FRC Model Development

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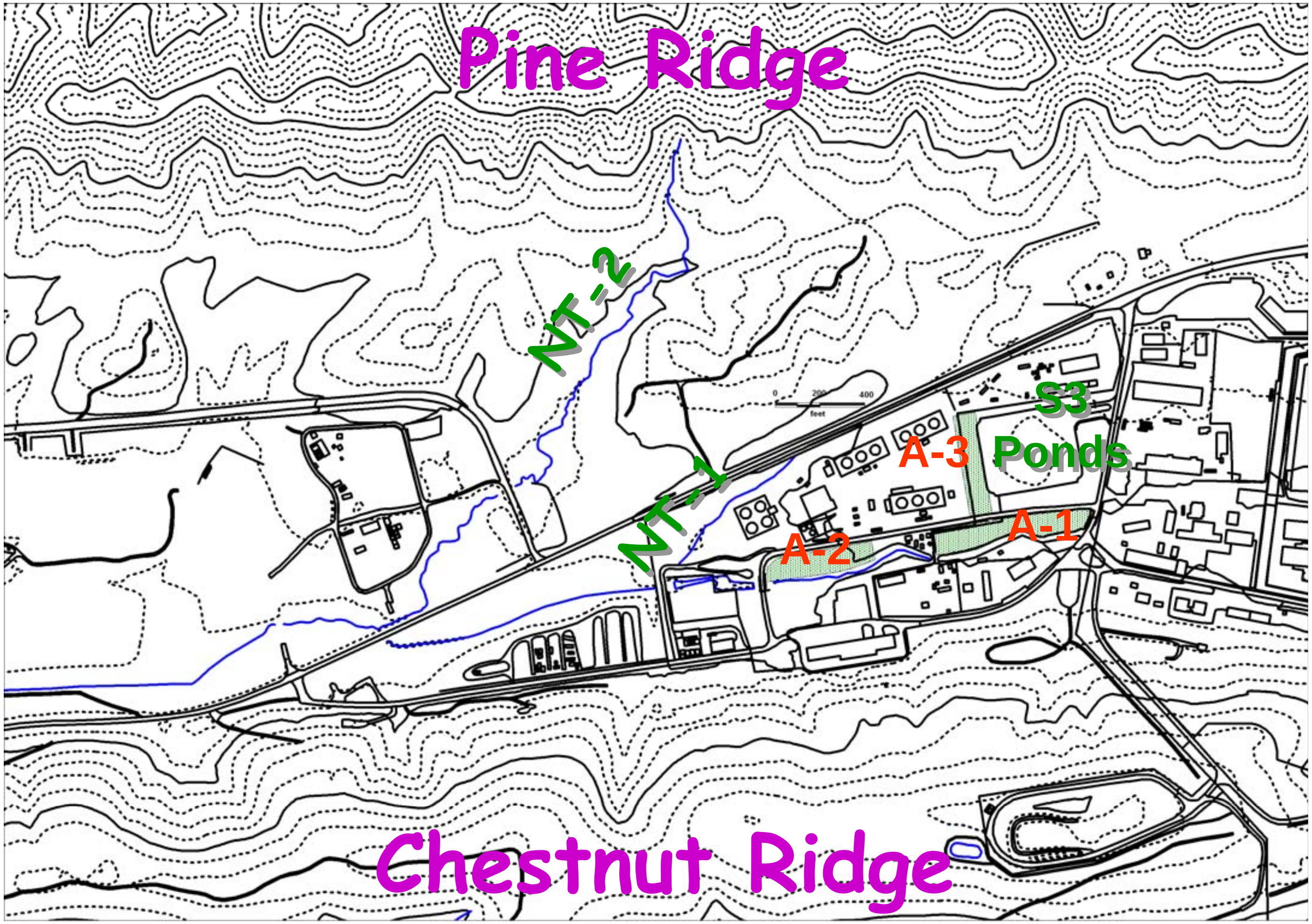
Site-Wide Modeling Effort Objectives

- Provide a means to interpret FRC site characterization data in an integrated manner to develop a more comprehensive understanding of the site
- Identify knowledge gaps to guide ongoing characterization efforts and to identify research priorities
- Quantitatively evaluate the validity of working hypotheses within the site conceptual model
- Provide a tool for NABIR PIs to define boundary conditions for plot areas and provide a modeling template for more detailed plot-scale modeling efforts

