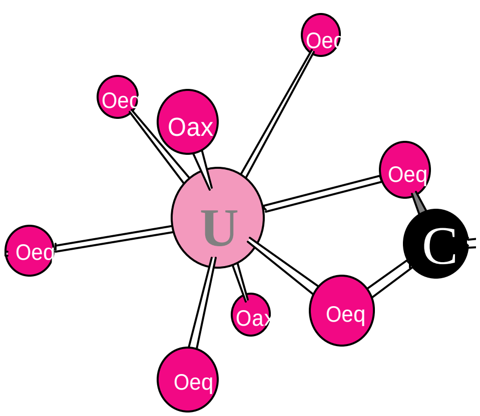
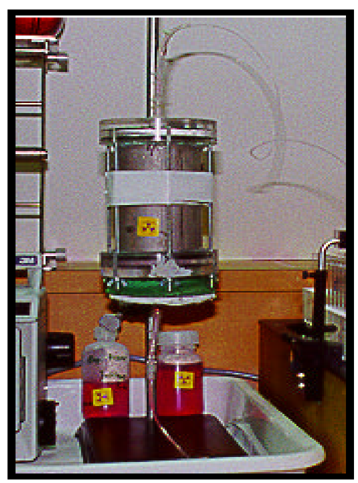
Geochemical/Geophysical Characterization Working Group

Research Briefs and Coordination

NABIR PI Meeting
March 2004





<u>Description of activities</u>

Project specific and general site characterization endeavors designed to quantify *in situ* contaminant speciation and select physical, chemical, and mineralogical properties of the FRC groundwater and solid phase before and after biostimulation.

Characterization endeavors encompass a vast range of scales from molecular scale contaminant speciation (e.g. high-resolution surface spectroscopy techniques) to field scale plume mapping (e.g. non-invasive geophysical techniques).

<u>Goals</u>

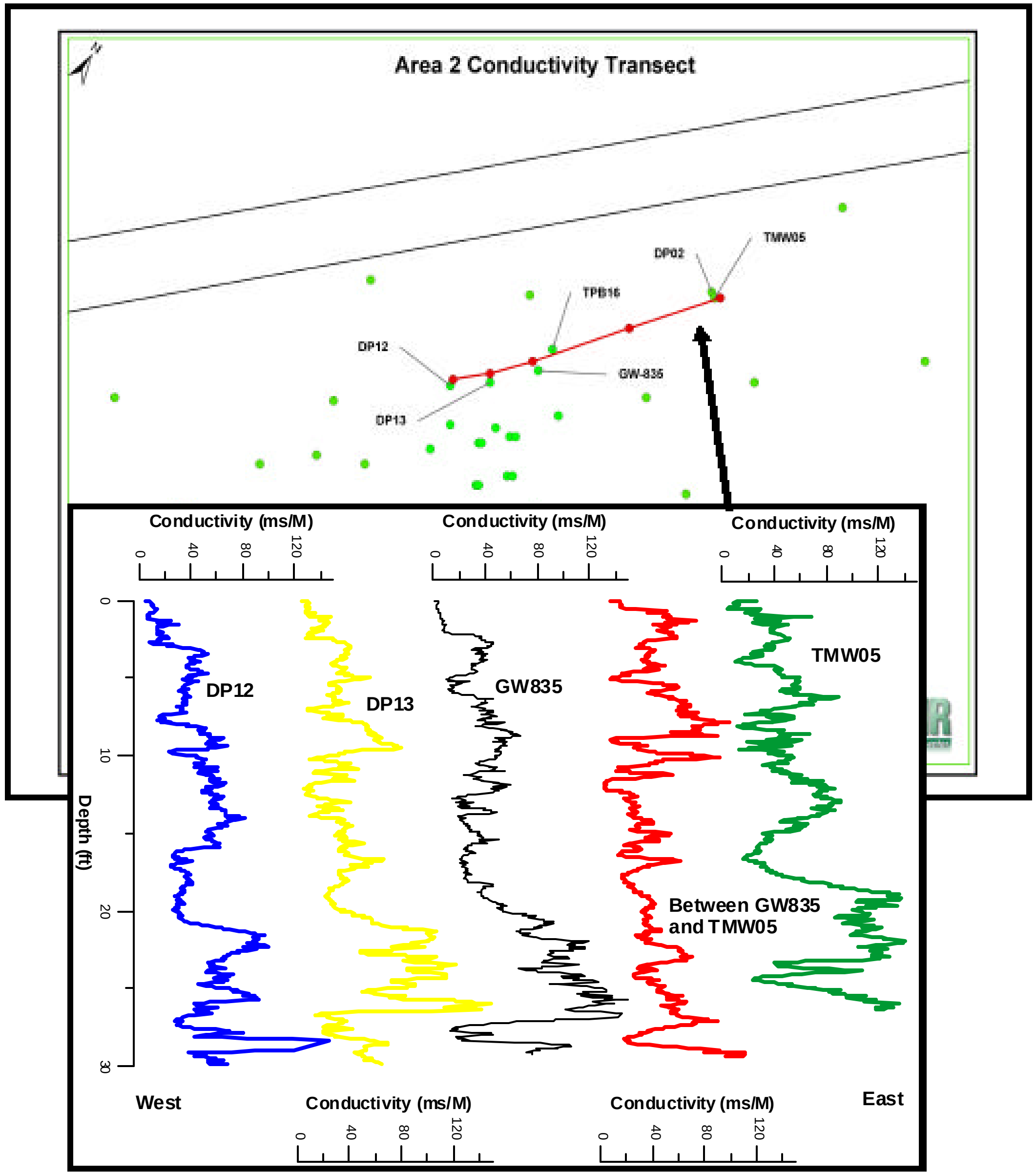
To provide an integrated set of research endeavors that provide an improved fundamental understanding of the geochemical and hydrological controls on bioremedation.

