The Oak Ridge Field Research Center Conceptual Model

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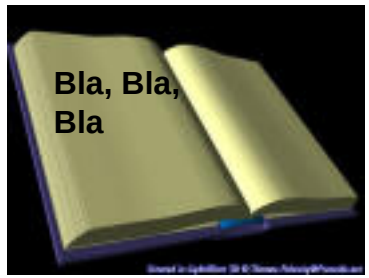
Purpose

To provide investigators from various programs (e.g. NABIR, EMSP, GTL) with state of the art knowledge of subsurface processes that are operative at the FRC background and contaminated sites in an effort to support their research mission.



Text description

Describes the current conceptual framework of coupled hydrological, geochemical, and microbial processes that control the fate and transport of contaminants at the Oak Ridge FRC.

Structured to discuss the FRC background area, the overall contaminated area, and each of the five contaminated field areas (Areas 1 through 5) with emphasis on field processes.

The text is a living document that will be updated as additional information is obtained.

Oak Ridge FRC Background Area

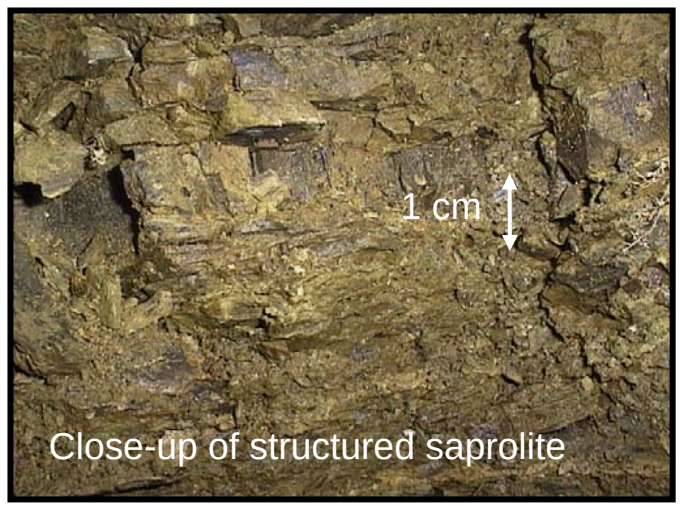
ORNL media consisting of interbedded fractured weathered shales and limestone

Geology

Bedrock and soil features
Fracture characteristics
Mineralogy and porosity

Overlying Saprolites

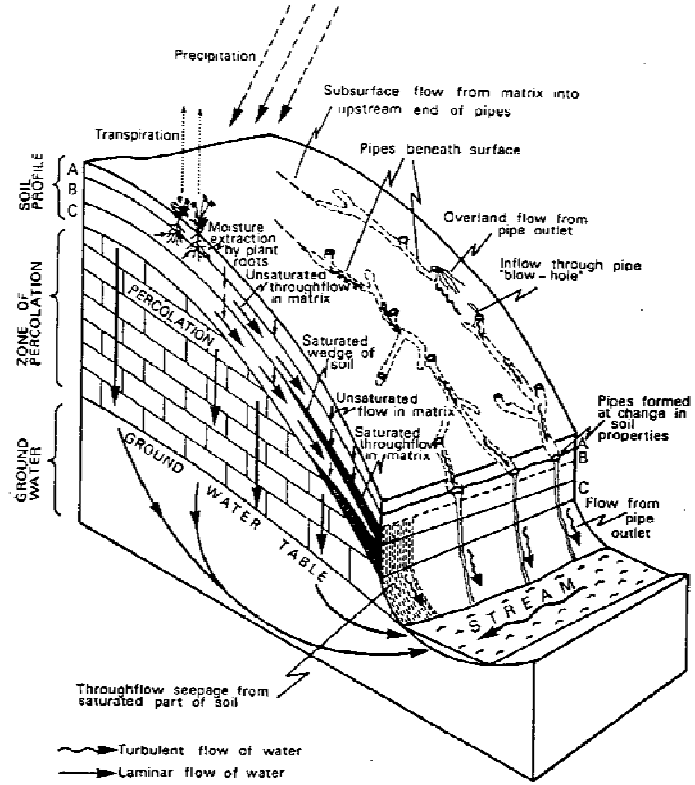
Underlying Bedrock



Oak Ridge FRC Background Area (cont.)

Hydrology

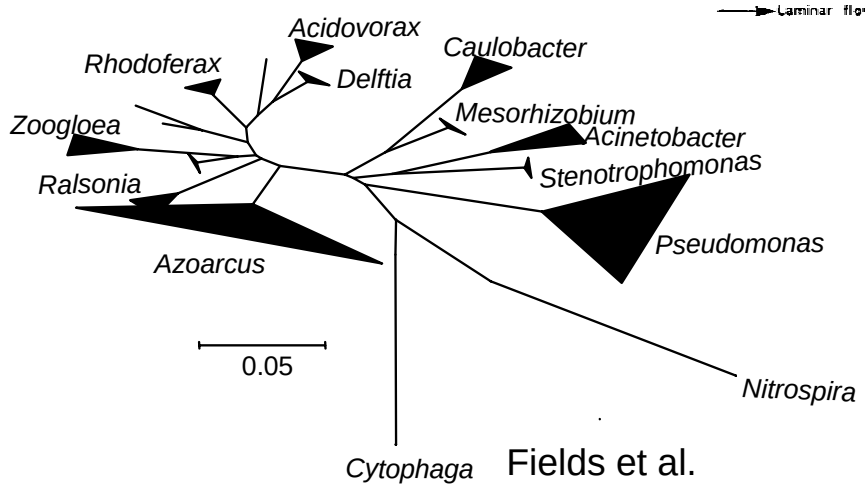
Vadose zone stormflow and recharge
Transition zone groundwater flow
Porosity and flow
Nonequilibrium processes
Multipore region flow and transport



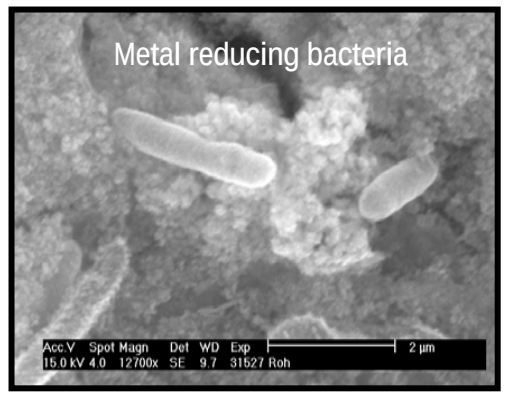
Geochemistry

Stormflow and groundwater flow
Interfacial geochemical reactions

Microbiology



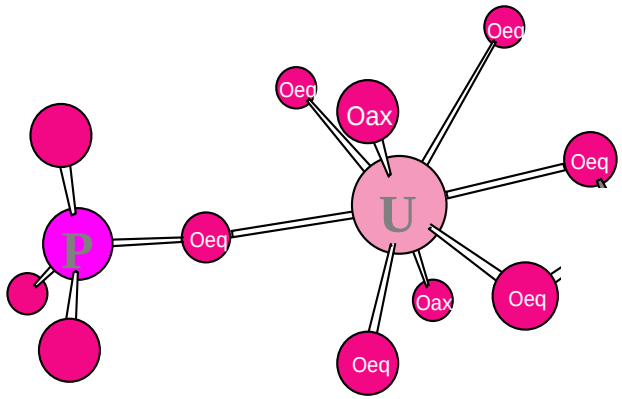
Fields et al.

