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Neural Operator Surrogate for Modeling Selenate Diffusion in Bentonite

MR. DAUREN SARSENBAYEV AND HARUKO MURAKAMI WAINWRIGHT

Massachusetts Institute of Technology

Reactive transport modeling is an integral part of performance assessment for high-level nuclear waste (HLW) disposal. Bentonite is widely considered a suitable buffer material in the engineered barrier systems for HLW, due to its high-sorbing, low-permeability properties. Sorption is the key mechanism of radionuclide retardation in bentonite. Se-79 is considered a high-priority dose contributor in PA due to its long half-life (3.27×10^5 years) and high mobility when present as soluble species in the form of selenate (SeO_4^{2-}) or selenite (SeO_3^{2-}). Selenium is also a vital micronutrient necessary for normal physiological functions. If Se-79 is introduced into the environment, it can readily become part of the natural selenium biogeochemical cycle. While extensive data exist for selenite sorption on montmorillonite, sorption of selenate on montmorillonite is less characterized. To address this knowledge gap, we use the L-SCIE international database, which compiles more than 17,000 sorption measurements across multiple minerals, to extract 18 experimental data points for selenate and assemble a distribution of K_d values. These K_d values are then propagated through CrunchODiTi, an electrostatic-effect-aware reactive transport code, after sampling via quasi-Monte Carlo (Sobol sequences) together with experimentally constrained ranges of bentonite structural parameters (porosity and tortuosity). We first generate an ensemble of breakthrough curves, which we then compare against experimentally reported diffusion behavior of selenate in bentonite [1]. From this comparison, we compute Gaussian likelihoods yielding posterior weights over the ensemble. Guided by these weights, we use the gpCAM software, which adaptively proposes new K_d samples in regions of the parameter space with the highest expected information gain. Because each reactive transport simulation is computationally expensive, we train a Fourier Neural Operator surrogate on the ensemble. The surrogate model accurately reproduces breakthrough curves with <1% root-mean-square error on unseen cases and achieves a 10^3-10^4 × speed-up relative to the full reactive transport model.

[1] Fox, Tournassat, Steefel & Nico (2024), Applied Geochemistry, 106090.