To couple this information with the research efforts within the other working groups in an effort to enhance the FRC site wide conceptual and numerical models and the research strategies of individual projects.

Site wide subsurface geochemical and hydrological characterization

Designed to provide macroscopic scale characterization of site specific groundwater hydrology and aqueous and solid phase geochemistry.

Results guide decision-making strategies for site selection and implementation of field scale biostimulation studies.



Example:

Electrical conductivity Profiling

Quick *in situ* method for interrogating subsurface geochemistry and the location and magnitude of potential contaminant plumes.

Watson and Hyder

Geophysical techniques for locating and tracking contaminant plumes

Example:

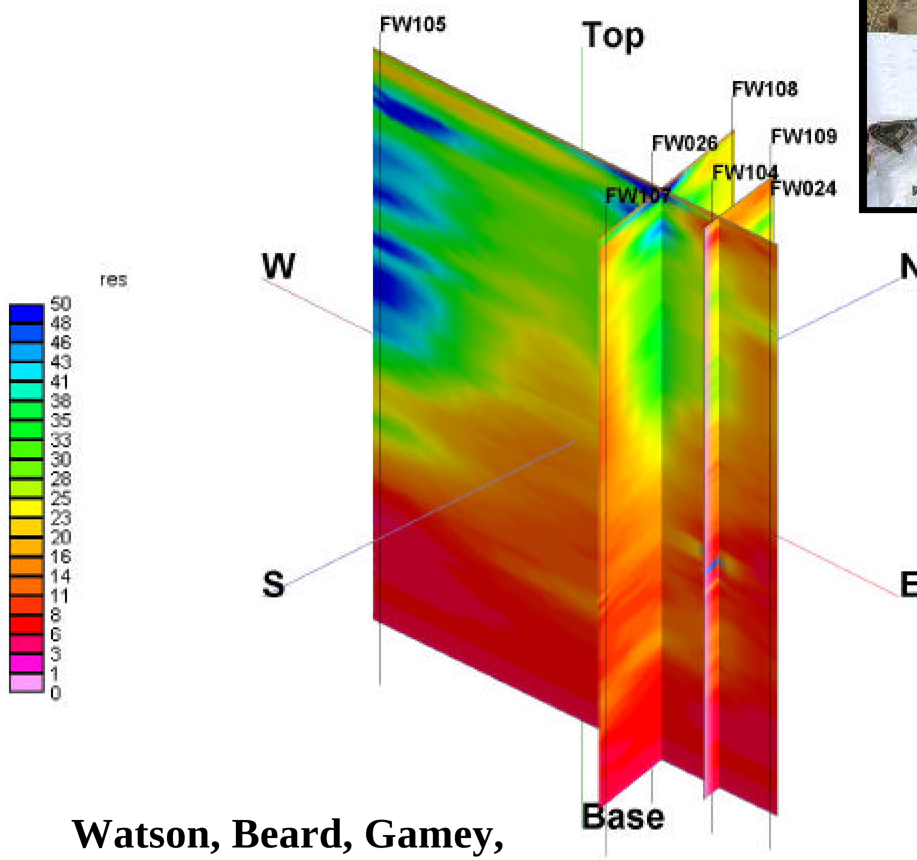
Electromagnetic Induction Logging, Seismic and Radar Tomography

