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ABSTRACT TITLE: Field-scale simulations of engineered bioreduction: Super 8, proteomics, genome-scale metabolic modeling, and beyond

ABSTRACT: The 2010 Super 8 acetate biostimulation field experiment was the first at the Rifle IFRC site to test the response of metal-reducing bacteria to elevated levels of aqueous U(VI) and calcium. The introduction of high bicarbonate and sodium concentrations on the west side of the experimental plot resulted in observed aqueous uranium and calcium concentrations up to 4 times ambient concentrations. While we are interested in the effect of evolving geochemical conditions on the biologically-mediated metal reduction rates, it is particularly difficult to quantitatively discern the individual contributions of competing processes from the monitored concentrations alone. These species are directly involved in aqueous and surface complexation, microbially-mediated TEAP, and mineral reactions, which are sensitive to controls (e.g., pH, Eh, alkalinity, etc.) affected by other reactions. The simulation addresses these issues through systematically coupled process models that have been developed in the context of observed behaviors from multiple field experiments at this site. For this simulation, the flow model parameters were not calibrated; we simply used the previously defined sandy gravel lithofacies properties and drove the model with time-dependent observed water levels. With the exception of changing the dependence in the goethite bioreduction rate law from >FeOH to FeOOH, all reactions, thermodynamics, and rate laws were identical to the previously published simulation of the 2008 Big Rusty acetate biostimulation field experiment. The modeling explores a large range of sodium, bicarbonate, acetate, and uranium exposure due to the different injection locations and schedules, as well as the slight misalignment of the flow field and the well layout. The removal of U(VI) from solution is demonstrated to be a trade-off between the U(VI) bioreduction rate and enhanced adsorption to the recently vacated surface complexation sites.

The Super 8 experiment was also notable for the relatively large number of proteomic samples (5, 8, 10, 13, 15, 17, 29, 36, and 43 days) collected at the well least impacted by the bicarbonate injection, CD01. In this simulation, we replaced the Fe(III) TEAP reactions and rate laws with a genome-scale metabolic ("*in silico*") model for *Geobacter metallireducens* (748 intracellular and exchange reactions). The *in silico* model of physiological metabolic pathways was embedded in the eSTOMP field-scale modeling framework. A linear programming solver is used to calculate feasible limits of intracellular metabolic flux distribution under a constraint-based flux balance analysis. Over 900 proteins specific to *Geobacter spp.* were detected. The annotation of genome-specific proteins to individual metabolic pathway reactions enables the abundance of a specific detected protein to be used to assess a specific predicted reaction flux. The effect of evolving biological and geochemical conditions on the trade-off between biosynthesis and respiration pathways is examined.

Finally, we show a preliminary 3-D variably saturated flow and transport simulation of the entire Rifle site floodplain. This will provide the foundation for the upcoming exploration of the floodplain microbial community in the hydrologic context of the upland watershed and the Colorado River.