Modeling Approach

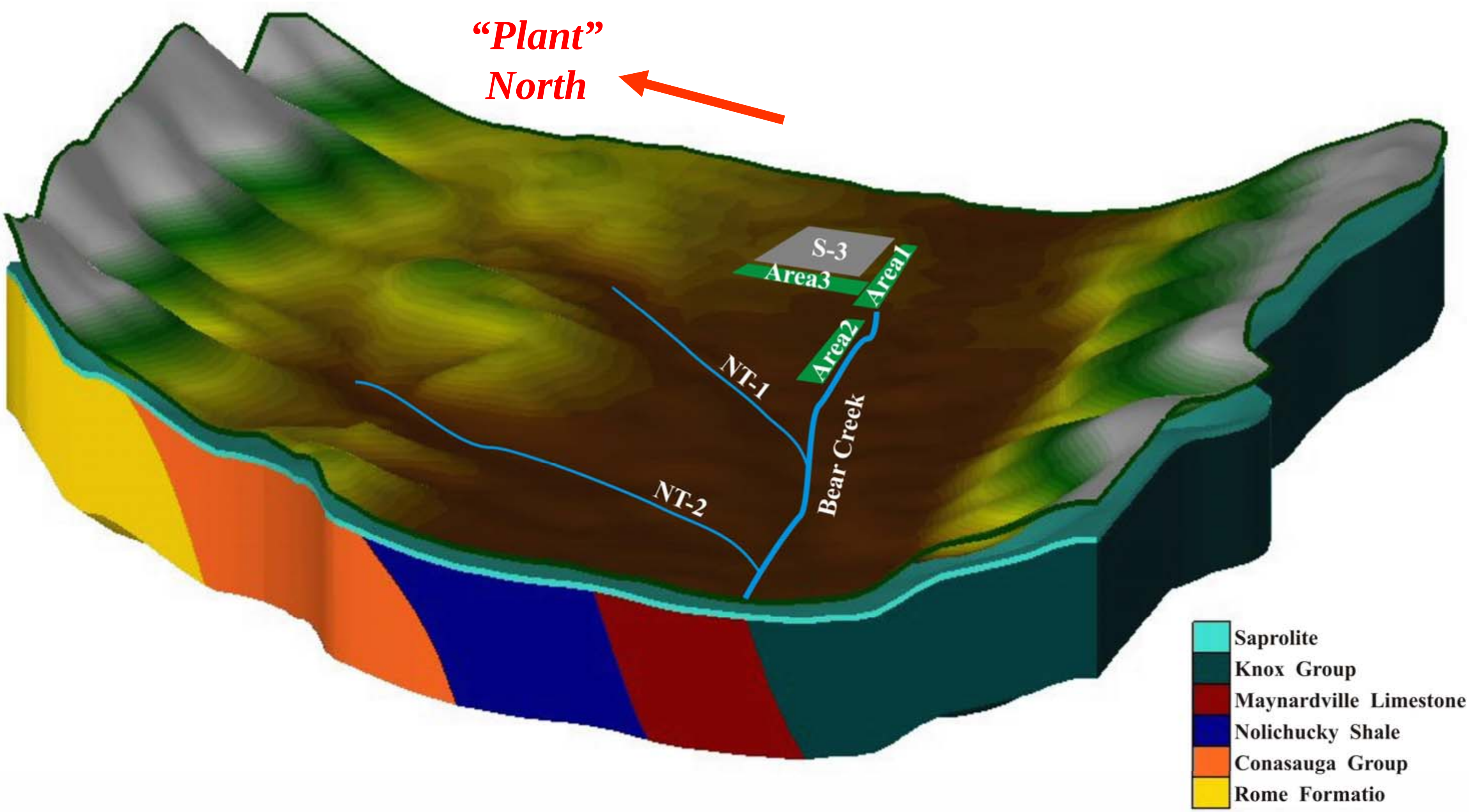
- Using HYDROGEOCHEM Version 5, which is an enhancement of HBGC123D
- Models 3D transient sat/unsat flow, heat transport, dissolved transport, and complex biogeochemical reactions
- Allows user-definable kinetic functions, which provides flexibility to adopt new formulations as our understanding improves
- Models fully anisotropic porous media suitable for representing densely fractured, dipping bedrock and saprolite

