

Modeling Working Group Update

NABIR Fall Meeting
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Overview of Discussions

- ❖ Status of site-wide FRC modeling effort
- ❖ Modeling efforts associated with column experiments and field tracer tests at WAG-5
- ❖ Deficiencies in process understanding and parameters?
- ❖ Effects of upscaling on model formulation and parameters?

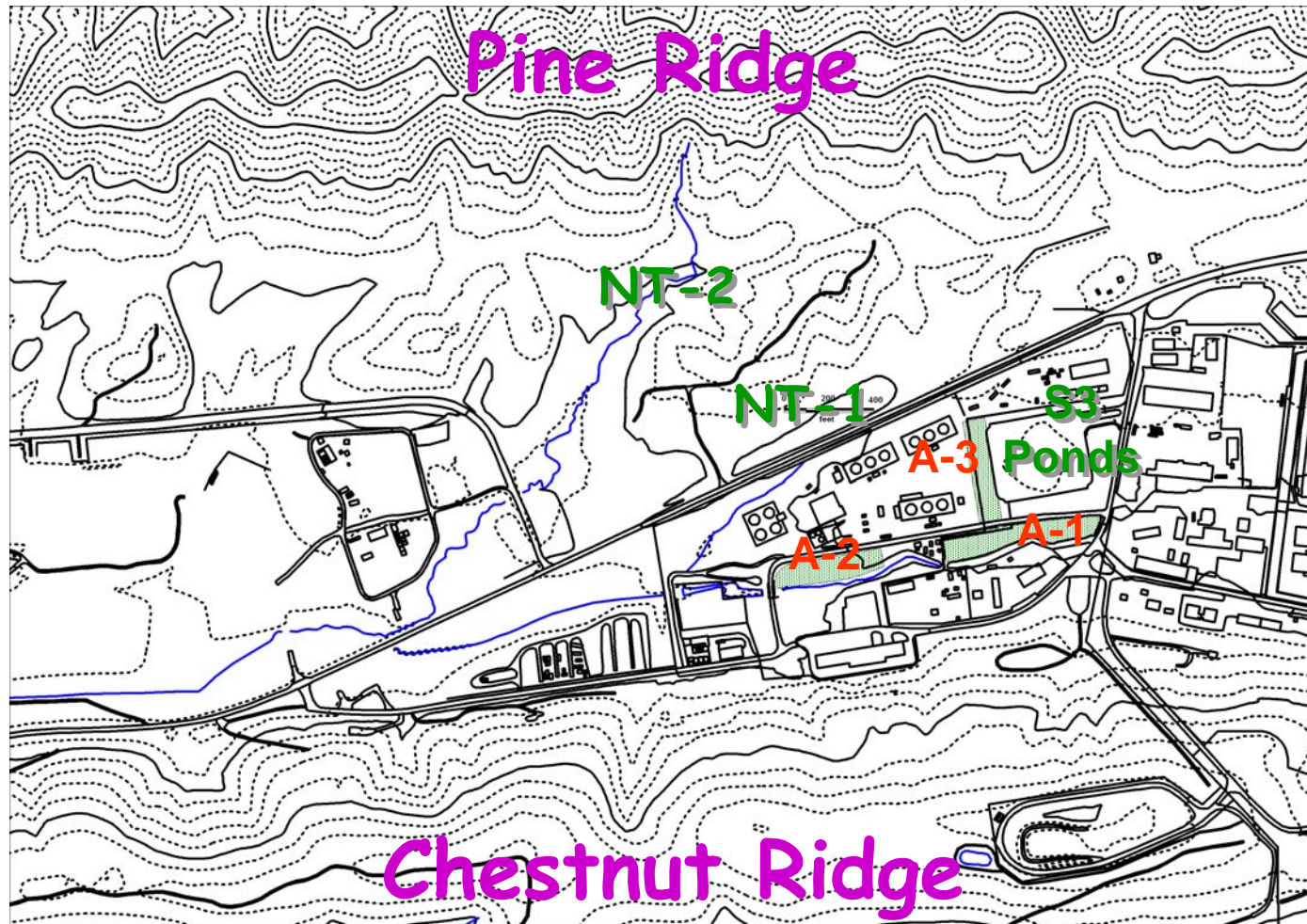
Site-Wide Modeling Effort Objectives

- ❖ 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 adapt to new formulations as our understanding improves
- ❖ Models fully anisotropic porous media suitable for representing densely fractured, dipping bedrock and saprolite

