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ABSTRACT TITLE: Detailed Modeling of Uranium Mobility Under a Combined Influence of Microbial Activities and Geochemical Transformations

ABSTRACT: The mechanistic model of in situ uranium bioremediation requires a detailed representation of subsurface microbial metabolism and an accurate characterization of interactions between microbial and geochemical processes. The overall objective of this project is to develop a fine-scale computational framework capable of predicting uranium mobility under a combined influence of microbial activities and geochemical transformations.

We have made progress in both biotic and abiotic processes for achieving the project goal. 1) A preliminary pan-genome-scale metabolic model for subsurface *Geobacter* community was developed. The unique features of the metabolism suggest more of a necessity from studies of subsurface communities than from the subsurface isolates or from the non-subsurface model species. 2) The quality of the metabolic network reconstruction for subsurface *Geobacter* community was improved by removing thermodynamically infeasible loops with unrealistic high fluxes. 3) Physiological studies of the sulfate reducing bacteria, *Desulfobacter postgatei*, were conducted to evaluate the metabolic activity under electron donor-limiting and electron acceptor-limiting conditions, respectively. A genome-scale model of *Desulfobacter postgatei* was developed, providing some insights into the sulfate reduction pathways. 4) An optimized genome-scale metabolic model for *Anaeromyxobacter dehalogenan* (a unique bacteria with diverse metabolic capabilities such as uranium reduction) was developed, and a bi-level optimization algorithm for resolving energetic model inconsistencies (REMI) was implemented to remove the reactions with unrealistic high ATP production. 5) Computational thermodynamics based on the coupled oxidation-reduction reactions for geochemical transformation was integrated into a comprehensive reactive-transport model of in-situ bioremediation of U(VI), providing predictions and insights into the role of abiotic redox reactions that occur in systems with interplay between microbiological and geochemical processes. This approach helps to address some questions of interest, such as the reason why abiotic U(VI) reduction often takes place under laboratory conditions but has not been reported to play an important role under environmental conditions. The above-mentioned recent advances in modeling biotic and abiotic processes will help to ultimately build a fine-scale predictive model for computer-aided design of field-scale uranium bioremediation.