Trait-based approaches to modeling the microbial biogeochemistry from terrestrial to aquatic ecosystems

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The mobility and speciation of nutrients within aquifers, from surface to subsurface to groundwater, is nominally dependent on the distribution and activity of microbial functional guilds (i.e. groups consisting of diverse microorganisms that carry out the same process). In turn, the composition of these guilds is a function of the organisms' physiological traits along with environmental, physical and geochemical conditions that exist across flow paths to create 'hot spots' of activity. Here we report the development of a trait-based model that simulates coupled guilds of microbes parameterized including traits extracted from large-scale metagenomic data. Our approach models the rate of nutrient uptake using equilibrium chemistry approximations and the thermodynamics of coupled electron donors and acceptors to predict the energy available for respiration, biomass development and exo-enzyme production. Each group within a functional guild is parameterized with a unique combination of traits governing organism fitness under dynamic environmental conditions. We scale up the trait-based model by coupling it to a reactive transport model to simulate microbial development across spatially structured landscapes. Finally, we use the model to explore abiotic controls on community emergence and impact on rates of reactions that contribute to the cycling of carbon across distinct redox zones of an aquifer.