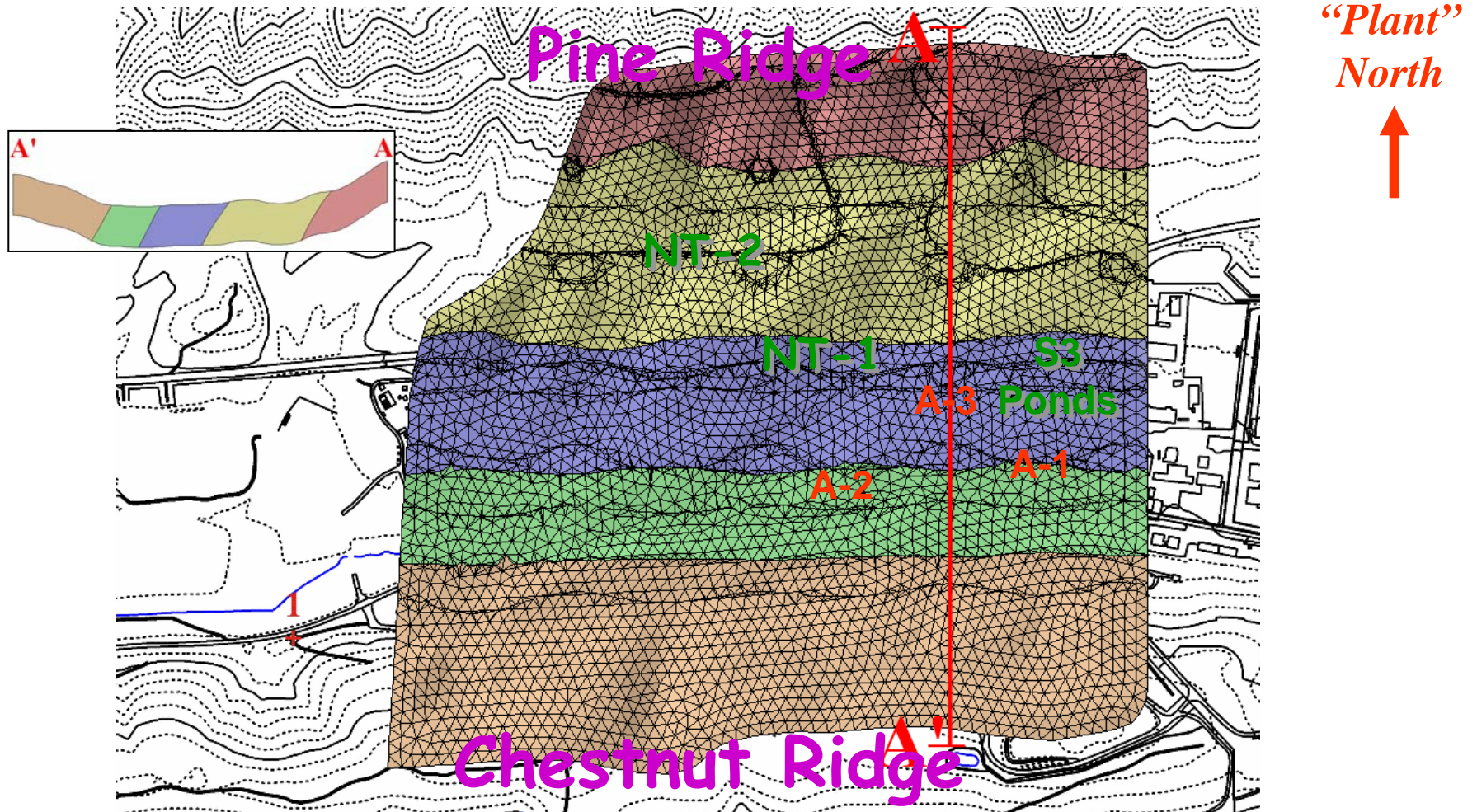
Overview of FRC Area



*“Plant”
North*

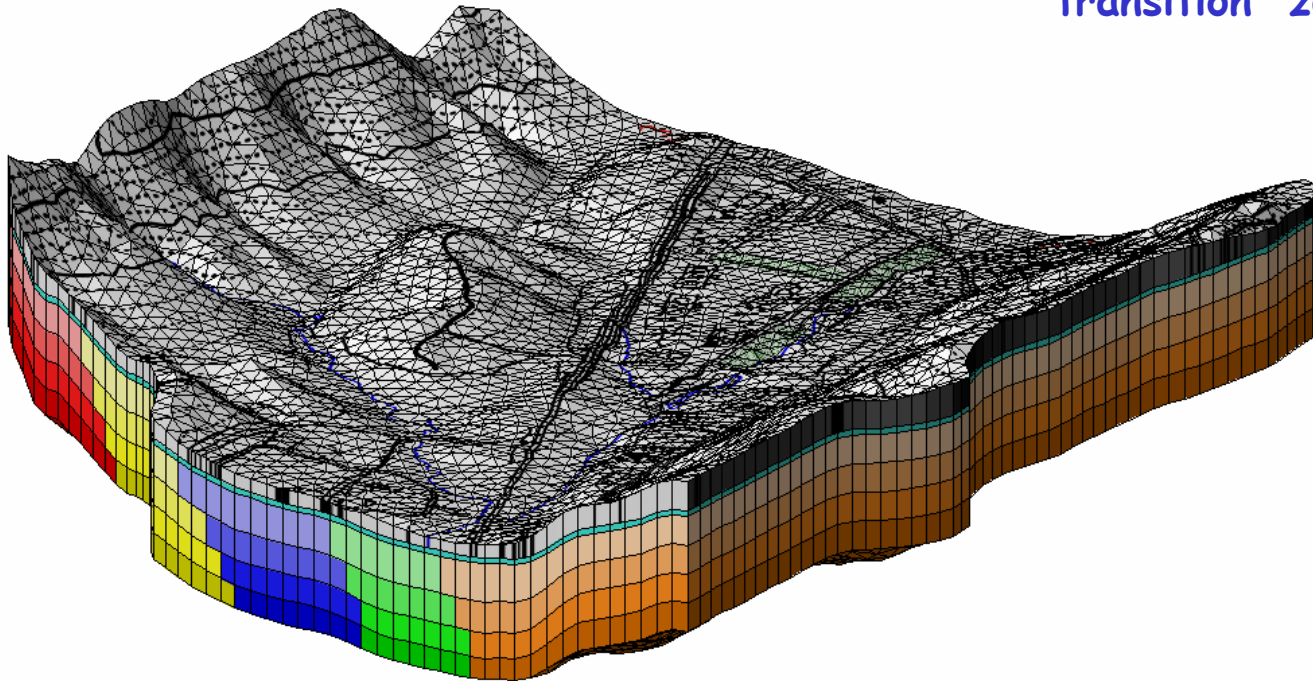