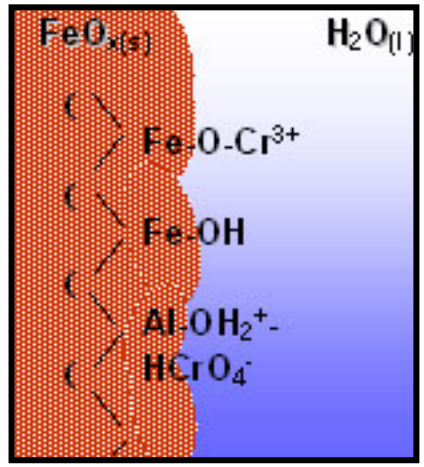


Oak Ridge FRC Contaminated Area

General Area Description

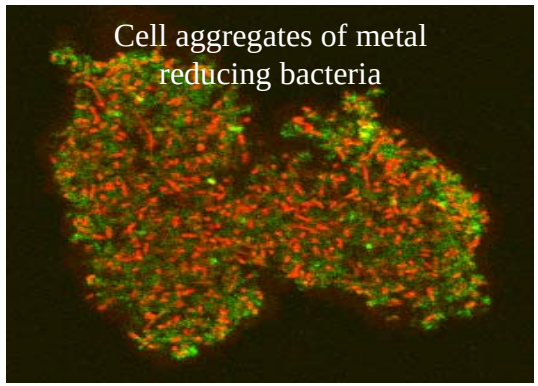
Waste Disposal Unit





Geology

Bedrock
Porosity
Overlying Saprolite



Hydrology

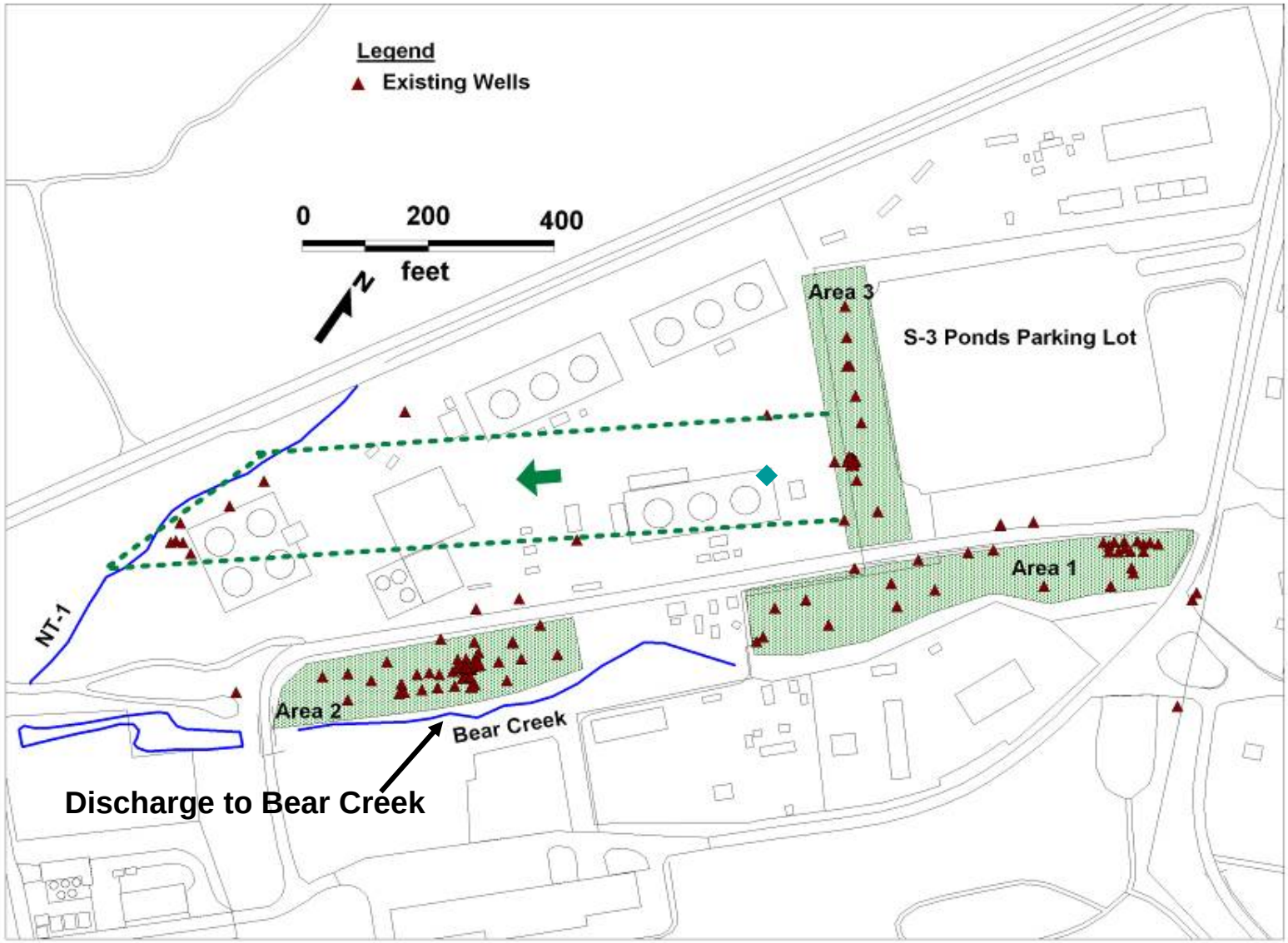
Recharge
General flow orientation
Groundwater flow in the unconsolidated zone and Nolichucky Shales
Groundwater flow in the Maynardville Limestone

