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# 1-D Reactive Transport Modeling of Ordinary Portland Cement (OPC) Leaching Experiments: Preliminary Results

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Cementitious materials are intrinsic to the engineered barrier system (EBS) of deep-geological nuclear waste repository design concepts. These materials are usually present as tunnel wall liners, shaft seals, and plugs. Given the relatively large amounts of cement material considered in these repository concepts, the interactions between cement pore fluids and other EBS components (e.g., bentonite) need to be evaluated as part of the long-term safety assessment. One aspect of this analysis is the model representation of cement leaching and its effect to the evolution of fluid chemistry, particularly at EBS material interfaces. Here we report preliminary results of a 1-D (diffusion-only) reactive transport model using the PFLOTRAN code for leaching of ordinary Portland cement (OPC) having a CEM I starting composition. Experimental data was obtained for an OPC sample (height = 2.3 cm) at 30°C and 63 days following the EPA method 1315 for leaching of monolithic and/or compacted granular materials. Model calibration was mainly accomplished by adjusting kinetic rate parameters (rate coefficients and surface areas) of the dissolution/precipitation reactions of the solid phase assemblage. Overall, the 1-D PFLOTRAN simulation results show good agreement with the temporal changes of concentration profiles for major solutes observed in the OPC leaching experiments. The formation of hydrous cementitious solids such as portlandite, CSH, and ettringite along with spatial changes in porosity and permeability are captured by the model. An initial larger increase followed by a subsequent decrease in porosity is predicted close to the cement-fluid interface, relative to locations farther from the interface. Ongoing and future work includes model sensitivity analyses of reaction kinetic and porosity/permeability parameters, 1-D reactive transport simulations of bentonite-cement interactions, and comparisons with experimental efforts.

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