Model Domain and Bedrock Geology

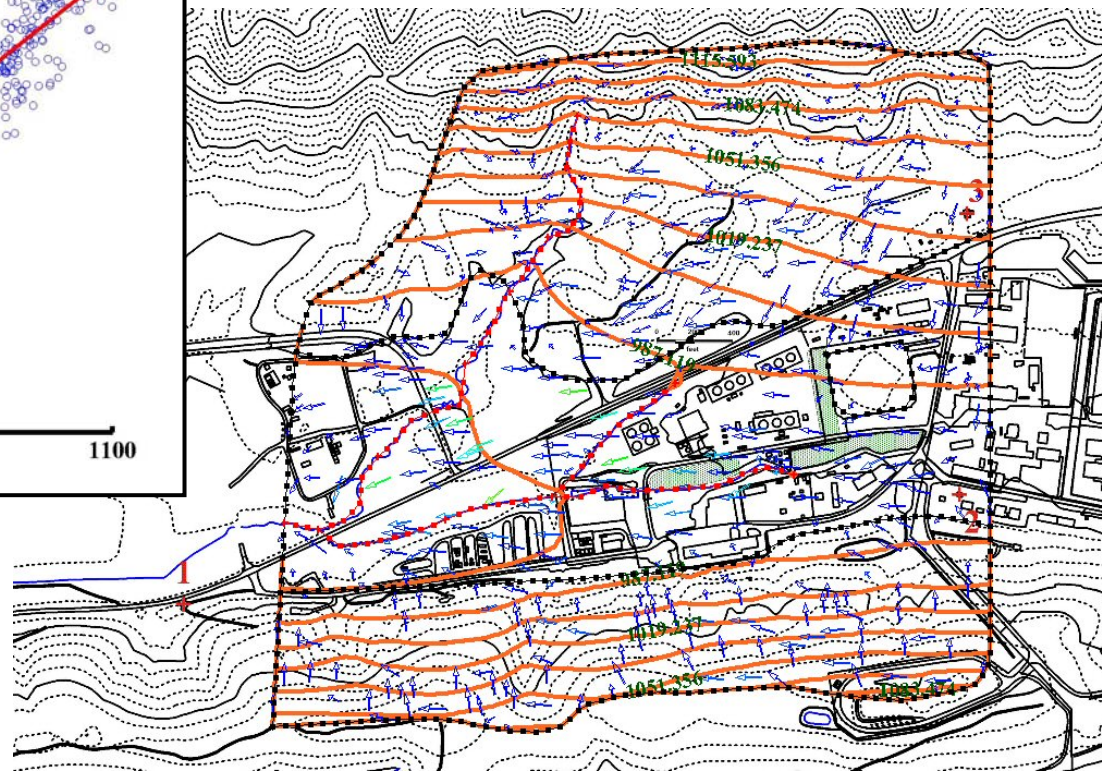
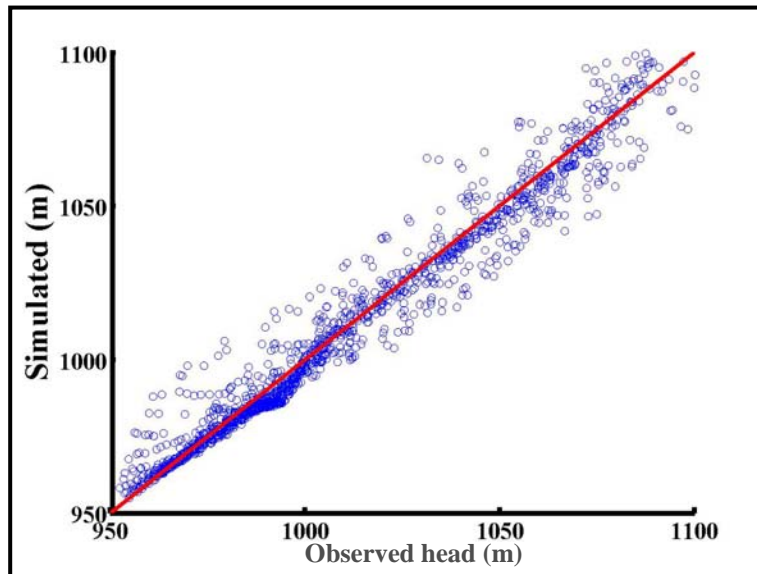