Geochemistry

Soils and sediments
Groundwater

Microbiology

Hydrological, Geochemical, and Microbial Characterization of Areas 1, 2, and 3



Hydrological, Geochemical, and Microbial Characterization of Areas 1, 2, and 3

Geology and Hydrology

Geochemistry

Microbiology

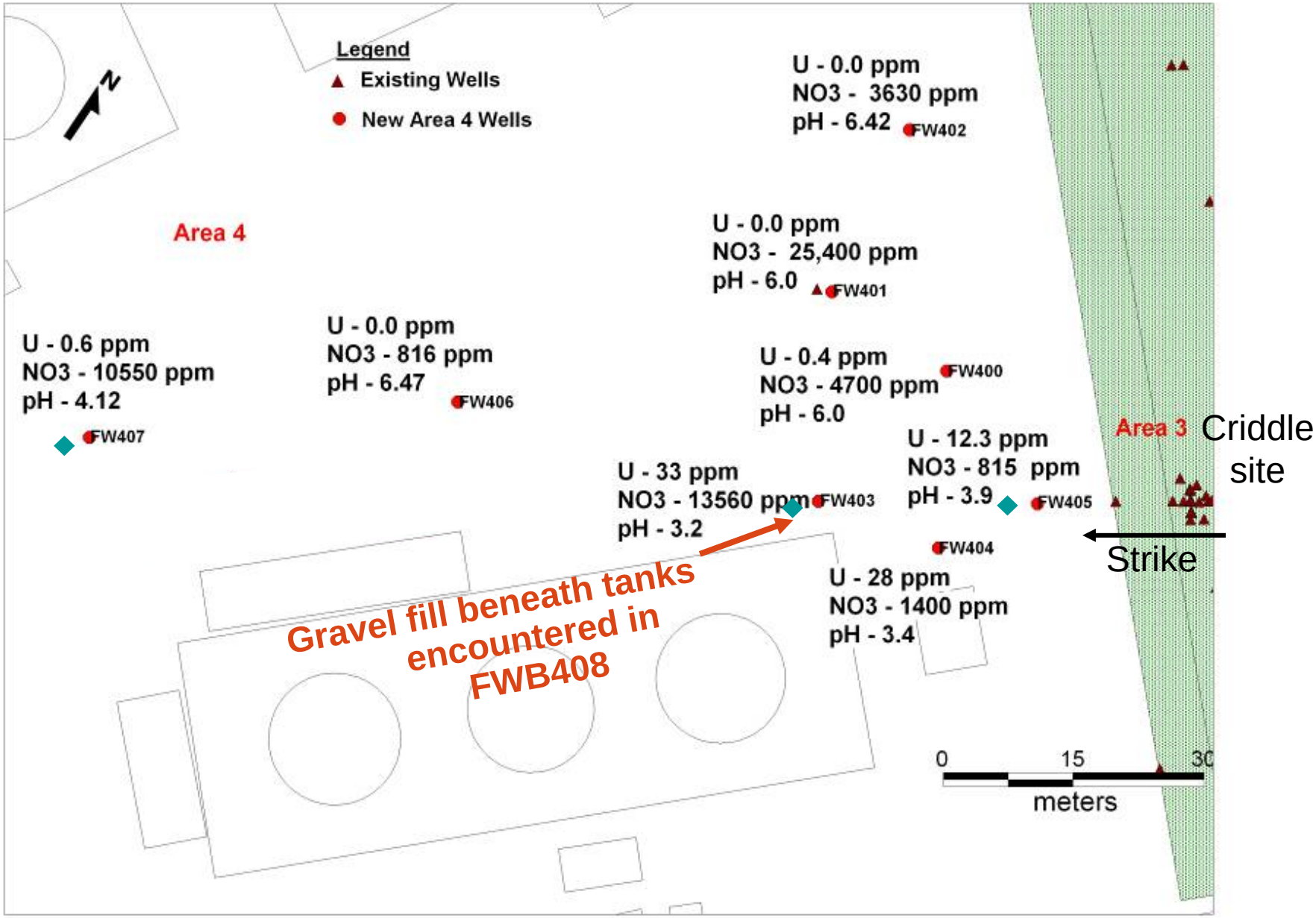
Sediments
Groundwater

Area 1: down-dip with moderate distance from source

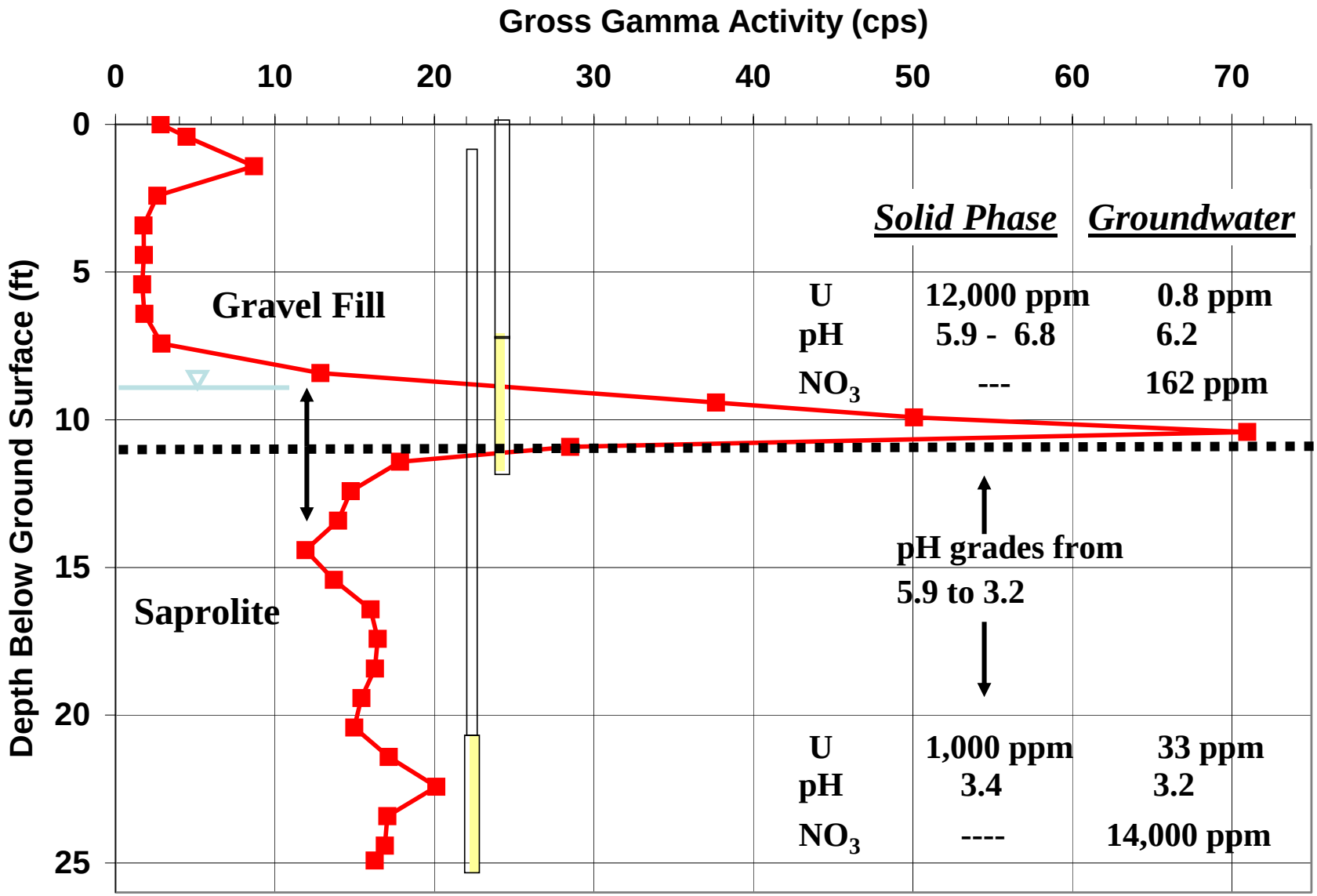
Area 3: Near-field U(VI) plume

Area 2: Far-field U(VI) plume in native weathered shale and fill

Area 4: Carbonate Gravel Fill Preferred Pathway



High U detected in Area 4 Dolomite Gravel Fill (FWB408)

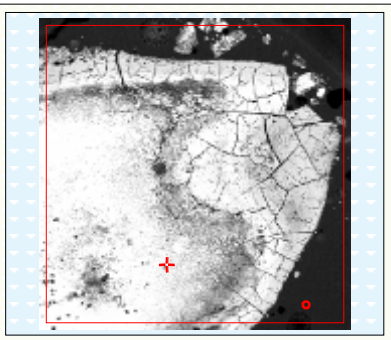


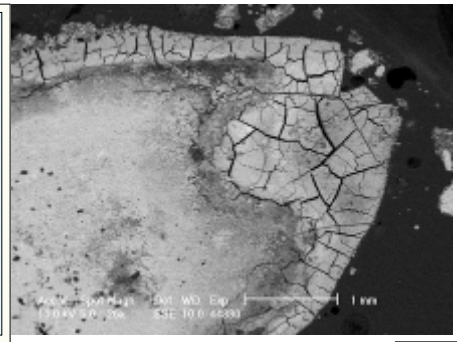
High U detected in Area 4 Dolomite Gravel Fill

