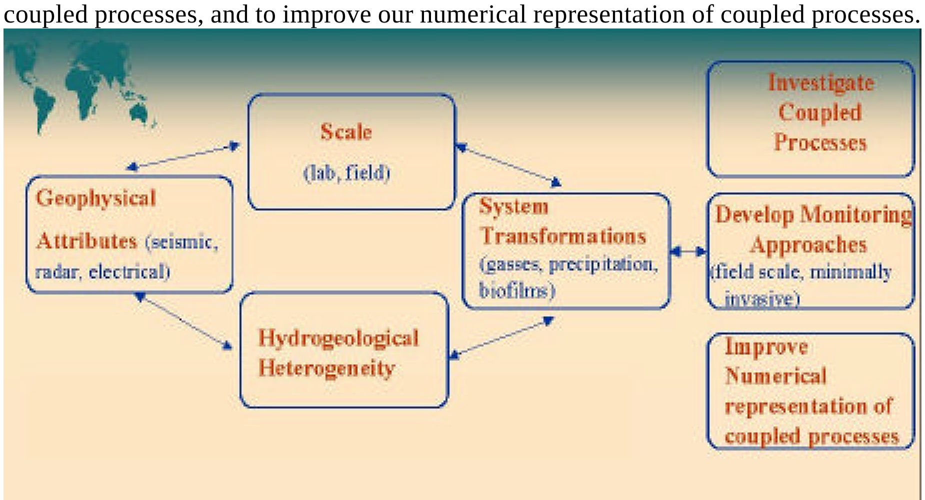
1. Research Objectives:

Biogeochemical and hydrological processes are naturally coupled and variable over a wide range of spatial and temporal scales. Additionally, many remediation approaches also induce *dynamic* transformations in the system. It is widely accepted that effective remediation requires a better understanding of coupled processes than is currently available. Further complicating the problem is the inability to collect the necessary measurements at a high enough spatial resolution yet over a large enough volume for understanding field-scale transformations. Our research includes two key objectives:

1) Improving the understanding of certain coupled processes, and
2) Investigating the capability to characterize and monitor coupled processes at appropriate resolutions and spatial scales using geophysical data.

Our work plan includes monitoring system perturbation experiments using microbial, geochemical, hydrological, and geophysical (seismic, electrical, radar) measurements as a function of scale (lab vs. field) and heterogeneity. Laboratory column experiments will be developed to test the geophysical responses and sensitivities to various processes that occur during system transformations, such as generation of gasses, biofilms, and precipitates. The resulting measurements will provide the database necessary for investigating coupled processes and for refining our numerical coupled modeling approach. The linkages between the components of the experiment and the research objectives are illustrated in Figure 1.

Figure 1: Our experiment focuses on monitoring system perturbation experiments, conducted under various hydrogeological conditions and at various spatial scales, using geophysical data. The developed database will help us to assess the potential of geophysical approaches for remotely monitoring system transformations, to investigate coupled processes, and to improve our numerical representation of coupled processes.



2. Research Progress and Implications:

This report summarizes work performed during the first year of a three-year project. The first part of the project is focused on lab-scale experiments so that we can develop an understanding of the sensitivities of various geophysical responses to system transformations under controlled hydrogeological-biogeochemical conditions. We have spent much of this year developing our laboratory column-scale experimental set-up, testing and calibrating our measurement and numerical modeling approaches, and refining our approach for integrating the diverse datasets that we will collect during the column experiments. Although each suite of column-scale experiments will include several columns for making disparate measurements (i.e., different columns for seismic, radar, electrical, hydrological, and biogeochemical data acquisition), as each column will be subjected to the same advection rates and the same treatments, we will assume that the acquired data are co-located in space and time and will analyze the datasets as a whole. Figure 2a illustrates the multiport set up associated with the biogeochemical column, which will allow sampling of fluid chemistry, biomass and nanoparticle and/or flocculate samples along the length of the flow-through column. The electrical column, shown in Figure 2b, includes gold current electrodes at each end of the column and non-polarizing AgCl potential electrodes along the length of the column. Spacing of the electrodes along the length of the column will permit complex resistivity measurements as a function of location during the experiment; a similar arrangement has been developed for the seismic and radar column measurements.

