Development of Genome-Informed Reaction Network and Dynamic Models for Simulating Biogeochemical Processes of Carbon, Nitrogen, Chromium and Technetium in Subsurface Systems

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Biogeochemical reaction network and dynamic metabolic models are being formulated and tested for simulating microbial community functions and the biogeochemical transformation of carbon, nitrogen, chromium, and technetium in the subsurface interaction zone – SIZ (zone of groundwater-surface water mixing). Biotic and abiotic experiments, functional gene and enzyme assays, and multi-scale kinetic analysis are being performed to characterize kinetic biogeochemical reactions controlling the transformation of organic carbon, nitrate, and contaminants (Cr and Tc); and the production of gaseous species (CO_2 and N_2O) in SIZ sediments from two Hanford Reach locations. The transformation of nitrate and nitrite to gaseous N_2O and N_2 coupled with organic carbon oxidation to CO_2 was observed to correlate with dynamic changes in functional genes and enzymes regulating the denitrification processes. The resulting robust data set provides both a model simulation target and a well-defined reaction system for rigorously evaluating genome-informed metabolic models. This evaluation will proceed over the next year using two different model conceptualizations of microbial community functions responsible for denitrification: cybernetic control and system-level entropy production. In our first experiments with newly collected Hanford Reach hyporheic zone sediments, we have observed that Cr(VI) is reduced rapidly to sparely soluble Cr(III), implying that SIZ sediments have significant reduction capacity that may limit Cr and Tc discharges from groundwater to surface water. In similar experiments, a multi-rate model has been developed to account for the effects of heterogeneous redox-reactive mineral phase distributions and fine-scale facies variations on the macroscopic rate of Tc(VII) reduction to Tc(IV). Collectively these results form the basis for an integrated multi-component kinetic reaction network model for describing the biogeochemical transformations of organic carbon, nitrate, and contaminants in the SIZ and up-scaled domains of the Hanford Reach.

This presentation is part of SBR/PNNL_SFA.