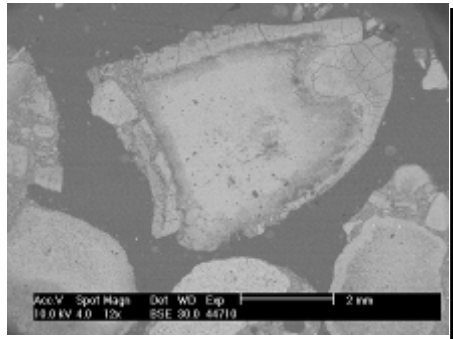
U co-precipitated with Al, S, and Si

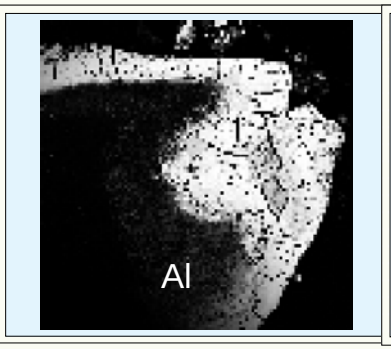
SEM-BSE element mapping

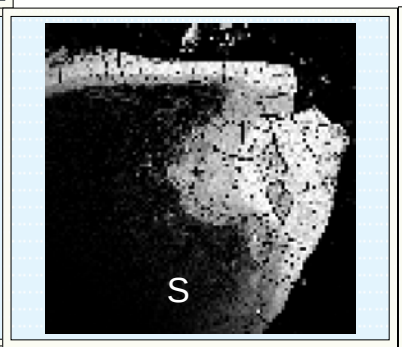
Saprolite/Gravel interface

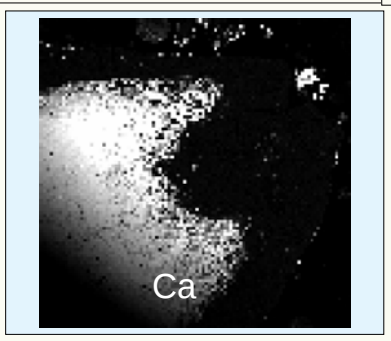


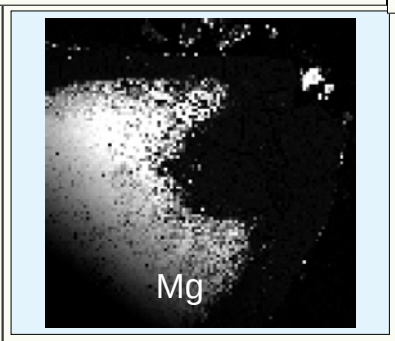


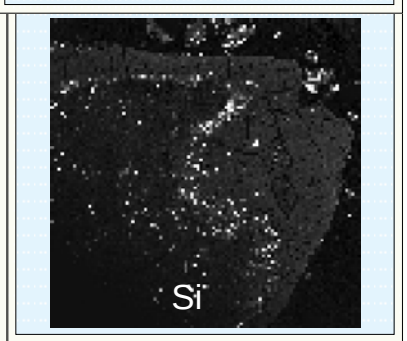


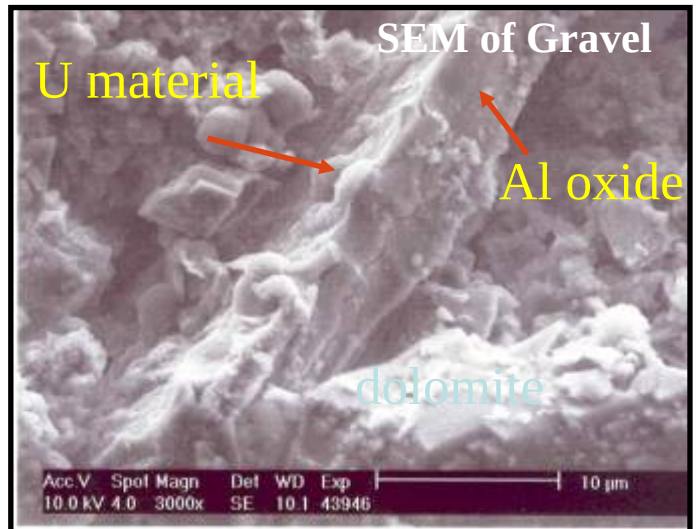






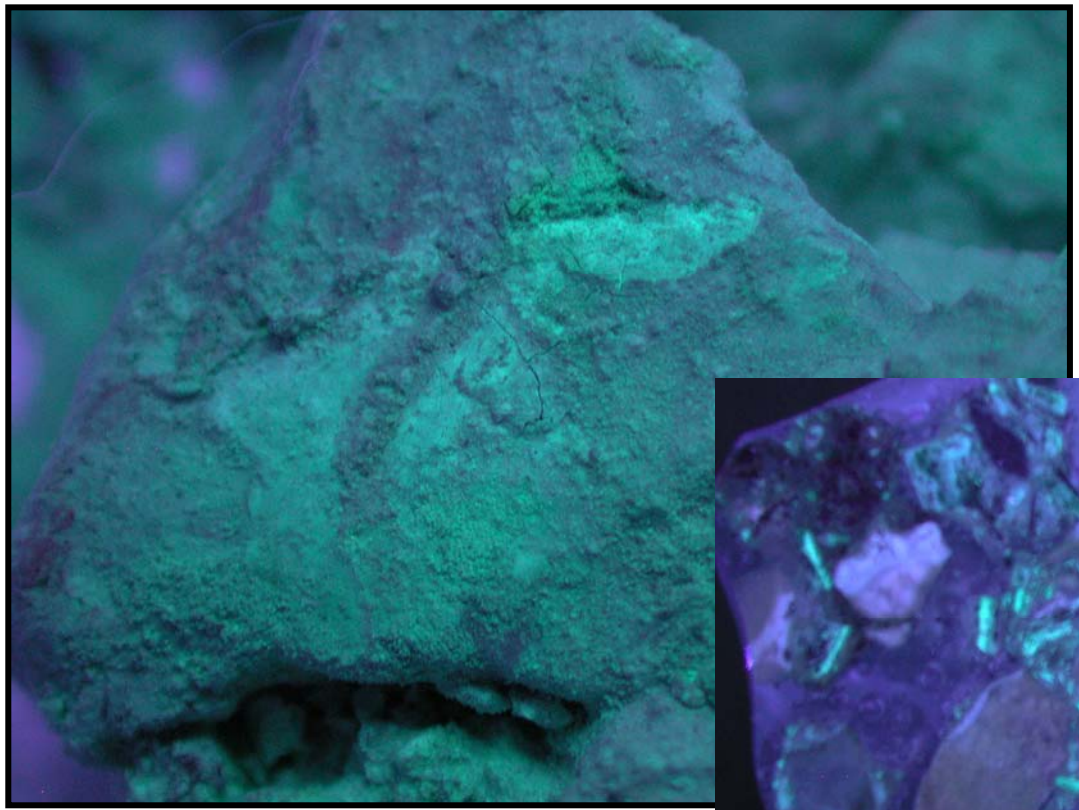






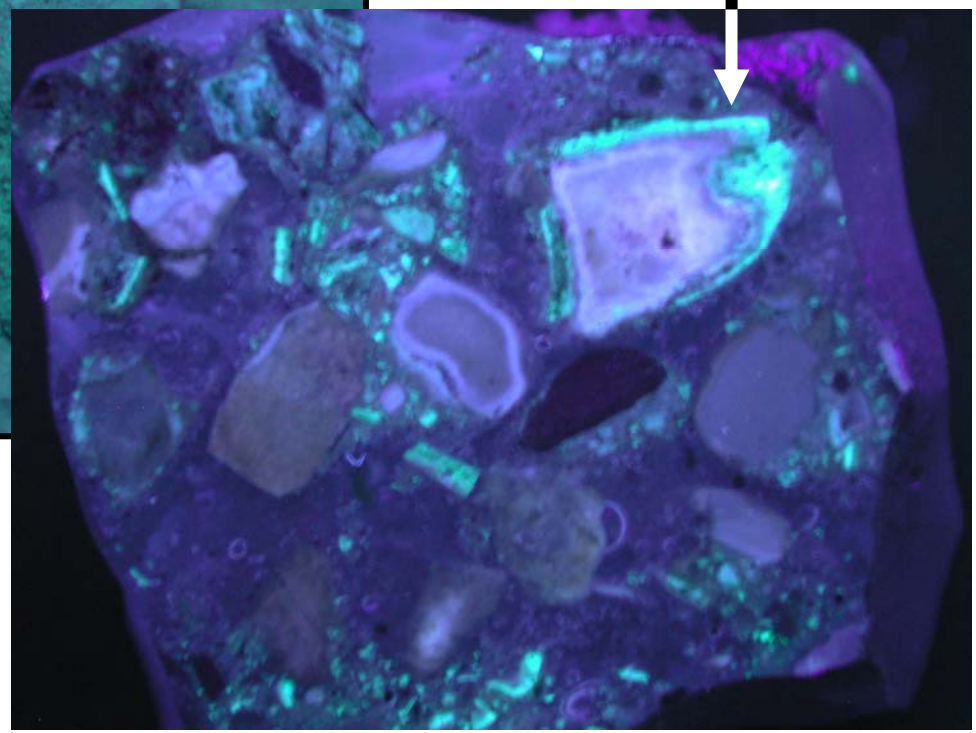
High U detected in Area 4 Dolomite Gravel Fill