Figure 2a. Biogeochemical measurement column showing multi-port samplers.

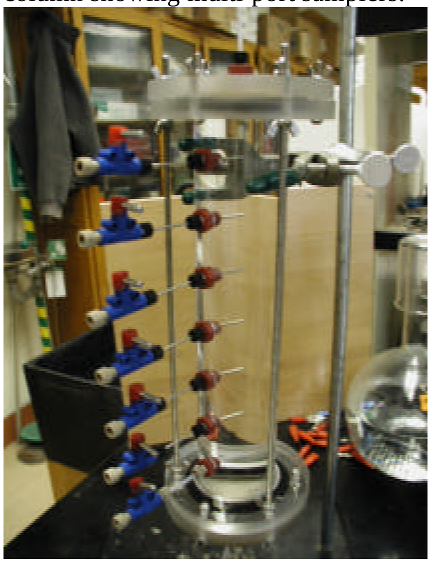
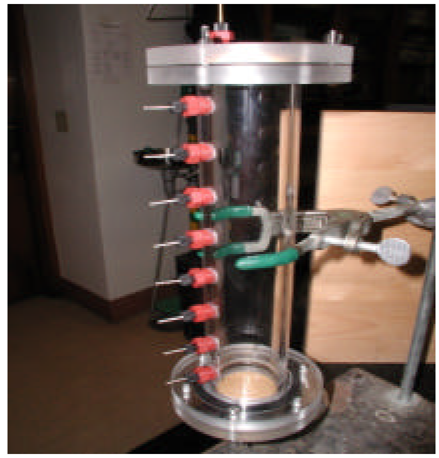


Figure 2b. Electrical measurement column with current electrodes on top and base and potential electrodes along length of column.



Our first suite of column-scale experiments is underway, and focuses on microbe-induced iron and zinc sulfide precipitation in porous granular saturated medium in both fine- and coarse-grained sediments. We have started with this suite of experiments to parallel the conditions found at the D-Area Coal Pile Runoff Basin at Savannah River Site, which is a proposed site for field testing in the third year of this project. The microbe that we have chosen to use for this experiment is the *Desulfovibrio vulgaris* (ATCC 29579), which is a sulfate-reducing bacteria (SRB) commonly found in natural aquifers. Our initial tests have confirmed that *D. vulgaris* reduces sulfate while oxidizing lactate to acetate and that the generated bisulfide reacts with aqueous metals to form metal sulfides such as ZnS and FeS. Laboratory tests have shown that there is rapid production of metal sulfides under stimulated conditions; we anticipate that these precipitates will clog pore spaces and throats, thereby decreasing the hydraulic conductivity of the flow-through column and altering the geophysical responses.

