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Experimental and Surface Complexation Modeling of Fluoride Release from Natural Soils: Mechanistic Role of Dissolved Iron.

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Fluoride (F^-) contamination poses environmental and health risks through soil-derived mobilization to groundwater. In soils, Fe-F interactions control F^- adsorption-desorption, yet Fe dissolution and complexation under specific geochemical conditions can enhance F^- release despite metal oxide retention. The mechanistic representation of these coupled iron-fluoride processes remains poorly constrained in current geochemical models of F^- desorption from natural soils. In this study, batch desorption experiments were combined with surface complexation modeling to investigate F^- release from natural soils under environmentally relevant conditions representative of semi-arid alluvial settings. Soils collected from areas affected by high-fluoride groundwater were subjected to controlled desorption experiments across a wide pH range (3.0 -pH 11.0) to evaluate the influence of dissolved iron and Fe-F surface complexes on F^- mobilization. The results of the batch experiments demonstrate that F^- release is greater in subsurface soil layers than in surface layers. Additionally, soil pH, organic matter content and specific surface area have been identified as significant factors governing the depth-dependent variation of F^- in soils. The release kinetics of F^- followed a pseudo-first-order-model. Furthermore, the SCM, utilizing a general composite approach, successfully simulated the experimental results for various soils with a root mean square error (RMSE) of 7.53%. The findings showed that F^- mobility in Fe-rich soils is strongly controlled by iron-mediated adsorption processes. At the experimental Fe concentration, fluoride is largely retained under acidic to near-neutral conditions (pH ~3-7) through the formation of Fe-F surface complexes (>SOFeF$^+$, >SOHF, and >SF), reducing its release into solution. At very low pH (<3), fluoride occurs primarily as HF, while aqueous Fe-F complexes are negligible (<1%), and surface adsorption dominates retention. Under alkaline conditions (pH >8), deprotonation of Fe-OH sites weakens Fe-F complexes, increasing aqueous fluoride. Overall, iron in the soil suppresses fluoride release at low to moderate pH by stabilizing it on soil surfaces, while fluoride desorption becomes significant only under strongly alkaline conditions. The combined results underscore the importance of Fe oxide rich soil horizons in regulating fluoride mobility, providing insights that can guide targeted remediation and control approaches in F^- affected agricultural and groundwater systems.