Functional Enzyme-based Metabolic Models for Simulating Biogeochemical Processes

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Microbially-mediated biogeochemical processes are regulated by enzymatic activities that control the biogeochemical transformation of carbon, nitrogen, and other elements in natural environments. However, enzymes are often replaced using biomass or functional genes as surrogates in biogeochemical models because the quantification of specific enzyme concentrations in environmental samples is difficult. In this research, we developed a signature peptide-based technique that can efficiently and directly quantify multiple functional enzymes and their dynamics in sediments. This new technique was then used to investigate the correlations between functional enzyme concentrations and biogeochemical species concentrations during nitrate bioreduction in Columbia River hyporheic zone sediments from the Hanford site. A functional enzyme-based metabolic model was developed to describe multi-component biogeochemical processes based on the correlation results, measurements of the corresponding functional genes, and a theoretical analysis of metabolic energetics. The model divides the microbial community into multiple functional entities, each characterized by a specific functional enzyme informed by environmental genomics. The functional enzymes explicitly link microbial metabolism with the biogeochemical reaction network. The resulting metabolic model was implemented using three alternative system-scale modeling approaches that differ in their conceptualization of functional enzyme production and reactivity in natural systems. The first approach uses the inhibition concept derived from experimental observations that some enzyme activities will be inhibited in the presence of certain types of biogeochemical species (e.g., O_2). The second approach uses the cybernetic concept that provides a rational description of the dynamic regulation of enzyme syntheses and activities based on control theory. The third approach uses the maximum entropy production principle derived from nonequilibrium statistical mechanics fluctuation theorem to regulate the evolution of microbial community functions and biogeochemical reactions. These approaches are currently being tested using the experimental data to evaluate their effectiveness and predictability. The metabolic model and system-scale modeling approaches provide a framework for describing the coupled evolution of microbial community functions and the biogeochemical transformations of organic carbon, nitrate, and contaminants in hyporheic zone sediments at both laboratory and field scales.