Spatial and temporal plume mapping during manipulation.

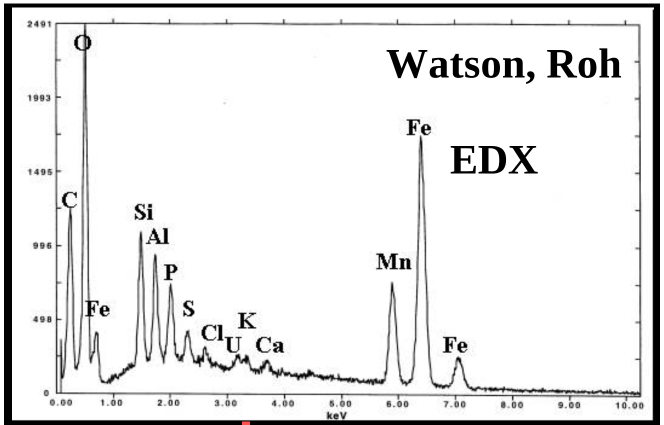
Mapping subsurface material heterogeneities.

Assists in quantifying fast flowing fracture regimes vs. slower flowing matrix regimes.

Complements direct groundwater geochemical tracer measurements.



Watson, Beard, Gamey, Hubbard



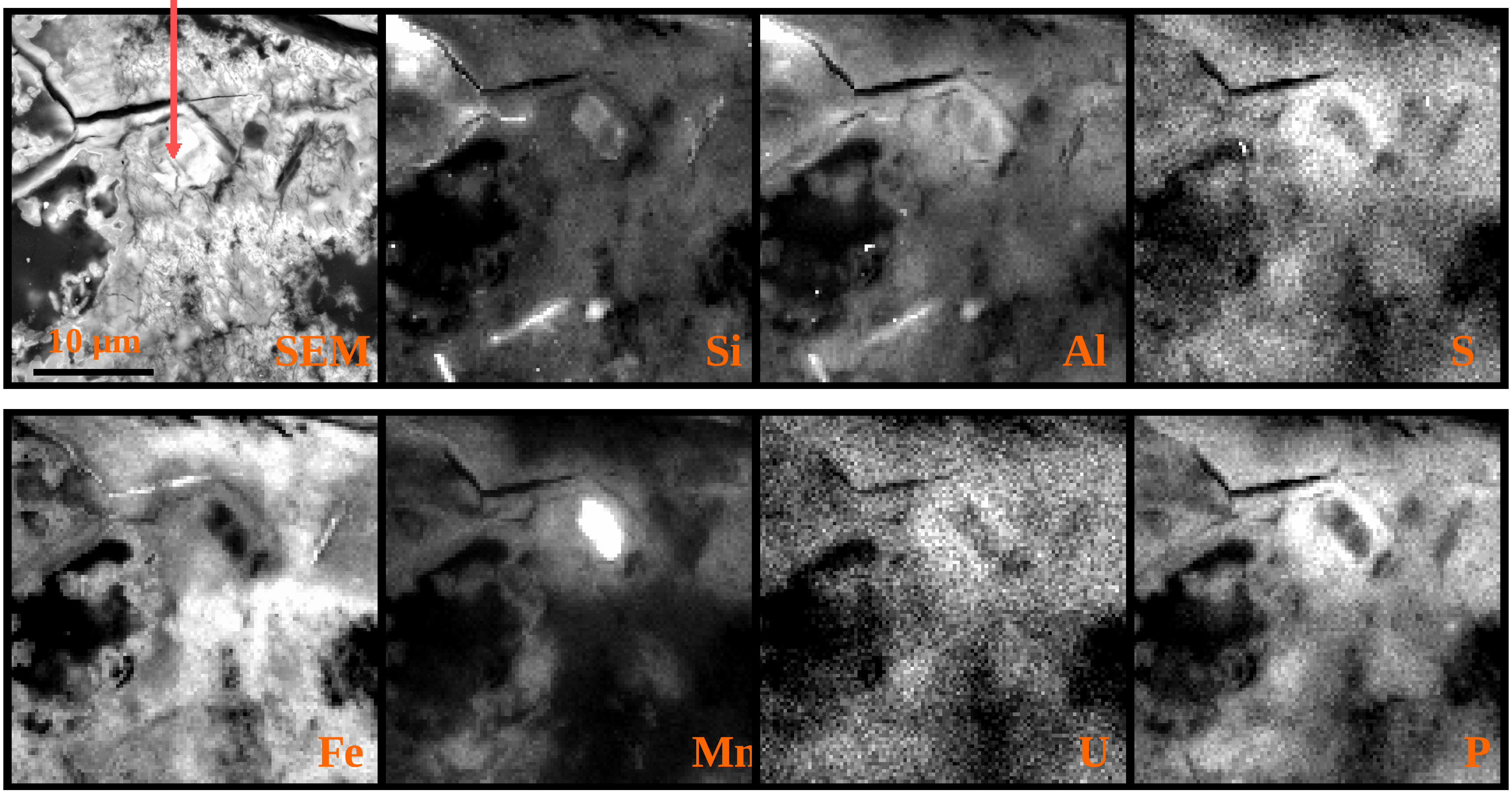
Mineralogical controls on contaminant distributions