Overview of FRC Area



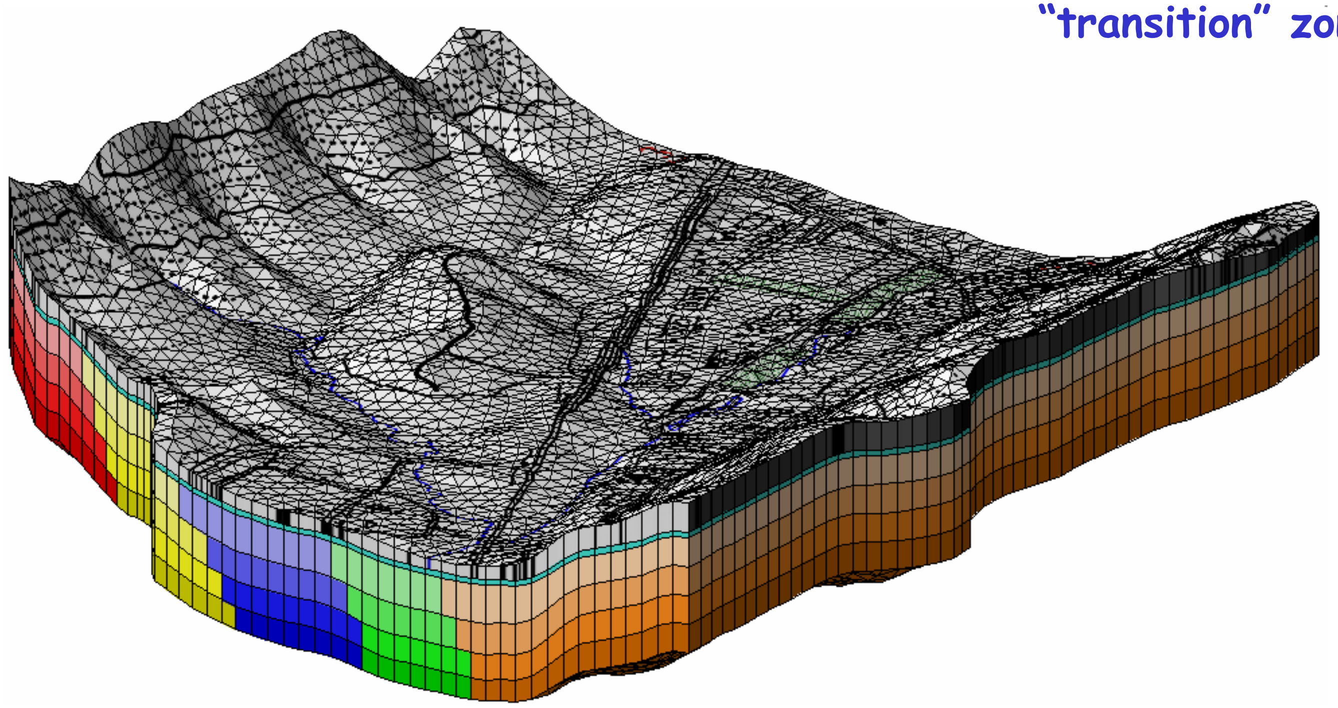
"Plant" North

Model Domain and Bedrock Geology



Discretized Model Domain

Bedrock is overlain by soil/saprolite zone and "transition" zone



Flow Model Calibration

- Recharge zones:
  - Hill slopes – 7.8 cm/yr
  - Valley (uncovered) – 2.5 cm/yr
  - Paved areas – 0 cm/yr
- Conductivity – anisotropy oriented w/ rock dip
  - Fill material (isotropic K = 2 m/d)
  - Saprolite
  - Transition zone
  - Rock units with $K(z) = K(0) \exp(-f\, z/z_T)$
  - where z_T= total thickness of all layers

