Reactive Transport Benchmarks on Heavy Metal Cycling

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Modeling metal fate and transport associated with sediment, tailings, and waste rock is often needed for the management of abandoned mines and remediation of mining-impacted areas. Although a variety of reactive transport models have been used to investigate acid rock drainage (ARD) and heavy metal cycling, a systematic model inter-comparison has not been conducted to date. This study presents two benchmark problems dealing with 1) the generation and attenuation of ARD, and 2) sediment-metal interactions in mining-impacted lake sediments.

The first benchmark problem focuses on comparing reactive transport simulations of sulfide mineral oxidation and attenuation of ARD in partially water-saturated mine tailings. This benchmark considers variably saturated flow, multicomponent solute transport, diffusion of oxygen and carbon dioxide in the gas phase, sulfide mineral oxidation, the dissolution of gangue minerals, and precipitation and re-dissolution of secondary mineral phases. Four reactive transport codes - CrunchFlow, Flotran, HP1, and MIN3P were used to evaluate this benchmark. Despite substantial differences in model formulations, favorable agreement was obtained between the various codes.

The second benchmark problem focuses on heavy metal cycling in mining-impacted lake sediments. A multicomponent biotic reaction network with multiple terminal electron acceptors (TEAs) is considered to simulate the reductive dissolution of ferrihydrite and release of trace metals. The model incorporates Fickian diffusive transport, kinetic and equilibrium mineral precipitation/dissolution, and equilibrium aqueous and surface complexation. Four reactive transport codes - TOUGHREACT, CrunchFlow, PHREEQC, and PHT3D were used to evaulate this benchmark. Favorable agreement was obtained between these codes. Simulations of a more complex scenario including sedimentation and compaction with CrunchFlow and TOUGHREACT were also compared with this benchmark. Slight deviations in model results can be explained by different formulations for compaction.