Example:

SEM-BSE-Element Mapping of FRC sediments

-U distribution matches P and S distribution

-Contaminant speciation influences propensity towards bioreduction

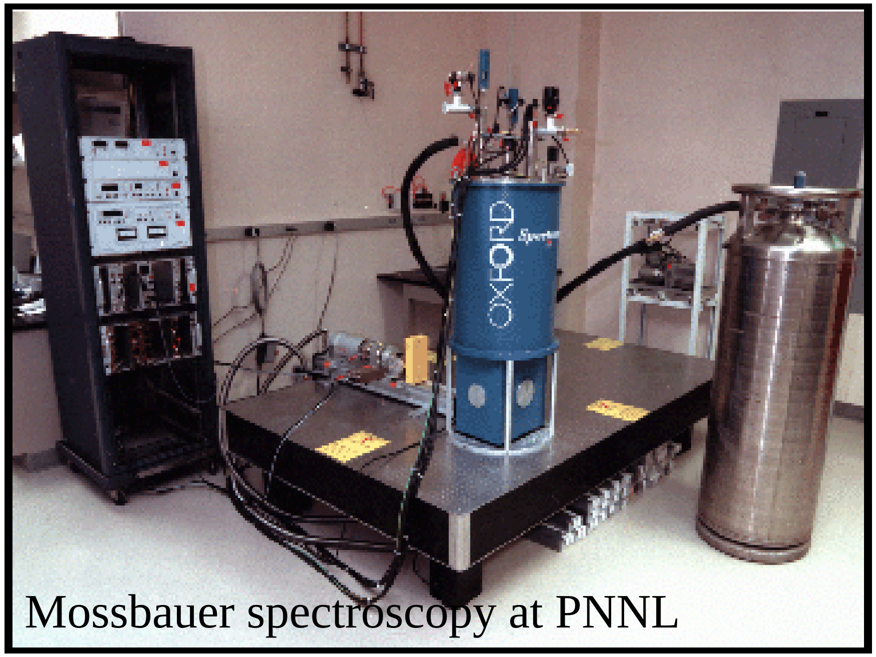


Characterizing the role of biogenic Fe(II) on contaminant bioreduction

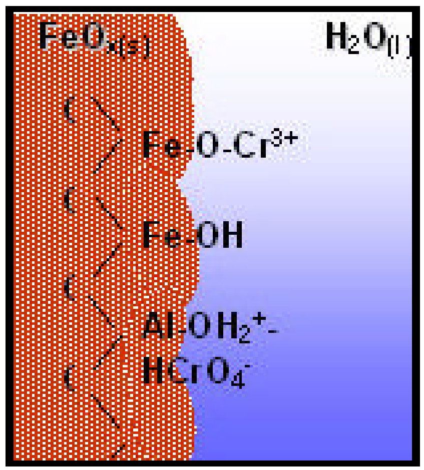
Mossbauer used to quantity the types, amounts, and distributions of various Fe-bearing minerals and oxides in heterogeneous FRC background and contaminated samples.

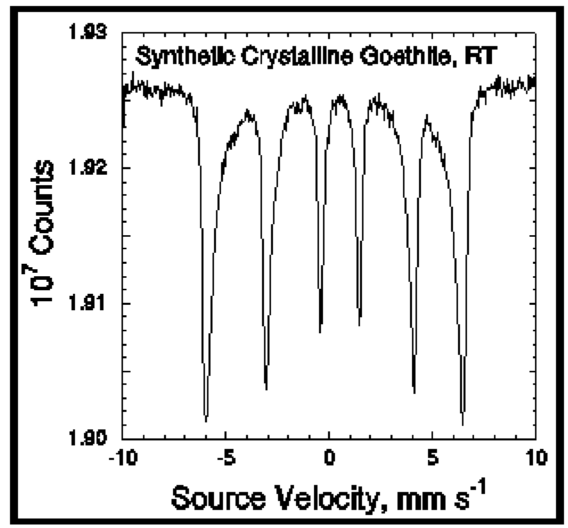
