Thermodynamic network model for predicting effects of substrate addition and other perturbations on subsurface microbial communities

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**Goal and Hypothesis**

The overall goal of this project is to develop and test a thermodynamic network model for predicting the effects of substrate additions and environmental perturbations on microbial growth, community composition and system geochemistry.

The hypothesis is that a thermodynamic analysis of the energy-yielding growth reactions performed by defined groups of microorganisms can be used to make quantitative and testable predictions of the change in microbial community composition that will occur when a substrate is added to the subsurface or when environmental conditions change (Fig. 1).

**Assumptions**

- Community consists of 39 microbial groups, each with a defined metabolism, growth equation, and biomass yield (Table 1).
- Groups that can obtain the most energy from a growth substrate in a particular "thermodynamic niche." grow.
- Growth is predicted using equilibrium thermodynamics

**Simulation Methodology**

- Simulations were performed for laboratory and field experiments at the Oak Ridge FRC, Old Rifle, and Hanford 100H.
- Equilibrium reaction paths computed using The Geochemist’s Workbench to predict the effects of ethanol, acetate, or lactate additions on microbial growth, geochemistry, and mobility of U, Tc, V, and Cr.
- "Batch" and "flush" simulations compared to experimental data.
- Initial geochemistry matched to initial conditions in each experiment (Table 2).

**An Interesting Observation …**

Predicted biomass and community composition are very different for batch and flush simulations and provide some insight into the difficulty of transferring the results of laboratory microcosm experiments to the field

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