Dolomite gravel under UV light



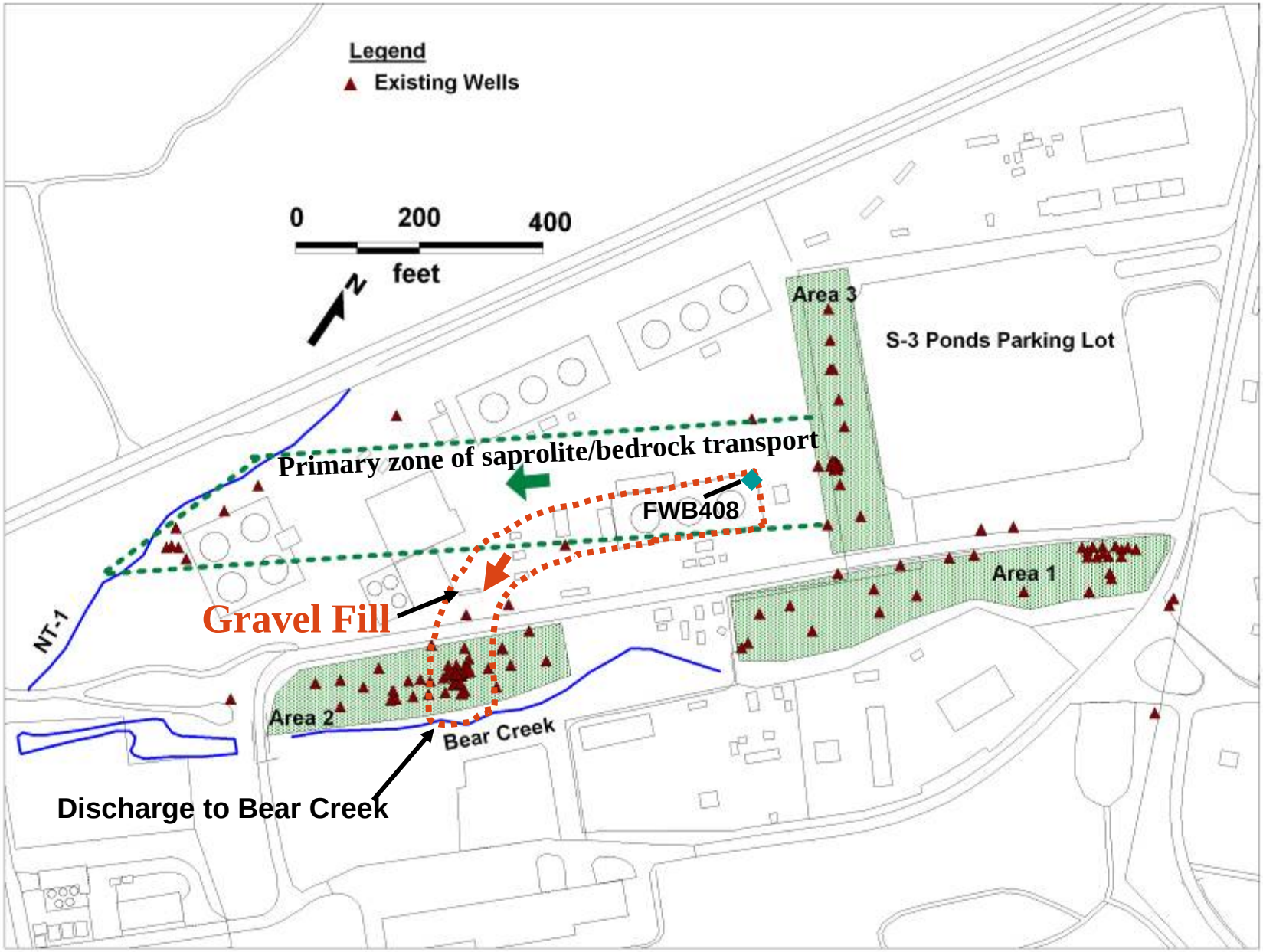
Solid phase U
>12,000 ppm

Thin section

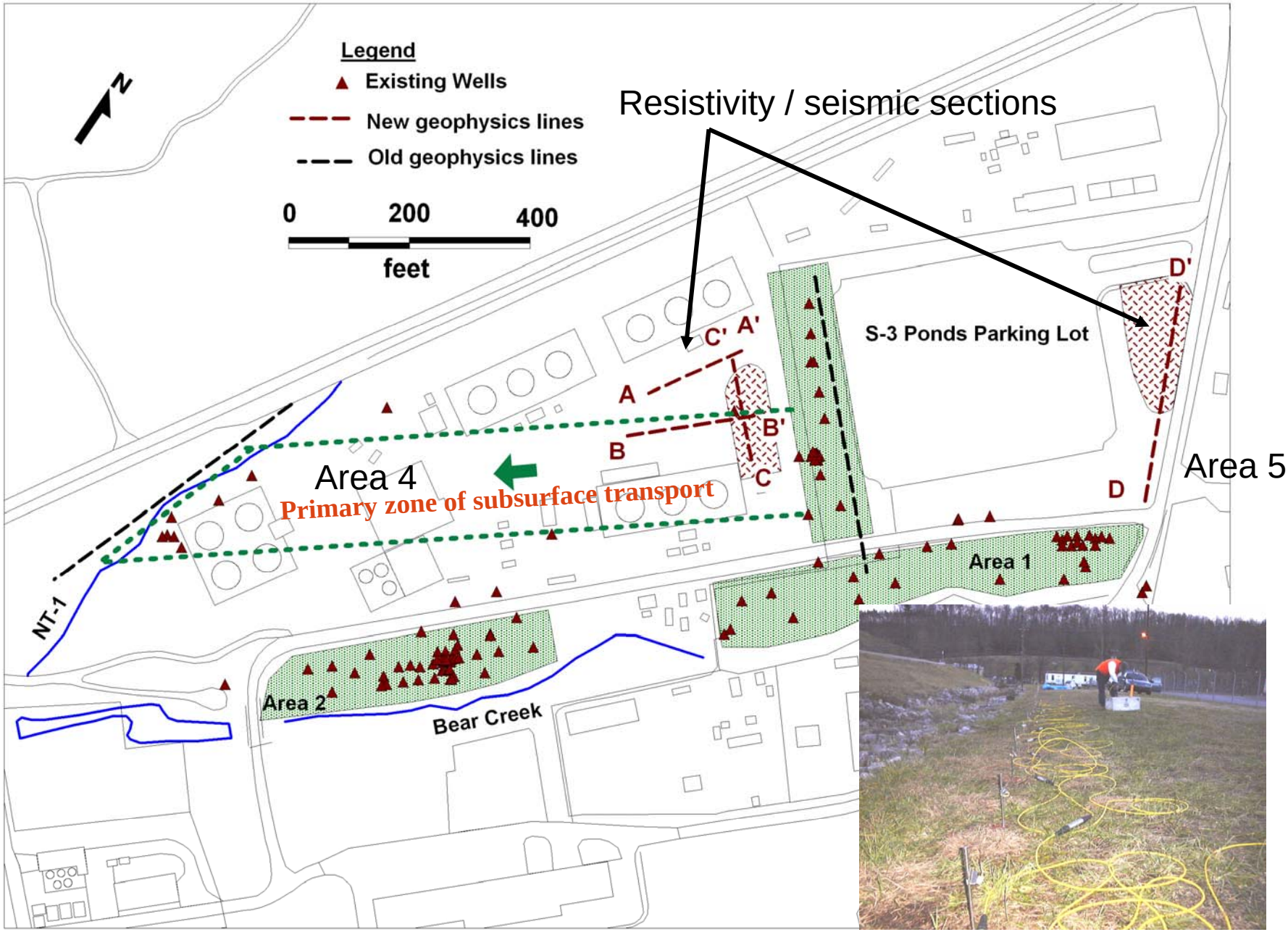


More than likely a U-Al-S-Si-OH amorphous solid phase (say what?)

Extent of Shallow Gravel Preferred Pathway

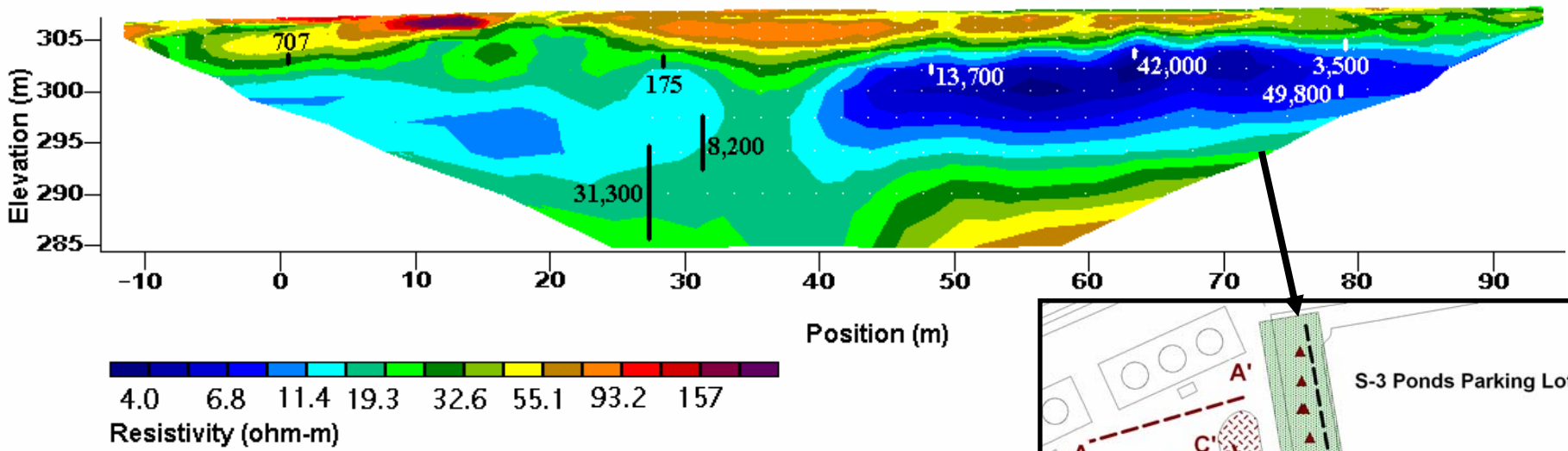


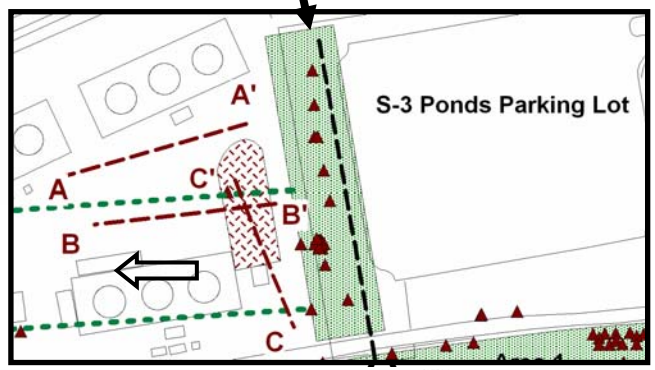
Area 4: Saprolite/Bedrock Preferred Pathway



