Benchmarking the simulation of microbial Cr(VI) reduction and Cr isotope fractionation

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Reduction of soluble Cr(VI) to less toxic and sparingly soluble Cr(III) is the main focus of in-situ (bio)remediation efforts at Cr(VI) contaminated sites. Bioremediation often involves injection of organic carbon into the subsurface to stimulate the growth of indigenous bacteria that mediate the relevant redox processes. Further, a powerful proxy for demonstrating succesful Cr(VI) reduction is the fractionation of stable Cr isotopes. The use of reactive transport modeling is often required to obtain a predictive understanding of Cr(VI) reduction including the processes associated with biomass dynamics and those associated with Cr isotope fractionation. To ensure the accurate simulation of these processes we developed two benchmarks, each consisting of a series of component problems with increasing complexity.

The first benchmark focuses on the simulation of microbially mediated redox reactions with the explicit inclusion of the microbial community dynamics and the impacts on reaction rates. Rate expressions for microbially mediated redox reactions include kinetic limitations (Monod and inhibition terms) as well as thermodynamic limitations. Both catabolic (energy) and anabolic pathways (biomass growth) are considered in the microbially mediated reactions.

The second benchmark focuses on the simulation of Cr isotope fractionation in 1D and 2D domains. It is based on a recent field study where Cr(VI) reduction and accompanying Cr isotope fractionation occurs abiotically by an aqueous reaction with dissolved Fe^{2+}. The problem set includes simulation of the major processes affecting the Cr isotopic composition such as the dissolution of various Cr(VI) bearing minerals, fractionation during abiotic aqueous Cr(VI) reduction and precipitation of Cr(III) as sparingly soluble Cr-hydroxide.

Correctness of the numerical solutions for the two benchmark problem sets were ensured by running the problems each with 4 well-established reactive transport modeling codes: CRUNCHFLOW, TOUGHREACT, MIN3P, and PHT3D or FLOTRAN. In general, model to model comparisons showed excellent agreement.