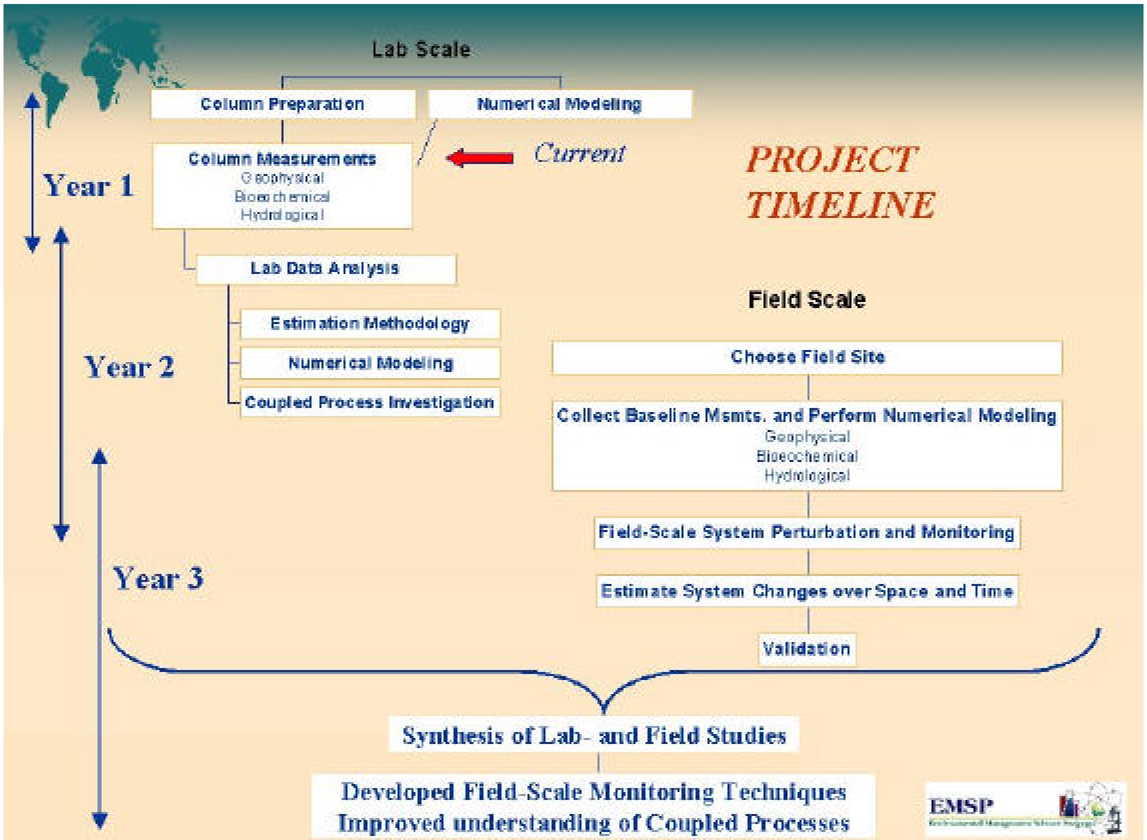
In addition to experimental data collection, we have worked this year on improving our numerical modeling and parameter estimation techniques, both of which are crucial components for this study. We have simulated the experimental conditions using the coupled numerical BIOCORE model, which takes into account the interactions between aqueous and adsorbed/attached chemical and microbial species as well as minerals. The simulations have helped us to understand what reactions to expect as well as to design our sampling protocol. We have also developed a novel data integration approach using Monte Carlo Markov Chain methods. This approach has been tested on two different data sets, and is advantageous for data integration and parameter estimation in cases such as this project, where there are a large number of variables and complex/non-linear relationships between the different variables.

Analysis of our experimental data will help us to understand how the different geophysical measurements (seismic, radar, and electrical) will respond to the generation of two different precipitates and associated reduction in pore space. Additionally, we will use the developed measurement database to investigate a few specific coupled processes. In particular, we will investigate the onset of correlated mineralogical-biogeochemical gradients within the columns associated with the precipitation of the two different metal sulfides, and will investigate the interactions and dynamics of hydrological-biogeochemical alterations.

3. Planned Activities:

Figure 3 illustrates the timeline associated with this project. As shown in the timeline, year one and part of year two focuses on column -scale measurements and analysis, development of estimation methodology, and numerical mo deling. The last part of the second year and the third year will be devoted to testing the potential of the geophysical methods for monitoring system transformations at the field scale.

Figure 3 Project Timeline



4. Information Access:

A pdf file of a presentation given at the EMSP PI meeting in May 2003 is available at: http://esd.lbl.gov/people/shubbard/vita/webpage/hubbard_susan_86922.pdf, and a project website is available for viewing at: http://geo.lbl.gov/pnandi/emsp.html.