Honing In On Model Adsorption Parameters for Nuclear Fuel Cycle Contaminants

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Reactive transport models are ideal for predicting the fate of radionuclides and other metals and metalloids at contaminated sites associated with the nuclear fuel cycle. Reactive transport models are not always feasible, however, because ideally, they require thorough characterization of geochemical and hydrogeologic parameters at spatial scales (e.g., km) that can be cost prohibitive. Furthermore, stakeholders may prefer to build on an established groundwater flow model, if it exists, rather than develop a new model with more sophisticated reactive transport capabilities.

In this case study, several different approaches were utilized to develop attenuation parameters for constituents of concern in a flow and transport model (FTM) with some capacity for modeling attenuation. The FTM inputs comprise a linear equilibrium partition coefficient (Kd) or a non-linear equilibrium Freundlich coefficient (Kf) and exponent. Together, these inputs are referred to as adsorption parameters. Uncertainty in estimation of adsorption parameters was evaluated using four different methods: (1) an in situ method (in situ-SE) where solid and aqueous concentrations of a constituent were derived from sequential extraction and groundwater sampling, respectively; (2) an in situ method (in situ-SPLP) where solid and aqueous concentrations of a constituent were derived from a modified synthetic precipitation leach procedure and groundwater sampling, respectively; (3) a surface complexation model (SCM) in PHREEQC using site-specific estimates for ferrihydrite concentrations; and (4) a method where adsorption parameters were fit to a calibrated FTM to obtain the best match to historical groundwater concentrations.

The best estimates of adsorption parameters were those with overlapping values among the in situ-SE, in situ-SPLP, and SCM methods. These best estimates were applied to the FTM and adjusted where necessary. The resulting FTM shows that for some constituents of concern, including uranium and molybdenum, monitored natural attenuation is not acceptable for the site. As a result, the current FTM forms the basis for ongoing modeling scenarios aimed to identify the best remediation strategies for the most mobile groundwater constituents of concern.