Reactive Transport Modeling of Microbial Processes: Cell Aggregate-scale Models and Upscaling Using Pore-scale Simulations

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Project Goals

The overarching project goal is to expand our understanding of the key microorganisms, metabolic strategies, and interspecies relationships involved in the formation and oxidation of methane. Our research evaluates potential mechanisms controlling anaerobic oxidation of methane (AOM) medicated by archaeal-bacterial consortia at the aggregate-scale and studies the influence of pore scale physico-chemical heterogeneity on macroscopic rate estimates in marine sediments.

At the aggregate scale, three different mechanisms for extracellular interspecies electron transfer are investigated and the results are compared to the cell-specific anabolic activity obtained by FISH-nanoSIMS. The sensitivity of model outputs towards poorly constrained model parameters is also explored to constrain model parameters for use in larger scale models. Next, we investigate the interaction between microorganisms and pore scale microenvironments, which may not be properly resolved by macroscopic rate measurements. The role of heterogeneous distribution of microorganisms on macroscopic rate estimates is explored in various flow and reaction conditions and important parameters for upscaling with improved accuracy are proposed.

Microorganisms dynamically interact with their microenvironments in nature through complex physical, chemical, and biological processes. Because of the complex and heterogeneous nature of porous media, predicting microbial activities across different scales remains challenging. We address the challenge of identifying mechanisms of syntrophic microbial interactions and upscaling microbial metabolism at the microbe-to-pore scale using reactive transport modeling approaches.

First, we simulate the activity of archaeal and bacterial cells mediating anaerobic oxidation of methane coupled with sulfate reduction at the scale of microbial aggregates. Three different mechanisms are investigated including electron transfer through the exchange of solutes such as H_2, the delivery of disulfide from methane-oxidizing archaea to bacteria for disproportionation, and direct interspecies electron transfer. We identify the mechanisms of synthrophic interactions that are consistent with both macroscopic rates and microscopic measures of anabolic activity. To that end, simulation data are compared to multi-modal image data from FISH-nanoSIMS observations, for which a machine learning approach to automate this analysis is being developed. The results

indicate electron transfer through the exchange of solutes such as H_2 is unlikely because the simulated intra-aggregate microbial activities differ from the observed distribution of nitrogen incorporation, and because oxidation rates are limited by the build-up of metabolites, inconsistent with observed rates. Instead our proposed DIET model yielded cell specific rates and archaeal activity distributions that were consistent with empirical observations, with little impact of the spatial distribution of bacterial and archaeal cells and consortium sizes. Our results demonstrate the successful integration of numerical modeling and experimental observations that improve our understandings of microbial activities, and point to direct interspecies electron transfer as a possible syntrophic mechanism (He et al. 2018).

Next, the role of heterogeneous distribution of microbial aggregates at the pore scale to upscaled microbial reaction rates is investigated under various flow and reaction kinetics conditions. Lattice-Boltzmann simulations reveal that scaling errors depend strongly on Peclet and Damkohler numbers, and to a less extent on the distribution of microbial aggregates (Jung and Meile, submitted). It is also shown that the systematic integration of macroscopic parameters improves the accuracy of upscaling biochemical reaction rates, demonstrating the importance of mechanistic understandings of upscaling physical and biochemical processes in porous media.

References

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Funding statement

This work was supported by the Genomic Sciences Program in the DOE Office of Science, Biological and Environmental Research DE - SC0016469. The authors declare no conflict of interest.