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# A Mechanistic Approach for Integrating Molecular Information into Surface Complexation Modelling (SCM) of PFAS-Ferrihydrite interactions

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Per- and polyfluoroalkyl substances (PFAS) are a unique class of synthetic organo-chemicals. Due to their high thermal stability and chemical resistance, they have been used in many fields including fire extinguishing foams, waterproof clothing, nonstick cookware, and other consumer products [1]. PFAS are considered a significant threat to public health and environment due to their properties of bioaccumulation, high toxicity, and long-term persistence in the environment [2]. Both short- and long-chain PFAS (e.g., PFPeA, PFOA, PFOS) are highly mobile contaminants that are present in the sub-surface environment, and their fate and transport is primarily governed by interfacial interactions in the air-water, solid-water, and Non-Aqueous Phase Liquid (NAPL)-water interfaces. Despite the environmental significance of these compounds, limited research has been conducted to unravel PFAS molecular-level interactions in reactive transport applications. Ferrihydrite (FH) is an amorphous iron oxyhydroxide that is highly reactive due to its surface area and site density [3]. In this study, in-situ Attenuated Total Reflection Fourier-Transform Infrared (ATR-FTIR) spectroscopy and adsorption batch experiments are conducted to investigate PFAS interactions with ferrihydrite, under various environmental conditions. Using experimental data, a Surface Complexation Model (SCM) is developed to predict PFAS partitioning. The ATR-FTIR data identified the formation of a hydrogen bonded outer-sphere complex together with a Na co-adsorption outer-sphere complex. SCM incorporated spectroscopic evidence and predicted PFAS adsorption under a wide range of pH and ionic strength values. The findings of the study, which integrate molecular-level understanding with batch adsorption data, are pivotal for bridging the gap between fundamental surface chemistry and application for a robust predictive reactive transport model.

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