Quantify changes in Fe mineralogy following in situ biostimulation using various electron donors.

Quantify mechanisms of biogenic Fe(II) reactivity with the solid phase and its influence on the rate of contaminant bioreduction.



Mossbauer spectroscopy at PNNL

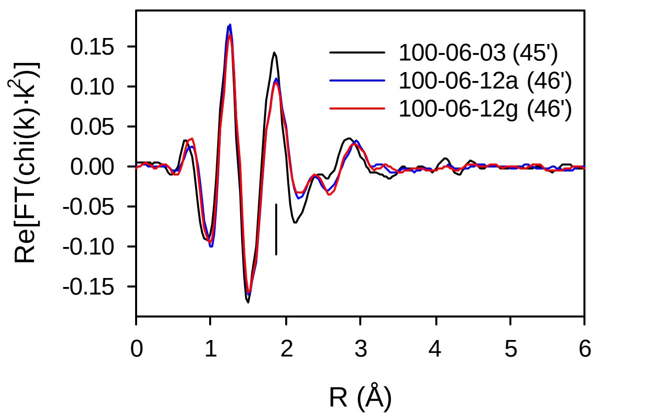




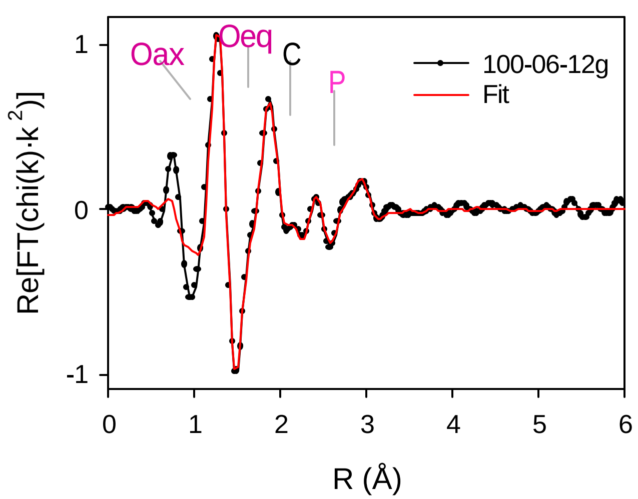
Stucki, Zachara

High resolution surface spectroscopy techniques for quantifying contaminant speciation and chemical environment

Real part of Fourier transform of data from samples taken at 45, and 46 (with replicate) feet

