Microbial dynamics and syntrophic interactions at the pore scale: towards an integration of reactive transport and microbial cell models

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Project Goals:
The overarching goal is to expand the understanding of interactions and fundamental activities involved in cycling of carbon and nutrients by syntrophic methanotrophic archaeal-bacterial consortia and associated viruses in anoxic sedimentary environments. Specific objectives are to (1) quantify energy and nutrient exchange [e.g., nitrogen (N), phosphorus (P), iron (Fe) and vitamins] within AOM consortia and between ANME-bacterial partners; (2) identify virus-host interactions associated with AOM and assess C and N transfer through viruses in methane-impacted sediment ecosystems; (3) model energy and nutrient exchange in AOM consortia and viral-host interactions (i.e., viral activity), and their environmental distribution patterns.

Abstract
Understanding the cycling of carbon and nutrients in the sediment environments requires an accounting of the feedback between microbial activities and environmental conditions. We approach this through the development of (1) a reactive transport model that establishes a connection between processes at the pore scale and the macroscopic environment and (2) novel flux balance community metabolic models of anaerobic oxidation of methane (AOM) consisting of methanotrophic archaea (ANME) and syntrophic sulfate-reducing bacteria.

The porescale modeling uses a Lattice-Boltzmann approach to solve the Navier-Stokes equation to establish the flow field, and advection - diffusion - reaction equations to model chemical distributions and account for microbial growth dynamics. Here, we apply the model to study the feedback between flow and microbial growth, in order to investigate the relationship between two key macroscopic characteristics of porous media, permeability and porosity, under conditions where bioclogging can occur. Simulation results for an idealized porous medium show biofilm growth at the pore scale which affects the evolution of porosity and permeability. The resulting spatially heterogeneous distribution of biomass leads to deviations from empirical macroscale models such as the Kozeny-Carman (KC) equation. For impermeable biofilms the deviations of porosity-permeability relations from the KC equation depend strongly on flow and reaction conditions, reflected in Péclet (Pe) and Damköhler numbers (Da). Simulations with porous and permeable biofilms reveal a substantially different evolution of porosity and permeability compared to nonporous and impermeable biofilms, highlighting the importance of microscale biofilm characteristics for macroscale hydrological properties of porous media. These results emphasize that accounting for microbial processes at the porescale (i.e. micrometer scale) can be important for understanding the evolution of chemical concentrations, microbial activities and flow at the macroscale.

Connecting micro- and macro-scales in the above application relied on a highly simplified, substrate-dependent process rate representing microbial activity. Thus, our ongoing efforts include the integration of omics-based in silico cell models to simulate sulfate-coupled AOM in a sedimentary environment.

Significant progress was made in our efforts to construct community flux models of AOM consortia. A critical first step is to improve our ability to construct accurate genome-scale metabolic models of the individual types of microbes that comprise these uncultured consortia: methanotrophic archaea (ANME) and sulfate-reducing bacteria. Toward this end, we curated pathways and model templates for these classes of microorganisms in our latest build of the ModelSEED genome-scale model reconstruction tool in the DOE Systems Biology Knowledgebase (KBase). The ModelSEED now has an archaea template with an archaea-specific biomass reaction. Additionally, it includes a more complete representation of archaeal metabolic pathways. On average, models of archaeal species constructed by the ModelSEED have 150 additional genes compared to before our curation efforts. Special attention was focused on the methanogenesis and related methanotrophy pathways in this curation, as these pathways are central to the ANME phenotype. ANME microbes are related to methanogenic archaea, but these organisms support "reverse methanogenesis" as the biochemical model for methane oxidation. This metabolic activity requires an efflux of electrons to a syntrophic partner, which is the role played by sulfate-reducing bacteria (SRB) in these systems. Thus, in addition to properly capturing the reactions and annotations for the methanogenesis pathway, we are also adjusting model flux constraints to ensure proper implementation of ANME behavior. We are performing similar curation to improve the representation of sulfur reduction metabolism in the ModelSEED, improving these pathways in all ModelSEED models. We applied this improved ModelSEED tool to construct models for exemplar ANME and SRB strains assembled and binned from metagenomic data collected for this project. Presently, we are combining these models together in community flux simulations, while integrating transcriptomic data, to predict potential trophic interactions between various ANME and SRB strains. Ultimately, these predictions will be tested in the reactive transport simulations described above, as well as new experimental studies.