

Field, lab, and computational tools and techniques for linking geochemical and microbial processes in a range of environments

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Defining the intertwining of geochemical cycling and microbial ecology is a problem of principle importance for a number of surface and subsurface geochemical processes. We will present and discuss the coupling of electrochemical techniques with microbial sampling and the application of artificial neural network (ANN) algorithms to quantify correlations between these datasets.

Microelectrodes are being used to define, *in situ* and in real time, geochemical microenvironments to guide microbial sampling in an effort to develop well correlated datasets to probe the dynamics between microbial activity and geochemical cycling. Information on a host of redox species (including a number of O, S, Fe, Mn, and As species) that are critical metabolic components for microorganisms can be obtained very quickly and at micron scales in water and saturated sediments using microelectrodes to determine spatial and temporal variability of these species. We additionally guide geochemical sampling of the water and sediment to determine other parameters at complimentary spatial and temporal scales using other techniques. Correlating geochemical data with microbial processes requires microbial sampling to also be done at comparable scales. These activities are guiding us towards a large database of geochemical and microbial data that are highly correlated in space and time. To utilize this database for quantitative assessment of the driving mechanisms that govern dynamics between these processes, we are developing and applying specifically designed ANN algorithms to assess the degree of change in geochemical process X that drives a change in microbial ecology Y (and vice versa). With this data we also guide laboratory kinetic experiments to assess how the population distribution of certain microbial organisms comprising a consortia is affected by changing key geochemical parameters. We will summarize current progress and describe ongoing research efforts based at several sites.

New approaches to characterizing microbial denitrification in the saturated zone

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Nitrate is the number one drinking water contaminant in the nation. It is pervasive in surface and ground water, and its principal sources (fertilizers, animal operations, and septic systems) have increased dramatically in the last 50 years. The extent and effectiveness of microbially-facilitated denitrification in mitigating nitrate loading to groundwater is not well known. In this paper, we report on a multi-disciplinary study of saturated-zone denitrification beneath a California dairy. The study integrates new methods for quantifying denitrification (membrane-inlet mass spectrometry for determination of excess nitrogen; quantitative real-time PCR for quantification of nitrite reducing bacterial populations) with existing methods for constraining groundwater flow and nitrate transport (³H-³He groundwater age-dating; 3D geostatistical models of aquifer hydraulic properties conditioned by direct-push CPT data; high-resolution models of groundwater flow and nitrate transport). A primary goal is to understand the extent to which saturated-zone denitrification is related to dairy management or to intrinsic properties of the aquifer. The aquifer is strongly stratified with respect to both nitrate and redox properties. Shallow groundwater is oxic and contains high levels of nitrate; slightly deeper groundwater is reduced and contains low or no nitrate and measurable excess nitrogen. In addition, we have developed rt-qPCR probes for the presence of bacterial DNA coding for the Fe- and Cu-containing nitrite reductase (*nirS* and *nirK*). Denitrifying bacterial populations at the site vary by at least four orders of magnitude, indicating that denitrification is strongly localized. Preliminary reactive transport modeling indicates that aquifer sediment properties, e.g. the distribution of fine-grained organic-rich sediment, must play a role in maintaining the observed redox stratification and controlling denitrification.

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