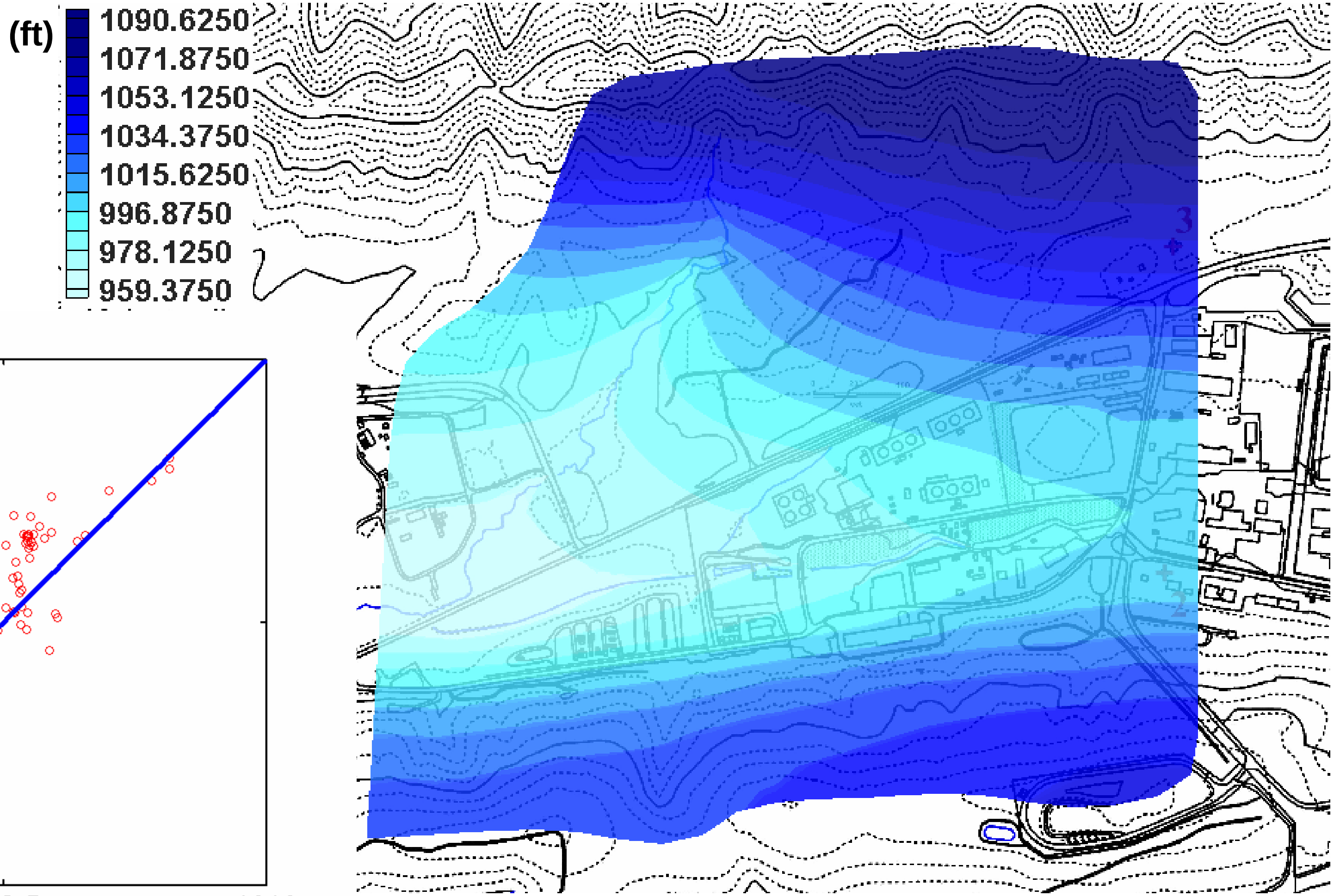
Calibration procedure

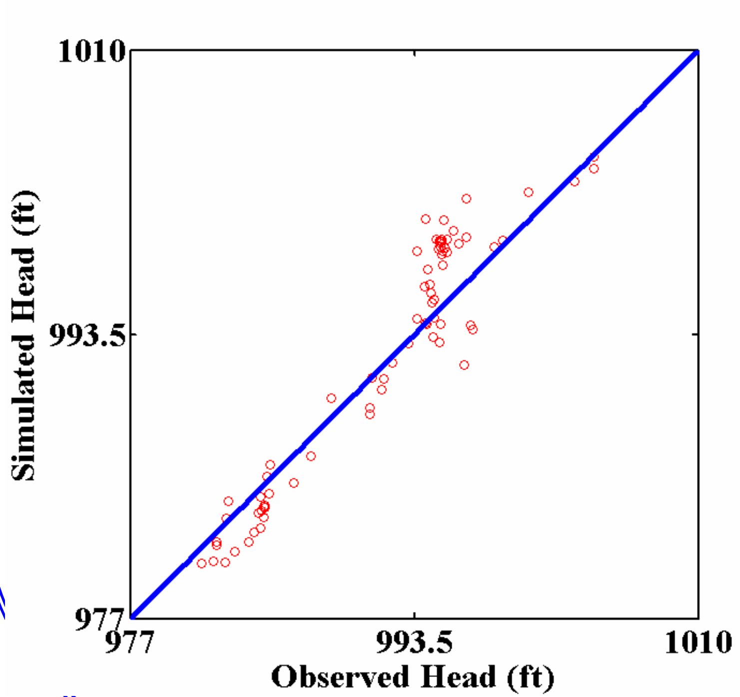
- Invert using nonlinear optimization code (PEST)
- Time-averaged water levels for 122 wells
- Average streamflow at Bear Creek NT-2 gauging station

Flow Model Calibration

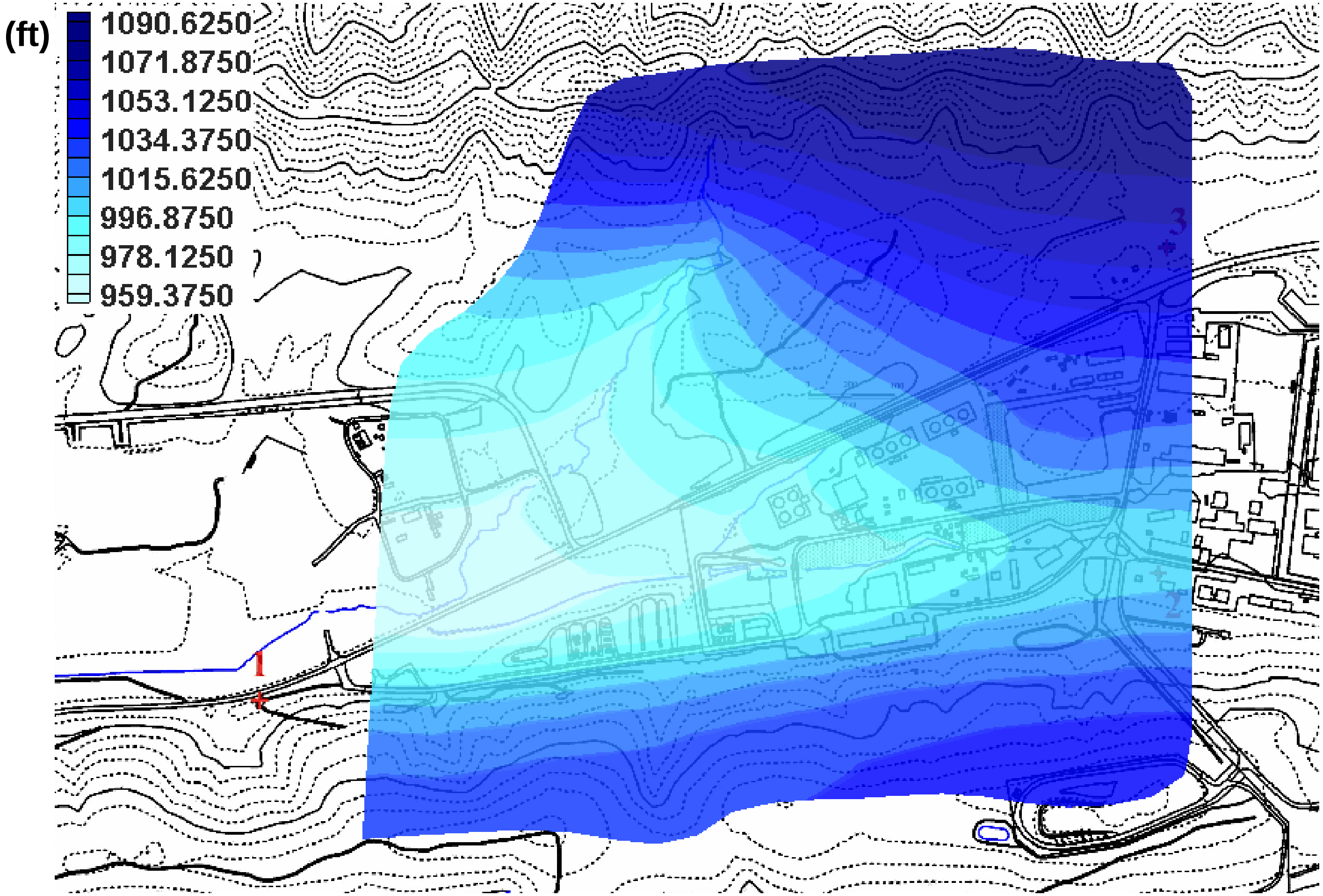
Unit	K_{strike} m/d	$K_{cross\text{-}bed}$ m/d	Depth factor
Saprolite	0.22	0.05	-
Transition	1.20	0.24	-
Knox Group	0.15	0.003	4.20
Maynardville Limestone	1.20	0.180	4.50
Nolichucky Shale	0.10	7.0E-04	3.50
Conasauga & Rome	7.5E-03	6.4E-09	4.50