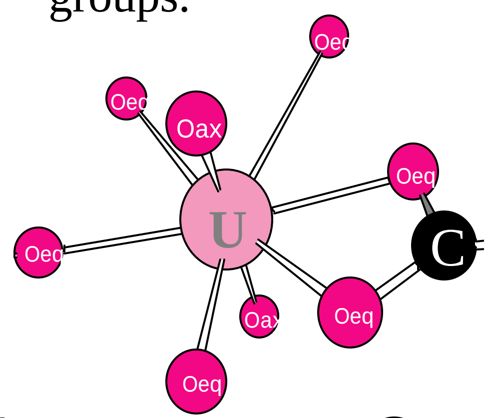


Real part of Fourier transform of data and model from sample taken at 46 feet

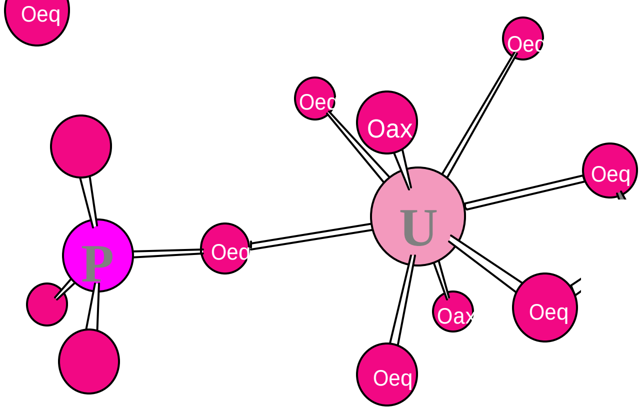


Example:

- EXAFS used to quantify the chemical environment of solid phase U at the FRC.
- U is coordinated by bidentate carbon containing groups and/or monodentate phosphorous containing groups.



Speciation controls rate of contaminant bioreduction.

