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Beyond Kd: Next Generation Performance Assessment Framework through Machine Learning

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Performance assessment (PA) methodologies for nuclear waste disposal has been developed and improved over the past several decades to compute the radiological risk to public health. Geochemical modeling is the core part of PA, describing the mobility of radionuclides influenced mainly sorption reactions. Most of the current PAs are based on the simplified representation sorption reactions through the Kd approach. Over the last 75 years, however, there have been several instances that the predictions in PAs failed at near-surface contaminated sites due to this simplified representation. A reactive transport model has been developed and validated for describing radionuclide transport, including surface complexation and cation exchange reactions. In parallel, significant efforts have been made to develop mechanistic models for describing complex and coupled processes— thermal (T), hydrological (H), mechanical (M) and chemical (C) processes — within or near engineered barrier systems (EBS) of the high-level nuclear waste repository. Still, there are computational challenges to include these complex THMC processes in large-scale PAs.

In this study, we develop a next generation PA framework to better represent these key geochemical reactions within large-scale radionuclide transport predictions. An important aspect is to account for uncertainties associated with natural systems as well as experimental data and geochemical models. The key developments using machine learning include (1) emulators for THMC models to compute time-varying Kd within bentonite buffers, which will be passed on to large-scale PA models [1, 2], and (2) an experiment-to-model pipeline based on the newly compiled global database L-SCIE [3], including Bayesian SCM/CE model calibration and model uncertainty quantification as well as data-driven representation of sorption reactions. The framework aims to improve the fidelity of PAs as well as to establish the realistic representation of repository performance for optimizing repository designs, site characterization and performance confirmation monitoring.

Reference

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