Steady State Groundwater Flow Model Calibration





Predicted Groundwater Flow During S-3 Pond Operation (1951- 1983)



Transport Model Calibration

- S3 source data computed directly (no calibration) from

  Total nitrate content of S3 pond in 1962, 1975, 1978, 1981, 1983

  Average hydraulic discharge rate to ponds

  Measured nitrate concentration in 1978

- Fit longitudinal and transverse dispersivity and unit porosities to measured nitrate concentrations in monitoring wells (536 measurements)

Transport Model Calibration

Parameters calibrated

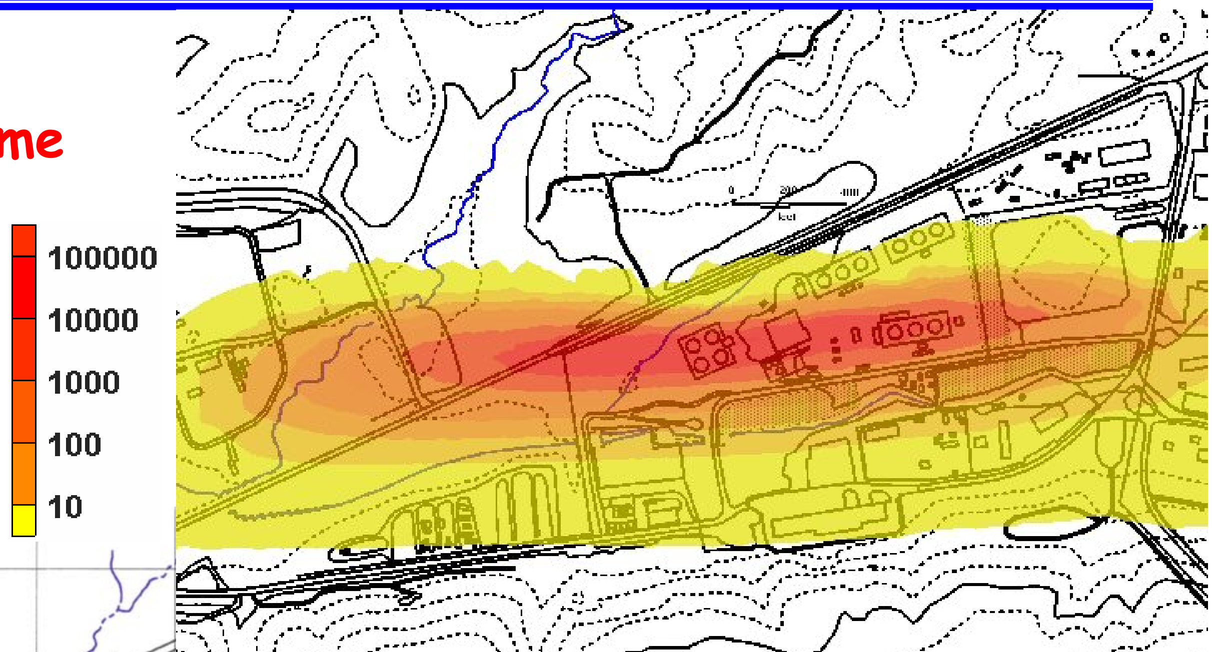
- Dispersitivites
  - A_L = 0.15 m
  - A_T = 0.003 m
  - note: A_L values from field tracer tests
    - 0.08-0.27 m Gwo et al. (1995, 1999)
    - 0.1 m Jardine et al. (1999)

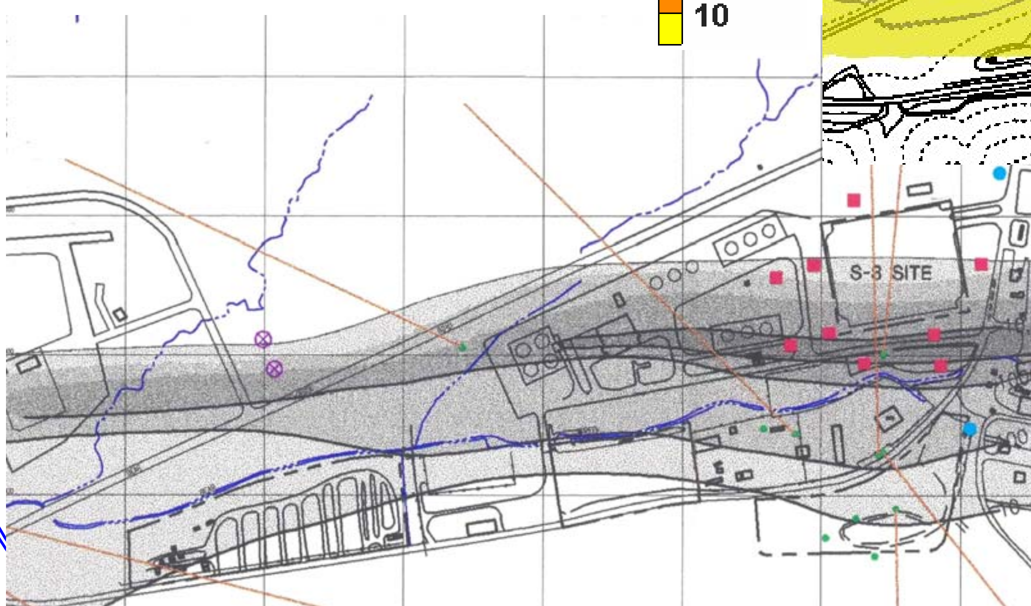
- Porosity
  - Saprolite: 0.45
  - Transition zone: 0.30
  - Rock units:
    - average porosity for top rock layer = 0.10
    - average depth reduction factor = 3