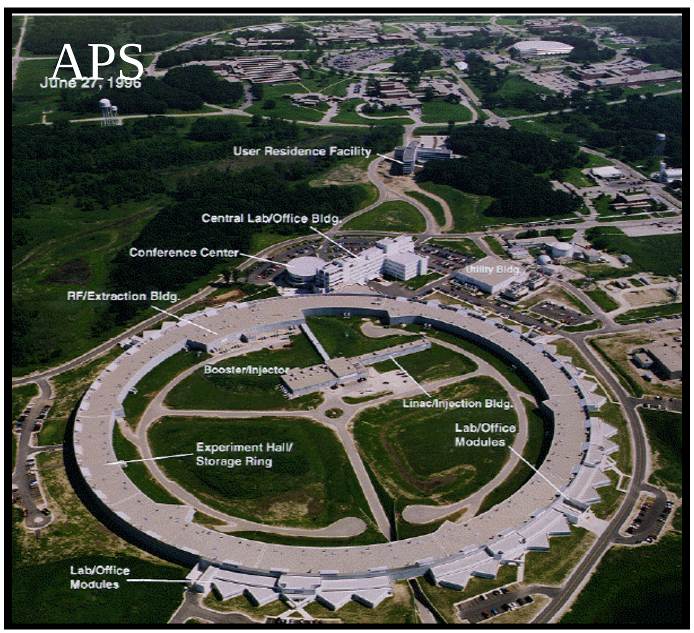


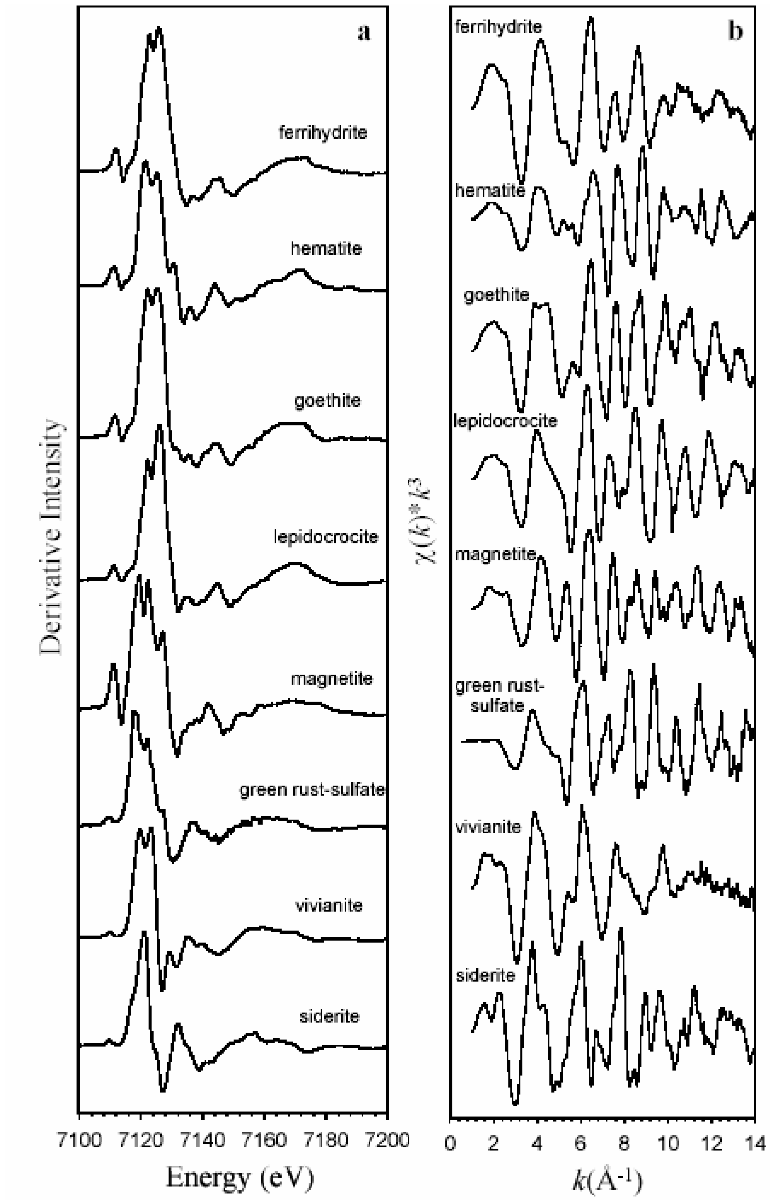
Kelly and Kemner

High-resolution spectroscopy for quantify reactive minerals in FRC soils

Extended X-ray Absorption Fine Structure (XAFS) used to quantify the Fe-oxide mineralogy in heterogeneous samples from the FRC.

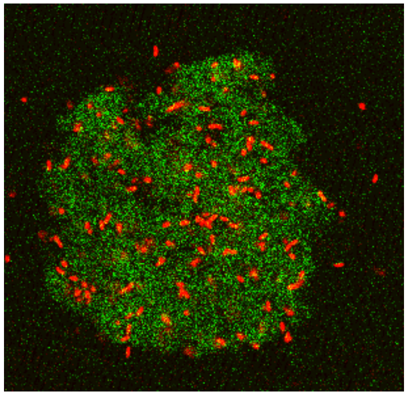
Quantifying biogenic Fe products and changes in mineralogy during biostimulation.