Resistivity Sections Near S-3 Ponds

Area 3





North-South section E-E':
Direction of flow into page

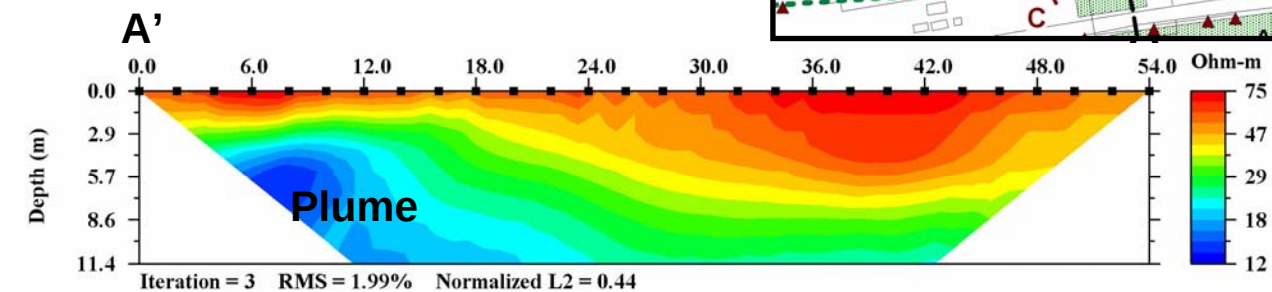
Area 4

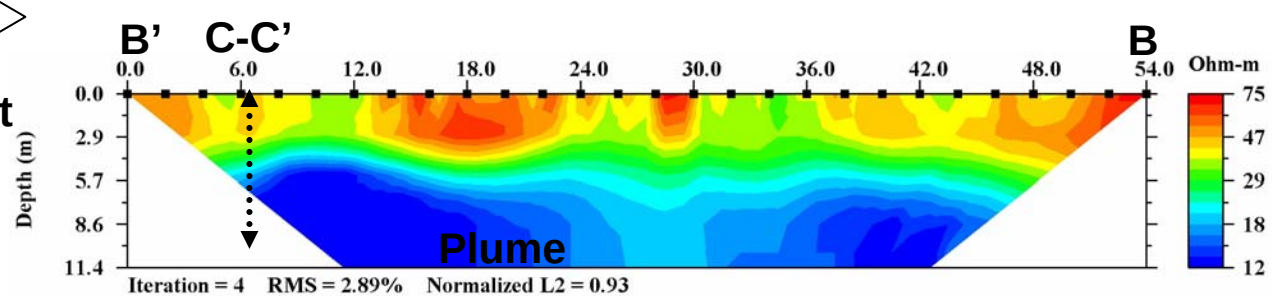
S-3 Ponds source

Northern transect outside pathway

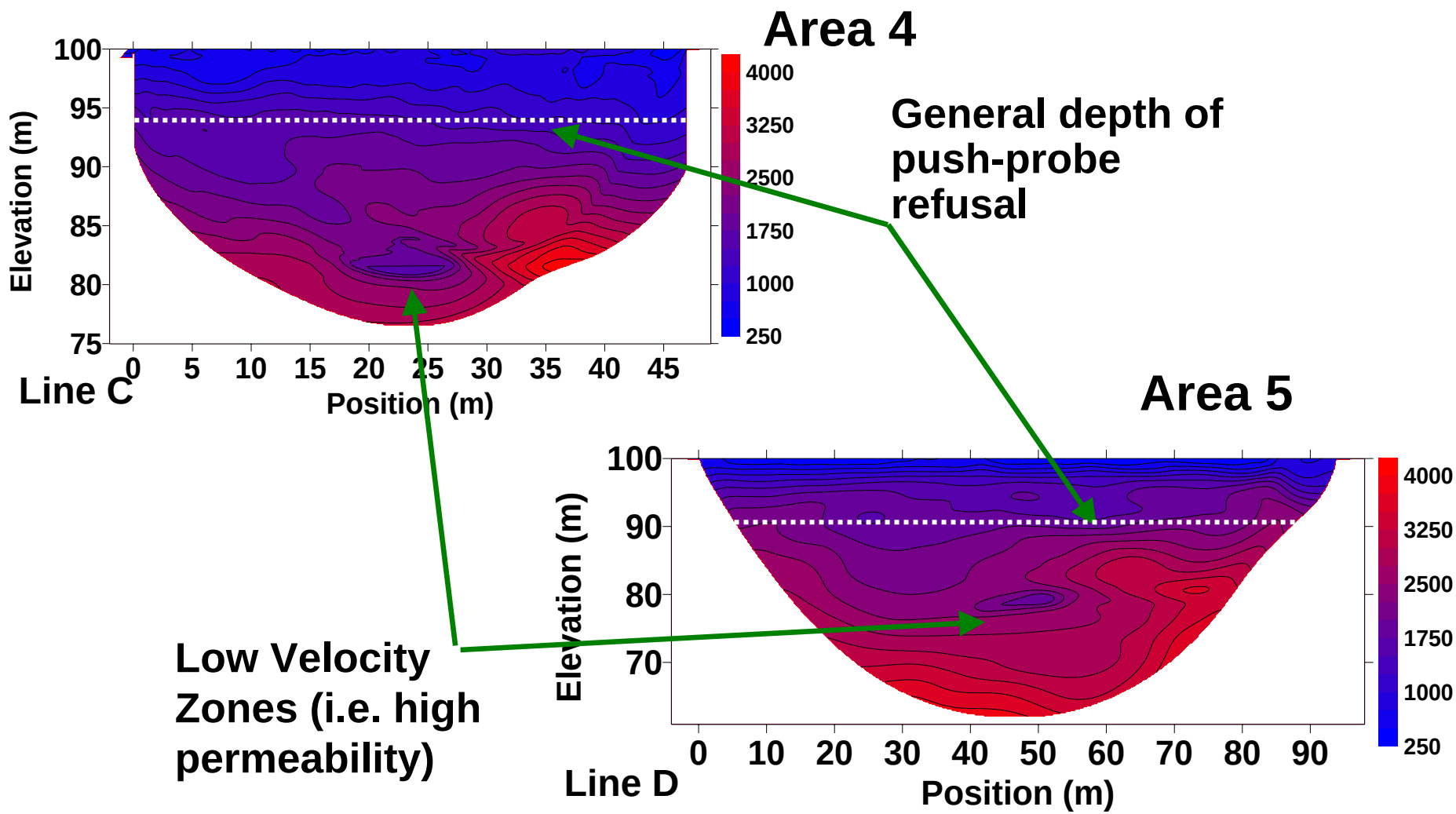
Flow direction

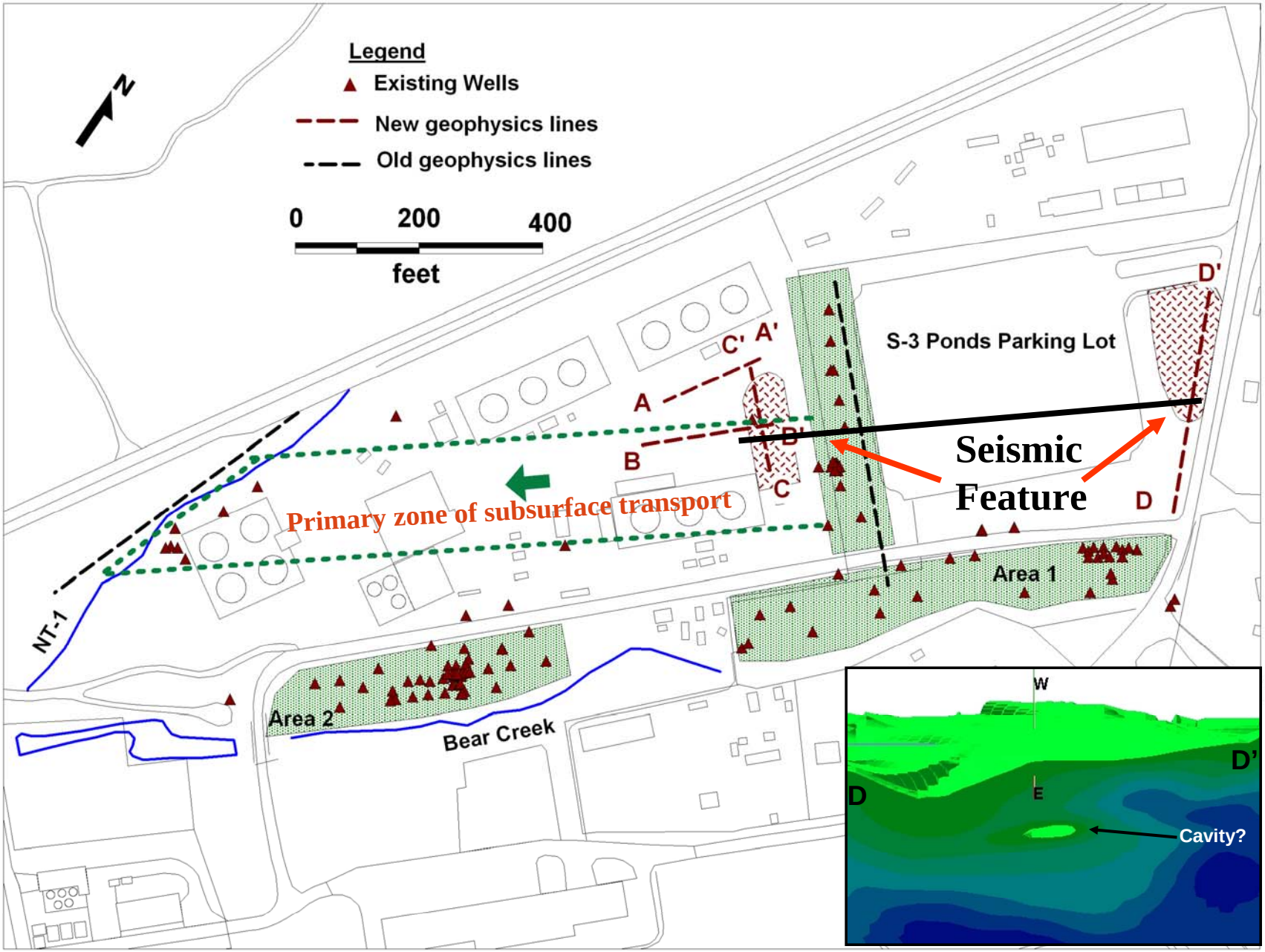
Southern transect inside pathway





Area 4 and 5 Seismic Tomography Results

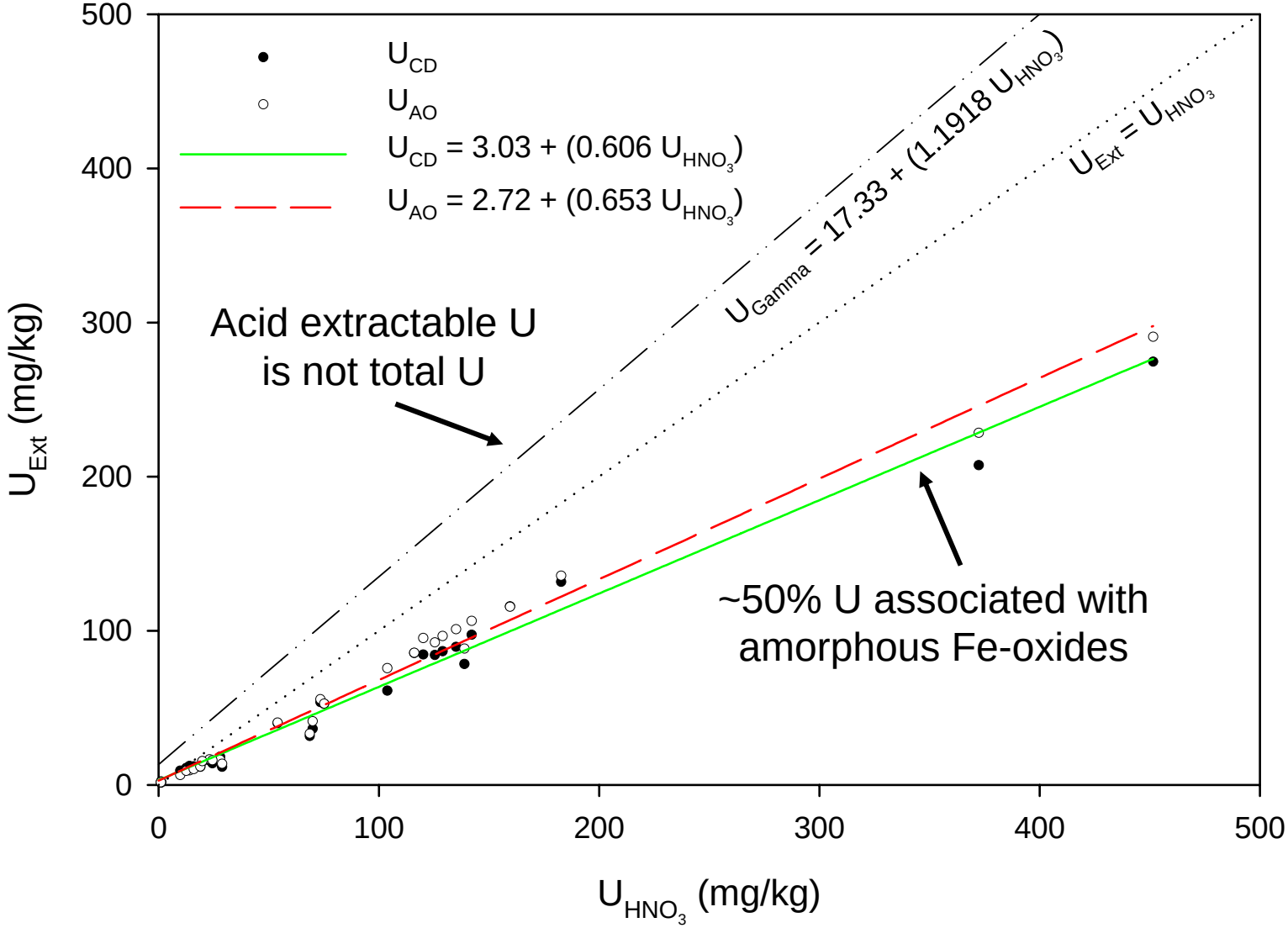




Seismic Feature Identified

Efficiency of Uranium Extractions

(Area 2 sediments)



RESEARCH NEEDS AT THE OAK RIDGE FIELD RESEARCH CENTER

General Microbiological Research Needs Across all the Contaminated Sites
General Hydrological Research Needs Across all the Contaminated Sites
General Geochemical Research Needs Across all the Contaminated Sites
General Numerical Research Needs Across all the Contaminated Sites

Future Needs: Unified Computational Approaches to Upscaling Subsurface Contaminant Transport (how do we pull it all together?)