$$\theta = \theta(0) \exp(-f\, z/z_T)$$

Nitrate Transport Model

Simulated Plume

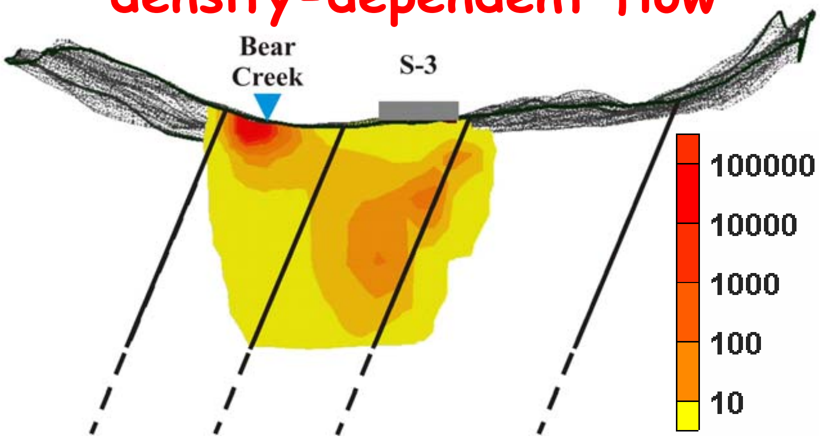




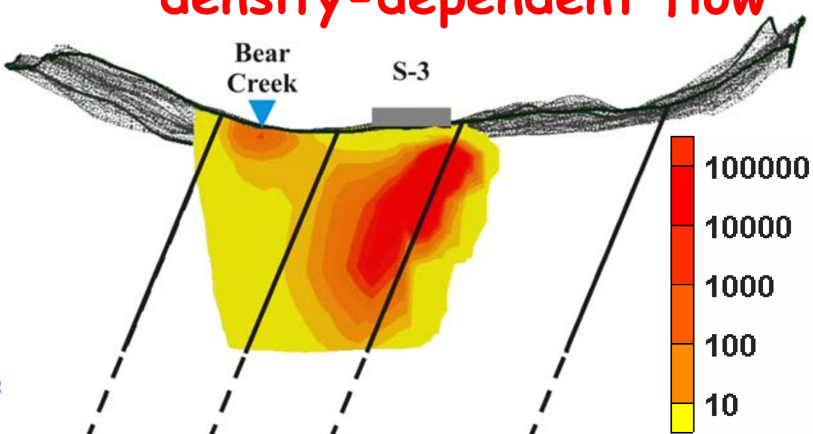
Observed Plume

Nitrate Transport Model Results, ca. 1995

Simulated plume without density-dependent flow

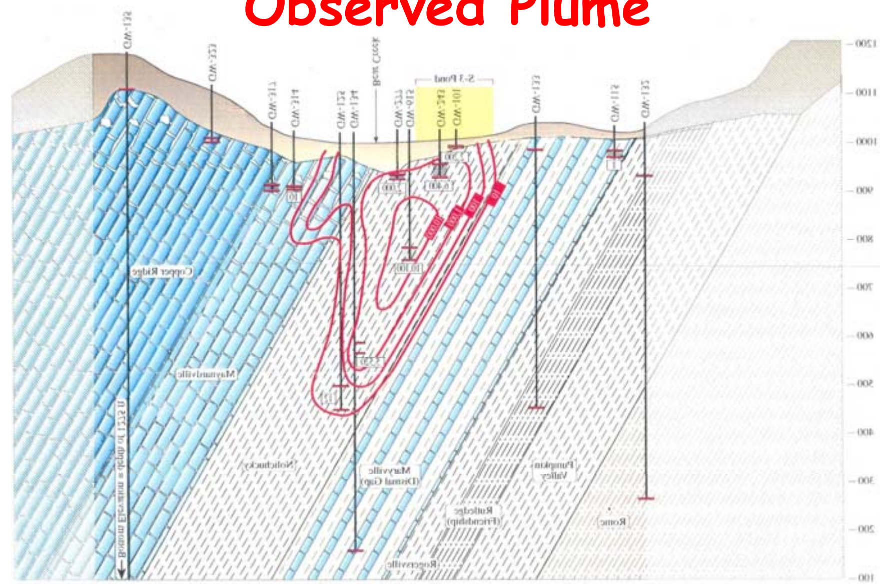


Simulated plume with density-dependent flow



Density-driven flow moves nitrate plume deeper near source as observed and impedes subsequent flushing

