study presents a Component Additivity approach in Surface Complexation Modeling (CA-SCM) using the Charge Distribution–Multi-Site Complexation (CD-MUSIC) frameworkto predict the partitioning of perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA) on quartz-dominated glacial sediments. Surface reactions are represented using mineral-specific, site-binding schemes, including 1-pKa formulations for Fe-(oxyhydr)oxide surfaces and quartz. Building on additive SCM approaches developed for ligand adsorption in subsurface systems, we hypothesize that PFOS and PFOA retention reflects the combined contributions of quartz, iron oxides, and clay fractions, modulated by pH and ionic composition.

Sediment characterization (X-ray diffraction, BET surface area analysis, and selective extractions) is integrated with controlled batch sorption experiments across environmentally relevant pH and ionic strength ranges. The dataset informs a PHREEQC-based surface complexation model that integrates individual mineral phases within the CA-SCM framework. By moving beyond empirical Kd approaches toward a mechanistic, mineral-specific representation, this work advances predictive reactive transport modeling of PFAS in sandy aquifer systems.

The framework is applied to sediments from a tanker truck rollover site in Cape Cod, Massachusetts, where the emergency application of aqueous film-forming foam (AFFF) introduced PFAS, including PFOS and PFOA, into a quartz-dominated glacial aquifer system. While previous studies have simulated advective transport processes in this site (LeBlanc et al., 1991), mineral-specific reactive mechanisms controlling PFAS retention remain unresolved. By implementing a CD-MUSIC–based CA-SCM framework, the resulting methodology provides a transferable approach for evaluating PFAS retention in quartz-rich environments impacted by AFFF releases.

References

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