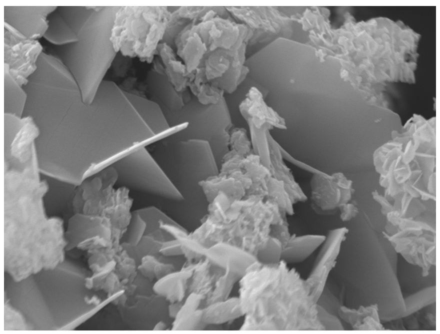


Fendorf

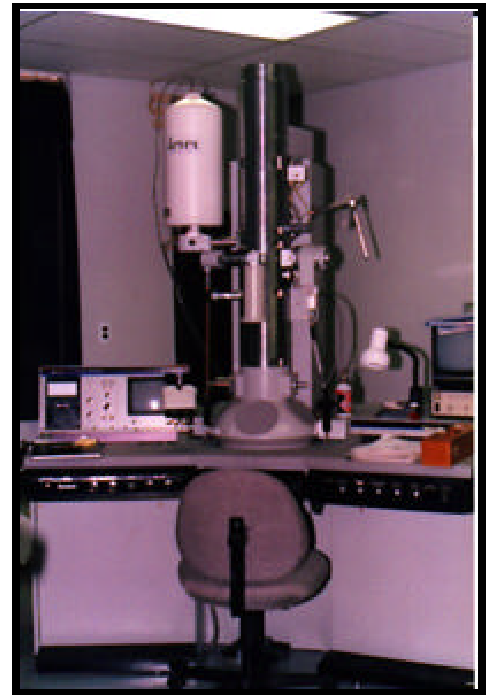
Scanning and Transmission Electron Microscopy

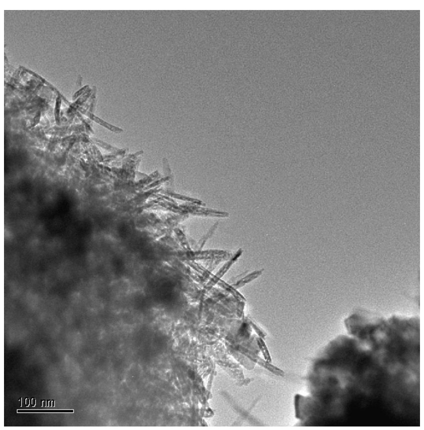


Bacterially populated iron oxide coated sand grain



Scanning electron microscopic image of biogenic green rust.





Transmission electron micrograph of iron oxide clusters showing goethite laths emanating from a ferrihydrite conglomerate.

Fendorf, Zachara

How are the hydrologic and transport data used?

- Data support the field scale modeling endeavor.

- Supply parameters for direct model input or scale-up (e.g. hydraulic conductivity, mass transfer rates, flow and transport anisotropy ratios, preferential flow vs. matrix diffusion).

- Improved conceptual understanding for enhanced numerical coding and simulation.

- Fast vs. slow flow zones may influence microbial community structure and dynamics.

- Provides essential information for the interpretation of geophysical measurements and monitoring that can now be used to assess processes at larger scales.

How are the solid phase geochemical and mineralogical data used?

- Mineralogy confirm whether hypothesized reaction pathways and associated stability/equilibrium constants are correct.

- Solid phase contaminant speciation used to understanding in situ geochemical and microbial processes.

- Supply parameters for direct model input (e.g. solute speciation, mass balance, spatial and temporal concentration distributions).

- Improved conceptual understanding for enhanced numerical coding and simulation.

- Important link to microbial community structure and dynamics and the rates and mechanisms of metal reduction.

How are the geophysical data used?

- Provides essential information on media structure and large-scale plume identification.
- Provides complementary information on in situ fate and transport processes.
- Provides large-scale view of subsurface features for guiding groundwater well placement.
- Proven and potential applications for monitoring hydrological, geochemical, and microbial manipulations.
- Supply integrated, large-scale subsurface data sets that can be compared to transport model simulations/visualizations.
- Used to estimate hydrogeochemical parameters for use in transport models.
- Improved conceptual understanding for enhanced numerical coding and simulation.

Links across working groups

Linkage to “modeling” working group involving direct parameter input and refined conceptual model; linkage from modeling group on parameter/process sensitivity and key data deficiencies.

Linkage to “rates and mechanisms” working group by providing enhanced knowledge on solid phase geochemical and physical characteristics, contaminant speciation, and biostimulation reaction products to close/balance reactions.

Linkage to “microbial characterization” working group by defining what hydrological and geochemical conditions control microbial community structure and dynamics.

Specific example of a linkage across disciplines:

("characterization" working group) Unraveling the mechanisms of biogenic Fe(II) production on contaminant reduction kinetics. Quantify dynamic changes in contaminant chemical environment and changes in Fe geochemistry during in situ biostimulation.

("rates and mechanisms" working group) Based on the above information, have the appropriate coupled geochemical and microbial reaction equations written, balanced, and parameterized.

("microbial characterization" working group) Based on the above, make sure microbial isolates and community structures are consistent with observed geochemical dynamics.

("numerical modeling" working group) Incorporated reactions above into site specific and site wide FRC numerical models. Parameterization and simulation of specific problems.