Observed Plume



Preliminary Geochemical Modeling Studies

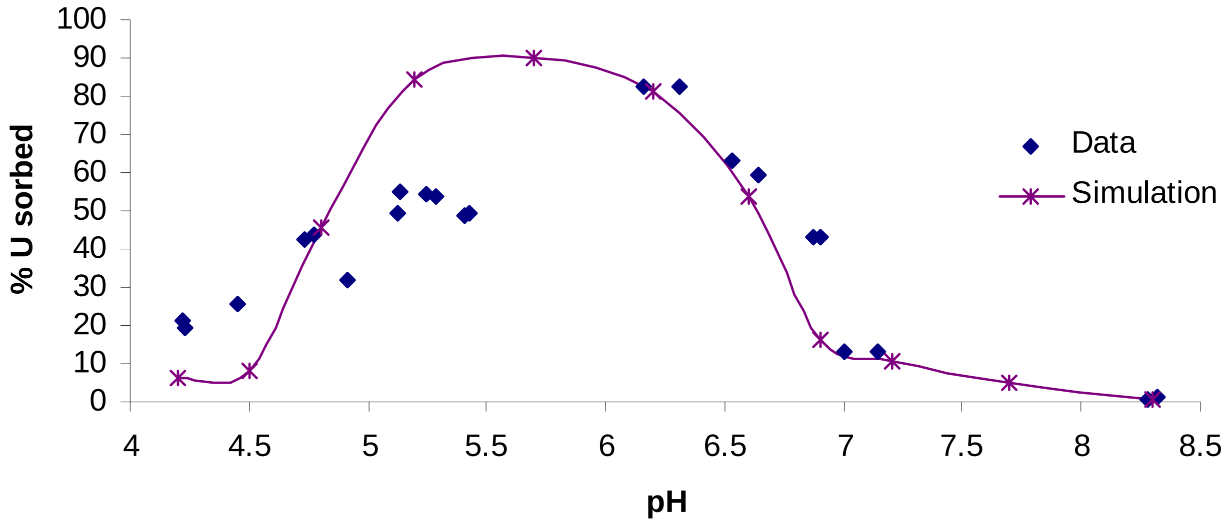
Objective: Determine if HGC v5 can predict uranium geochemistry using simple published reaction networks

- Evaluate predictions of pH-dependent U(VI) adsorption determined in batch experiments
- Simulate effluent elution curves from packed soil column experiments
- Simulate effluent breakthrough from undisturbed soil columns

(See poster by Fan Zhang for details)

Uranium Batch Adsorption Study

Simulate uranium adsorption with HGC v5 using equilibrium reaction network of Waite et al. (1994)

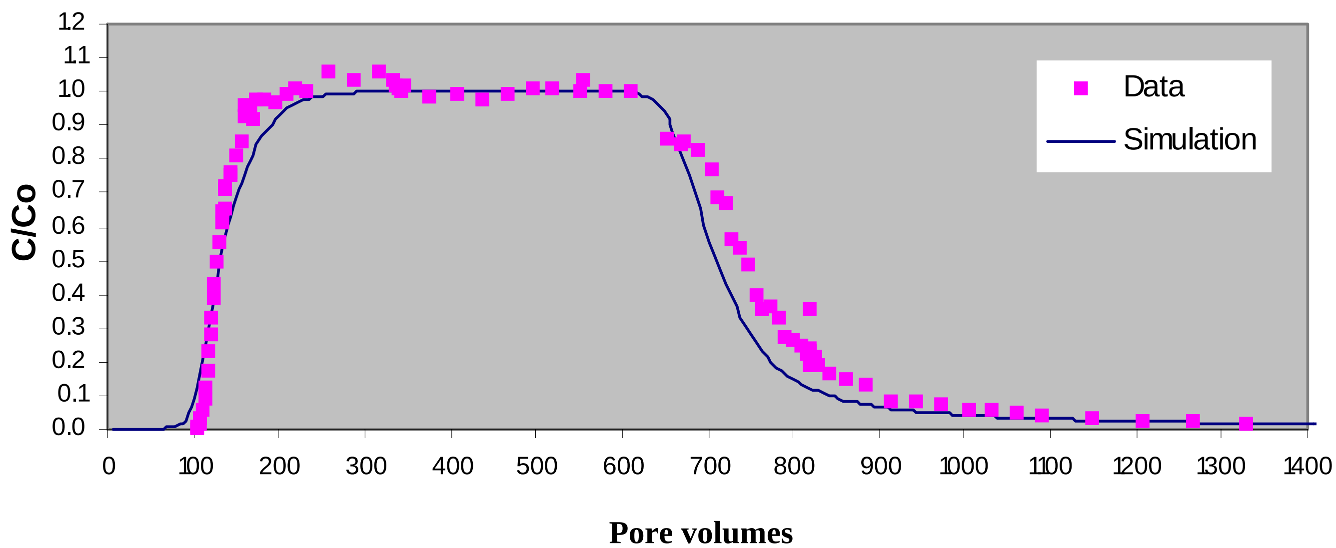


Adsorption on homogeneous synthetic soil material

(data from Scott Brooks' group)

Uranium BTC in Packed Soil Column

Simulate uranium breakthrough from packed soil column using Waite equilibrium rx network. Dispersion coefficient only fitted to data.