Discretized Model Domain

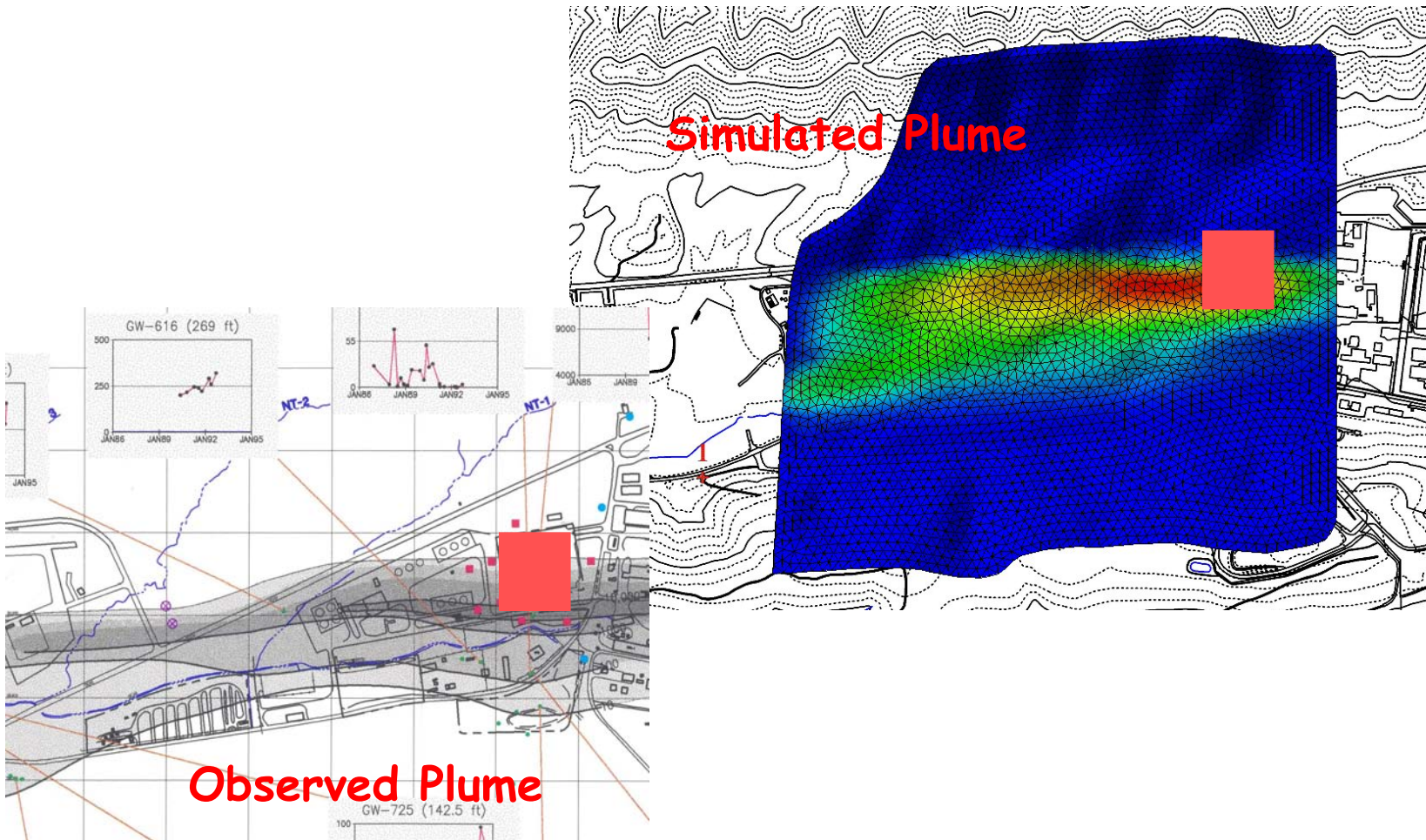
Bedrock is overlain by
soil/saprolite zone and
"transition" zone



