LBNL Sustainable Systems SFA 2.0: Genome-enabled watershed simulation capability (GEWaSC)

Eric King (eking@lbl.gov) - Lawrence Berkeley National Laboratory, Susan Hubbard (PI), S. Molins1, U. Karaoz1, N.J. Bouskill1, L.A. Hug2, B.C. Thomas2, C.J. Castelle2, H.R. Beller1, J.F. Banfield2, C.I. Steefel1, E.L. Brodie1 (Co-PIs). 1 LBNL, 2 ORNL, 3University of California, Berkeley.

The LBNL Sustainable Systems SFA 2.0 is focused on addressing uncertainties in how climate or land-use-induced changes in hydrology and vegetation will affect subsurface carbon flux, the spatial and temporal distribution of flow and transport, biogeochemical cycling, and microbial metabolic activity. Here we report on the initial development stages of a Genome-Enabled Watershed Simulation Capability (GEWaSC), which will provide a predictive framework for understanding how genomic information stored in a subsurface microbiome affects biogeochemical watershed functioning, how watershed-scale processes affect microbial function, and how these interactions co-evolve. This multiscale framework builds on a hierarchical approach to multiscale modeling, which considers coupling between defined microscale and macroscale components of a system (e.g., a catchment being defined as macroscale and biogeofacies as microscale). The multiscale framework is based on an object-oriented, modular software design that couples individual process models (e.g., biogeochemistry, microbial function). Initially, we are focusing on biogeochemistry within the Rifle floodplain system, a component of the greater Colorado River system. At the floodplain scale, our model schema considers microbial competition and activity in discrete zones (biogeofacies) identified using a combination of biological, chemical, and geophysical approaches. These zones include surface soils with vegetation, the vadose zone and capillary fringe, and naturally reduced zones with buried organic material.

We also report our initial progress in the development of a trait-based modeling approach within a reactive transport framework that simulates coupled guilds of microbes. Guild selection is driven by traits extracted from, and physiological properties inferred from, large-scale assembly of metagenome data. Metagenome information is also used to complement our existing biogeochemical reaction networks and contributes key reactions where biogeochemical analyses are unequivocal. Our approach models the rate of nutrient uptake and the thermodynamics of coupled electron donors and acceptors for a range of microbial metabolisms including heterotrophs and chemolitho(auto)troths. Metabolism of exogenous substrates fuels catabolic and anabolic processes, with the proportion of energy used for each based upon dynamic intracellular and environmental conditions. In addition to biomass development, anabolism includes the production of key enzymes, such as nitrogenase for nitrogen fixation or exo-enzymes for the hydrolysis of extracellular polymers. This internal resource partitioning represents a trade-off against biomass formation and results in microbial population emergence across a fitness landscape. We use this model in initial simulations to identify the processes regulating aquifer oxygen concentrations during seasonally fluctuating water table regimes at the Rifle floodplain.