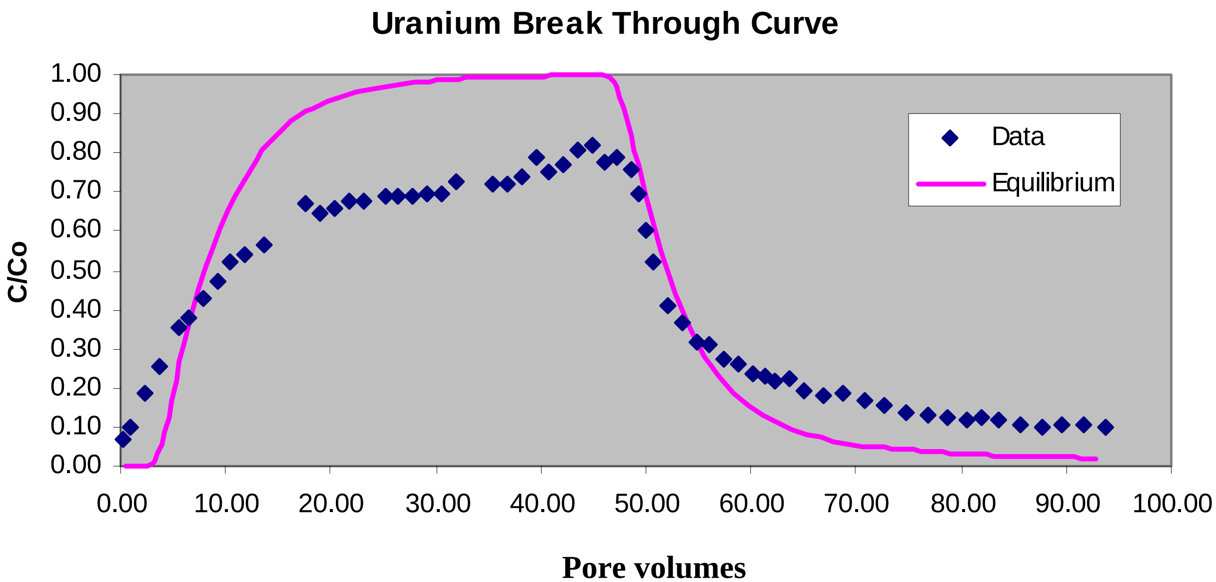


Same soil material as batch study

(data from Scott Brooks' group)

Uranium BTC for Undisturbed Soil Column

Same reaction network assuming local equilibrium didn't work as well for the undisturbed soil column

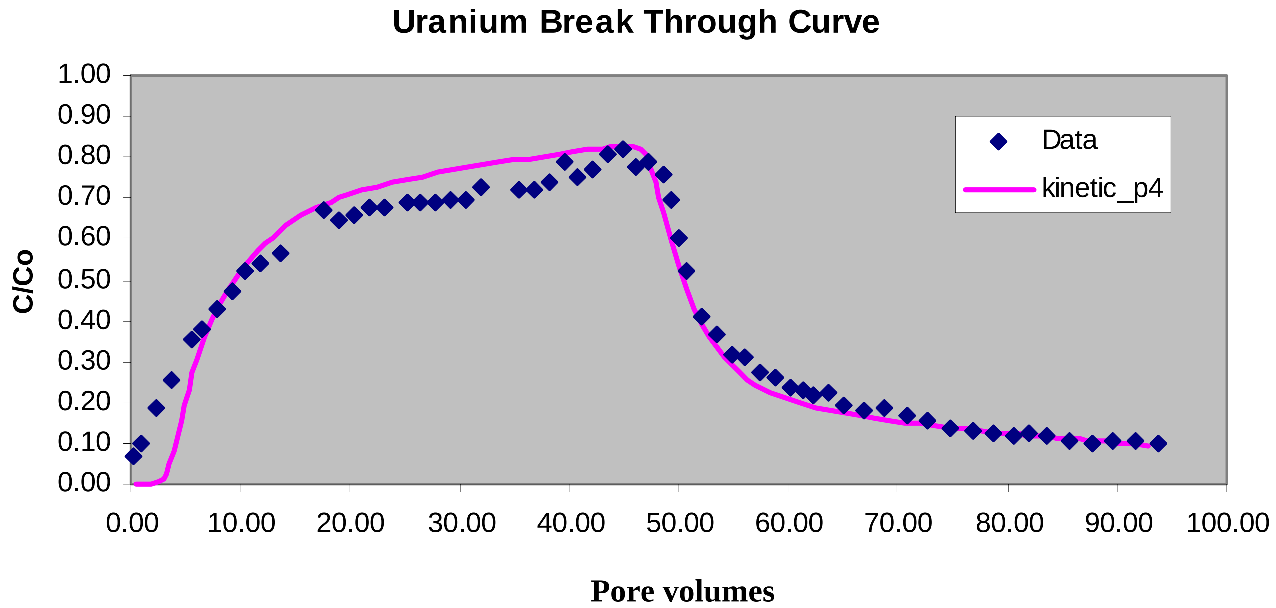


Undisturbed soil from FRC

data courtesy Phill-Dirt group (Jardine)

Uranium BTC for Undisturbed Soil Column

Fitting forward and backward rate constants to adorption reactions yielded good agreement with data



$$>Fe_s(OH)_2 + UO_2^{2+} = (>Fe_sO_2)UO_2 + 2H^+ \quad \log K_f = 3.04,\ \log K_b = -10.1$$

$$>Fe_w(OH)_2 + UO_2^{2+} = (>Fe_wO_2)UO_2 + 2H^+ \quad \log K_f = -0.494,\ \log K_b = 4.5$$

Work Plan and Issues

- Implement geochemistry into field-scale FRC model
- Refine calibration using new data as available
- Compare "bug-free" model to field data to assess impact
- Effects of uncertainty in biogeochemical rate functions and parameters (and effects of scaling up to field)?
- Effects of physical mass transfer limitations at field scale?