Representing geomicrobial processes in subsurface reactive transport models (RTMs)

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The chemical structure and evolution of subsurface environments is to a large degree determined by the activity of microorganisms. In particular, the distributions of redox-sensitive constituents are strongly affected by microbial metabolism, as electron transfer processes form the basis of biological energy generation. However, microbial reactions also modify acid-base and electrolyte properties of pore waters, thermodynamic driving forces, and the composition of particulate and colloidal matter in soils, sediments and aquifers. Comprehensive subsurface RTMs therefore require mathematical expressions that predict the rates at which microbial populations consume and produce chemical constituents. A common assumption is that microorganisms exhibit saturation kinetics with respect to the substrates they extract from their surroundings. This behavior is captured by the so-called Michaelis-Menten (or Monod) rate expression. Michaelis-Menten kinetics, however, have mostly been verified for pure cultures utilizing soluble substrates. More recently, experimental studies have shown that the Michaelis-Menten formulation also holds for redox transformation processes carried out by complex, natural microbial communities, and when solid-phase mineral substrates are utilized. The accumulating empirical evidence therefore supports the Michaelis-Menten formalism as the logical starting point for the development of mathematical representations of geomicrobial processes in RTMs. We present an extended Michaelis-Menten model, which accounts for substrate uptake efficiency, changes in microbial biomasses, the presence of inhibitors, and thermodynamic constraints on microbial reaction pathways. This kinetic model is incorporated into a RTM, which is then used to compare the spatial distributions of microbial biomasses and microbial reaction rates in aquatic sediments and aquifers. When advective flow dominates solute transport, as in aquifers, a strong correlation is predicted between microbial rates and the corresponding biomasses. In sediments, where diffusion and mixing process dominate dissolved and particulate transport, such a correlation is no longer observed. These results highlight the key role of the transport regime in controlling the microbial community structure and biogeochemical reactivity of subsurface environments

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Thermochemical data to describe actinide partitioning to bacteria: A mixed solvent approach

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Recent molecular dynamics simulations completed by others for the binding of metal ions in the outer lipopolysaccharide (LPS) layer of gram-negative bacteria have suggested unique metal binding mechanisms via cross-linking among the different LPS chains. Unfortunately, there are no current thermodynamic models available for calculating the stability of these cross-linked structures nor any capability for predicting how actinide ions and other species can bind or displace other metals from these structures. The problem is further complicated by the fact that the water content in the microbial membrane is highly variable, from full solvation in the outer membrane to essentially no water in the inner lipid core. Thermodynamically, the microbial membrane therefore represents an effective mixed organic-water "solvent" of variable composition.

To address these issues, we are developing experimental data for a thermodynamic model to predict the binding of cations (e.g., Ca^{2+}, Eu^{3+}, and Am^{3+}) in such mixed solvent systems represented by the microbial outer membrane. Experimentally, we are developing equilibrium data to describe the influence of sugar phosphate ligands (e.g., glucose-1-phosphate) on the solubility of well-characterized solids such as $Eu(OH)_3 \cdot xH_2O$. To represent the situation of cross-linking in the membrane and the variable water activity ranging from the bulk solvent to the inner lipid core, we are conducting our experiments in various mole ratios of water:methanol. Luminescence spectroscopy is used to verify solution species.

The experimental data will be used to describe the equilibria using the mixed solvent model developed by Wang, Anderko, and Young (2002, Fluid Phase Equilibria 203, 141-176). Our objective is to demonstrate the need for variable solvation systems rather than to develop a final representation of the microbial membrane. In this presentation, our efforts to-date will be summarized.