Building a Multi-level Model Framework for Computer-aided Uranium Bioremediation Design

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Reductive immobilization of hexavalent uranium to uraninite by stimulation of indigenous bacteria has been extensively investigated as an efficient remediation strategy for subsurface U(VI) contamination. The challenge is how to achieve a sustainable, cost-effective and efficient U(VI) immobilization under specific and various sedimentary conditions. The overall objective of the project is to address this complex and systemic challenge by developing a multi-level computational framework capable of predicting uranium mobility for a long period of time under different conditions.

We have made progress in six parts that complement each other for achieving the project goal. These six parts cover every detailed aspect of the study of bioremediation process through computational modeling approaches, i.e. from very small test environment to field sites, from individual microorganism to microbial community, from regular biostimulation to optimal control of chemical amendments, and from single computer processor to grid engine. These six parts can be summarized as follows: 1) We have built a more complex mechanistic model that incorporates the latest research findings on both biotic and abiotic processes in subsurface sediments, providing insights into uranium immobilization that cannot be obtained by experiments alone. We have shown the value of model by validating its predictions under dramatically different environmental conditions; 2) We have performed a preliminary construction and analysis of the *Anaeromyxobacter dehalogenans* model at the genome scale and we are planning to incorporate this organism into our computational framework due to its diverse and wide-ranged metabolic capabilities relevant to the reduction of iron oxides, selenium, nitrate, chlorophenols and uranium for growth; 3) We have investigated the interaction of *Geobacter* and sulfate-reducing bacteria both in sediment incubations and with *in silico* metabolic modeling, revealing that Fe(III) availability, rather than competition with sulfate-reducing bacteria, is the key factor limiting the activity of *Geobacter* during *in situ* uranium bioremediation; 4) We have developed an optimization framework based on optimal control theory to maintain the uranium concentration below the environmental safety standard while minimizing the cost of the acetate and Fe(III) addition rates as well as the difference between the predicted and target uranium concentration; 5) We have succeeded in optimizing and parallelizing our preliminary 3D research codes containing different kinds of kinetic and equilibrium equations. We then adapted the model to be executed on Grid Infrastructure through OpenMP implementation, achieving good speedups that are close to the theoretical maximum speedups; and 6) We have incorporated a genome-scale metabolic model of *Geobacter sulfurreducens* into a pore-scale simulation of reactive transport and microbial growth to assess the manifestation of pore-scale variability (microenvironments) in terms of apparent Darcy-scale microbial reaction rates. We are trying to ultimately integrate all of these individual components to build a multilevel model framework for assisting the design of an effective and efficient bioremediation strategy.