Towards a unifying theory of geomicrobial kinetics

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Geomicrobial kinetics studies how fast microbial metabolism proceeds in natural environments – a key question of low-temperature geochemistry [1]. It differs from microbial kinetics by considering wide spectra of tempertaures, pHs, availibilities of energy sources and growth nutrients, and other environmental factors. Geomicrobial kinetics also differs from geochemical kinetics in that it accounts for life's essential functions, including energy conservation, growth, and maitenance, and considers how thermodynamics impacts reaction rates.

Geomicrobial rates can be predicted on the basis of rate laws that applicable to natural environments [2]. These rate laws carry relatively large numbers of kinetic and thermodynamic parameters in order to account for various environmental and microbial factors. But application of the rate laws present a special challenge – how to assign values for the parameters.

Jin and Roden propose a best-choice approach to assign parameter values [1]. In theory, microbial parameters can be seperated into two groups, extant and intrinsic [3]. Extant parameters describes how rates are influenced by microbial adaptation to the environments, and include half-saturation constants for electron donor oxidation, acceptor reduction, and nutrient consumption, and specific maitnenance rate. These parameters vary with the availability of energy and nutrient sources, and should be determined directly using samples from the environment.

Intrinsic parameters describe the dependence of microbial rates on cellular enzymes and pathways, and include rate constant, growth yield, ATP yield, phosphorylation energy, and average stoichiometric number. These parameters bear the relationships determined by microbial physiology. Taking anaerobic respiration as an example, ATP yield and average stoichiometric number vary with electron donors and acceptors, and can be determined on the basis of respiratory pathways. Also, because microbial growth depends on ATP synthesis, growth yield increases linearly with ATP yields. As a result, we can taken intrinsic parameters as constants of microorganisms, and extraploate the values determined for pure cultures directly to the environment.

Taking the simulation of microbial sulfate reduction and methanogenesis as examples, I demonstrate how to select parameter values that are consistent with our current knowledge of microbial physiology and relavant to the environment of interest. I then apply the parameter sets and simulate microbial metabolism in batch reactors of mixed culture, flow-through sediment columns, and lake sediments. The results demonstrat that the best-choice approach reduces the task of parameter fitting and ensures the quality of simulation.

[1] Jin and Roden (2012) *Geomicrobial Journal*, in press. [2] Jin and Bethke (2007) *American Journal of Science* **307**, 643-677. [3] Grady, Smets, and Barbeau (1996) Water Research **30**, 742-748.

Experimental study on carbonation of Portland cement in sodium chloride solutions

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Carbonation behavior of cement has been extensively studied because cement carbonation affects the conrete stength and corrosion resistance of the steel reinforcement. Various factors can affect the carbonation of cement. This study presents the influence of salinity on the carbonation behaviors of cement material.

The leaching and carbonation tests were conducted on ordinary Porland cement(OPC) using a Teflon reacter at various NaCl concentrations (0 ~ 2.0 M) under ambient temperature and pressure conditions. For the carbonation tests, CO_2 gas (99.9%) was injected in the slurry, which was obtained by mixing the soluiton and OPC.

For the leaching tests, the slurry pHs increased to 12.0 ~ 12.9, regardless of the NaCl concentration, after 24-hours leaching due to dissolution of $Ca(OH)_2$. The electrical conductivities (ECs) of the slurries increased steadily during the leaching test at low NaCl concentrations (< 1.0 M), whereas decreased at high NaCl concentrations (> 1.0 M). The Ca concentration in the slurry increased with increasing the NaCl concentration. After the leaching tests, dissolution of C_3S and $Ca(OH)_2$ and formation of C-S-H and Friedel's salt were indentified by XRD, SEM-EDX, and TGA analysis. The NaCl concentration affected the extent of the C-S-H formation during the leaching tests. The C-S-H content in the reacted OPC was the highet at the 1.0 M NaCl solution. During CO_2 injection, the pH decreased due to the dissolution of CO_2 and the carbonation reaction. Precipitation of well-crystallized calcite ($CaCO_3$) and halite (NaCl) in the reacted OPC obtained after the carbonation tests were identified by XRD, SEM-EDX, and TGA analysis. The C-S-H content decreased but the $CaCO_3$ content increased with incresing the NaCl concentration after the carbonation tests. Theses results sugesst that the presence of NaCl enhances the dissolution of $Ca(OH)_2$ in the OPC during hydration and the precipitation of $CaCO_3$ by the elevated dissolution of C-S-H during CO_2 injection.