-Pull together multi-scale experimental data

-Using existing multi-component, multi-process numerical models

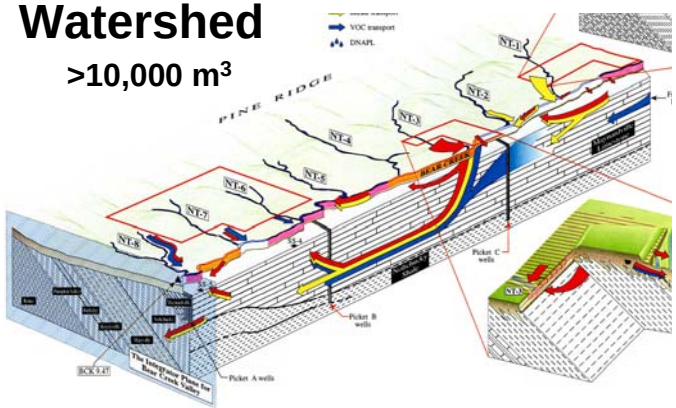
-Need for improved upscaling techniques

Field

10-10,000 m^3

Watershed

>10,000 m^3



Pedon

1-10 m^3

Undisturbed soil column

0.001-1 m^3

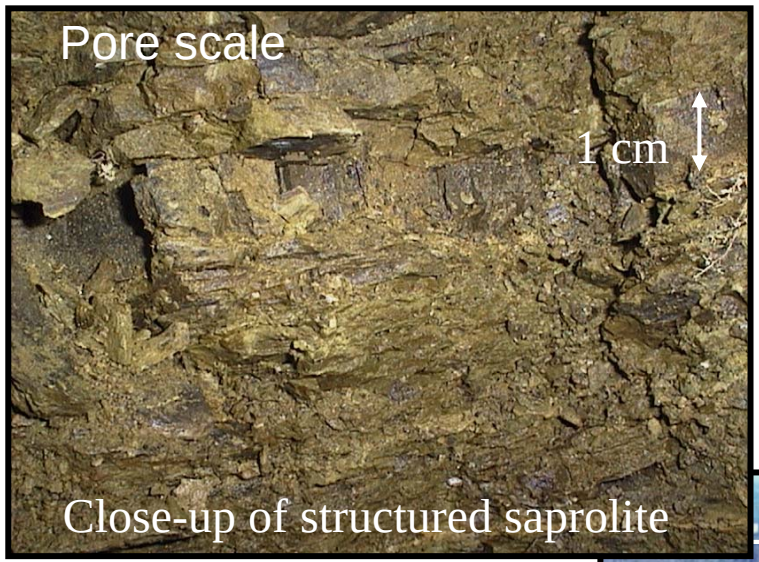
Multi-scale modeling

Batch Disturbed core

<0.001 m^3

Oak Ridge FRC scaling issues

cm scale matrix blocks
surrounded by fractures



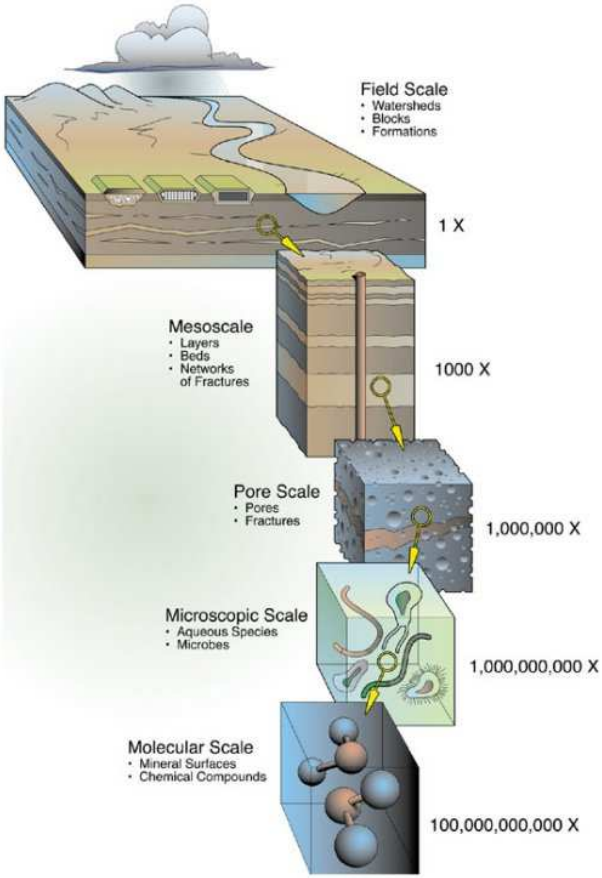
Scale up results in increased heterogeneity in physicochemical processes with new phenomena captured (e.g. macroscopic geologic features such as bed dip and topography, convergent flow).

Watershed and regional scale

Convergent flow and formation of empherial and perennial streams

(Discuss other examples)

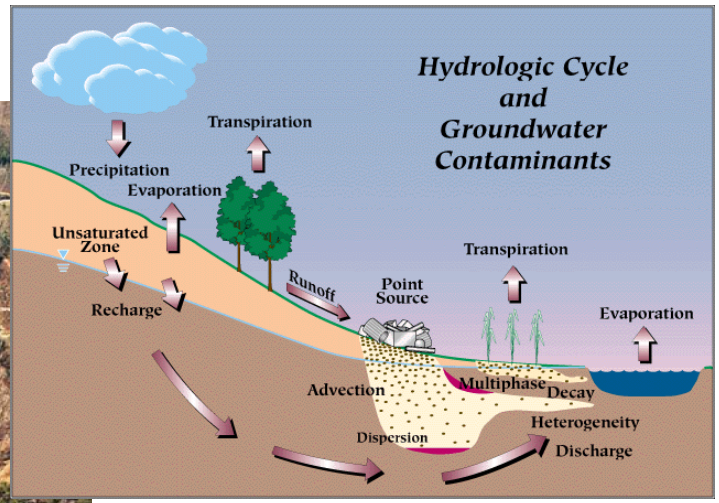
Basic science needs related to process scaling

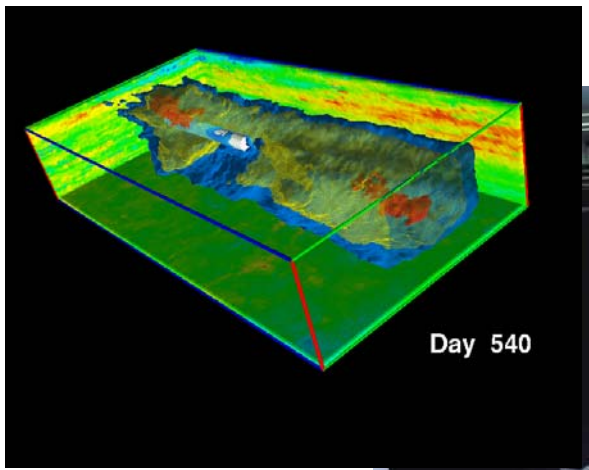


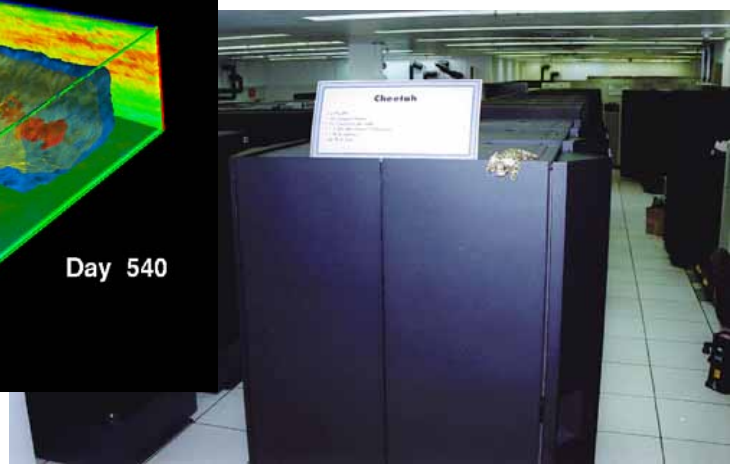
New experimental and predictive understanding of field-scale contaminant behavior

- Characterization of multiscale variability of properties.
- Identification of critical parameters that control contaminant plume migration and that need to be up-scaled to field/landscape scale (e.g. permeability's, mass transfer coefficients).
- Scale-up of fundamental physical, chemical and biological processes to field scale representations using improved techniques (e.g. fractal analysis, percolation theory, neural-network pedotransfer functions).
- Field-scale experimental research that focuses on the interaction of coupled hydrological, geochemical, and microbial processes on contaminant fate and transport.
- Applying molecular analytical techniques (e.g. synchrotrons, neutrons, electron sources) to macroscopic scale, undisturbed samples in an effort to better relate observations to the field.
- Close integration of experimental and numerical endeavors.

Future needs: Continued improvement of conceptual models and better integration with subsurface computing







Rationale: Contaminated site characterization and long-term monitoring will require the need for multiprocess, multicomponent validated numerical models and data sets to assess large scale, long-term fate and transport issues with an increased degree of certainty.

Watershed scale experimental endeavors to define important processes and provide parameterization to high performance computer models.

Understanding and using natural attenuation and enhanced natural attenuation

Development of new containment and remediation technologies / strategies

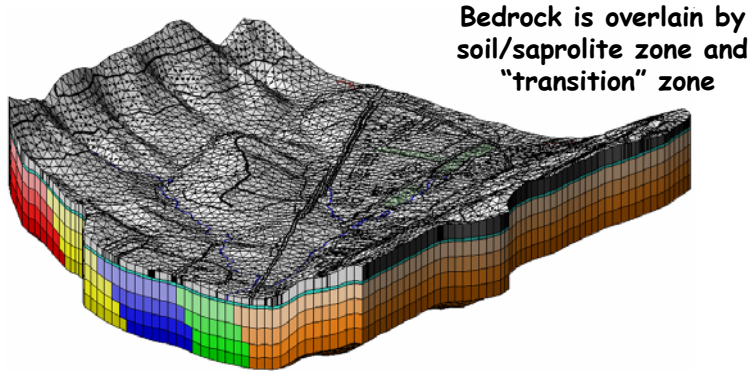
Site-Wide Numerical Model

Formulation of a site wide high-performance multiprocess, multipermeability flow and transport numerical model (Parker).

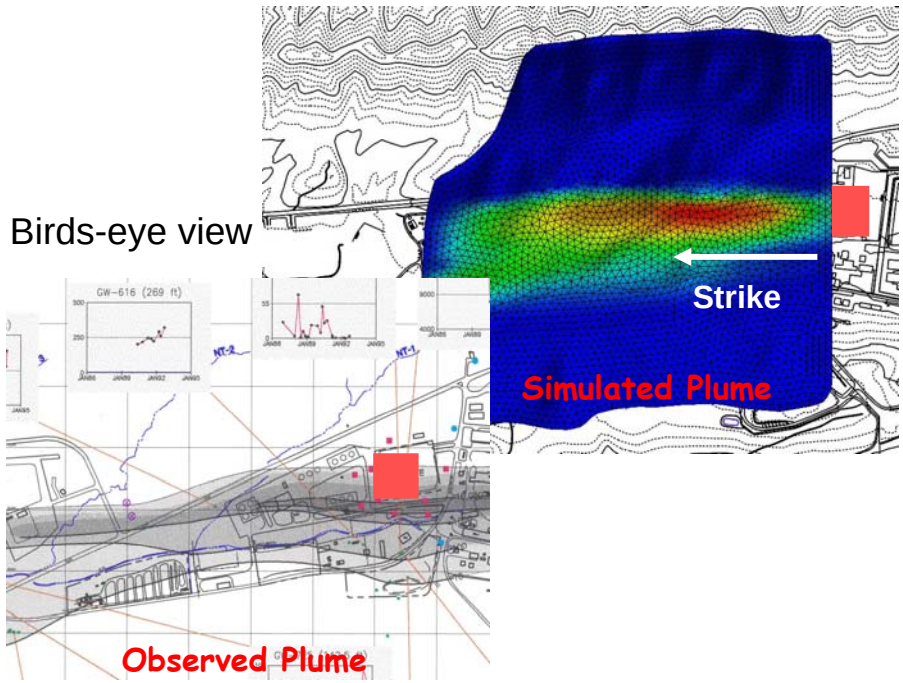
The FRC conceptual model provides the framework for the site wide numerical model.

Parameterized with experimental data acquired from the various research activities at the FRC and that are being organized within the working groups.

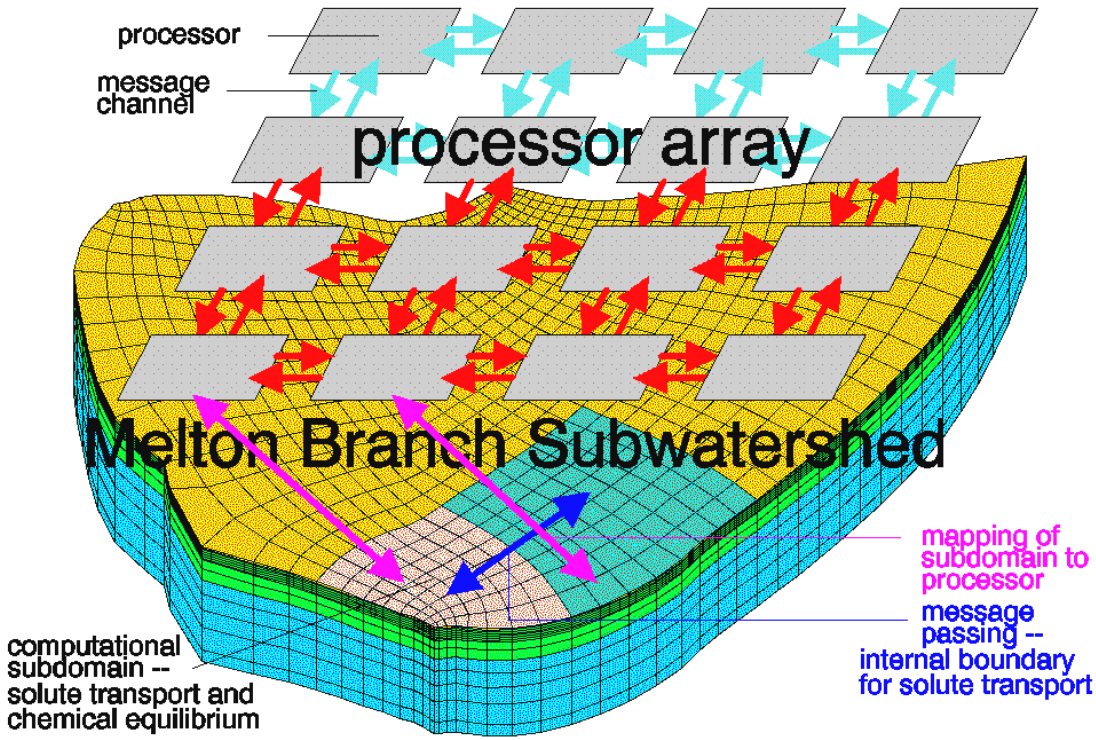
Discretized Model Domain



Birds-eye view



Link to high performance fate and transport modeling seems imperative



Watershed-scale models are built with imperfect information of the subsurface and uncertainties associated with model parameters and processes.

High-performance computing is necessary for quantifying parameter uncertainties when using mechanistically rigorous transport models at the field scale.

Multiprocess and inverse modeling (calibration) coupled with sensitivity analysis at large scales will need significant computational power.

Parallel processing supercomputers provide the capability of solving larger, more realistic problems faster and more economically.

Basic science needs associated with conceptual and numerical models

Comprehensive field-scale experimental data sets that quantify key processes that are necessary for model parameterization. Typically, limitations are data access/availability, not models or computational efficiency.

Aggressive coupling of multiscale experimental datasets that encompass coupled chemical, physical, hydrological, and microbial processes.

Sensitivity analysis of existing models should be used to guide and prioritize future site efforts.

Include new science in set of codes maintained for usability, high performance, extensibility, and portability.

Efficient mathematical alternatives to brute force methods.

Flexible and adaptive treatment of boundaries and moving fronts.

Software tools, utilities, and libraries for developing new simulation software and managing, analyzing, and visualizing large data sets.

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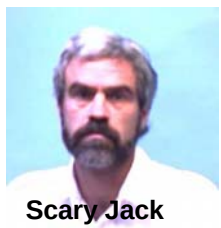
The Working Groups

Objective: To bring together scientists and engineers to resolve specific topical issues and work toward the overall goal of providing an improved understanding and predictive capability of the mechanisms that control microbially-mediated, *in situ* contaminant immobilization.

Four working groups have been established to implement collaborations and knowledge transfer among various projects associated with the Oak Ridge FRC.

(1) Microbial Community Analysis (Kostka)
(2) Rates of Microbially Mediated Metal Reduction and Oxidation (Burgos)
(3) Geochemical/Geophysical Characterization (Jardine)
(4) Numerical Modeling (Parker)



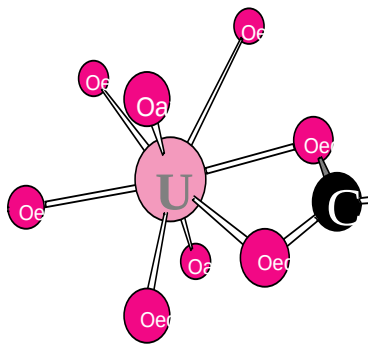
Geochemical/Geophysical Characterization Working Group (Leader: Phil Jardine)

Working Group goals

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.

Working group objectives:

To provide specific and general site characterization endeavors designed to quantify *in situ* aqueous and solid phase contaminant speciation.

To provide select physical, chemical, and mineralogical properties of the FRC groundwater and solid phase before and after biostimulation.