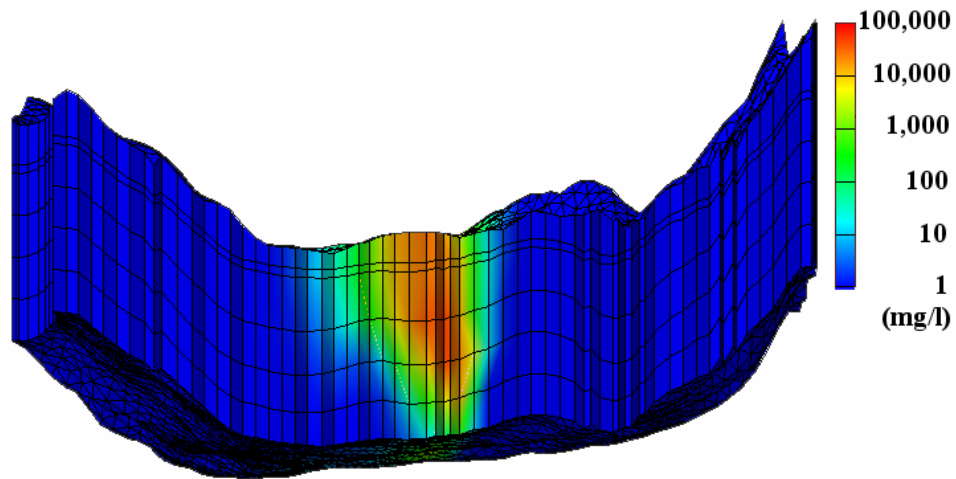
Preliminary Steady State Groundwater Flow Model Calibration



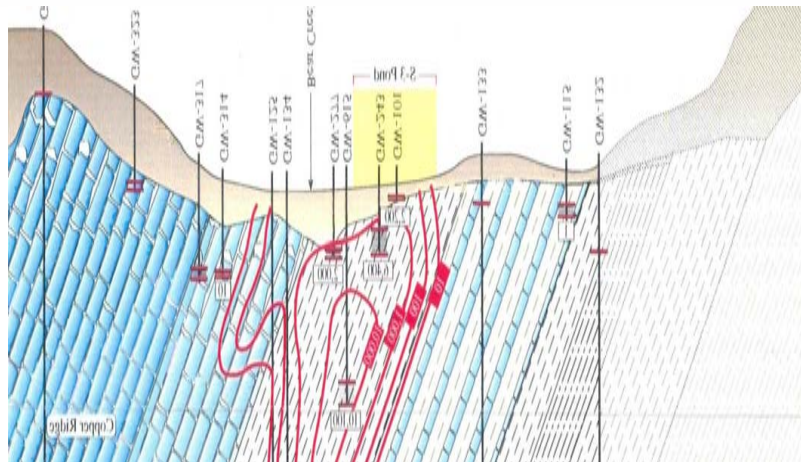
Preliminary Transport Model Results for Nitrate Plume from S3 Ponds ca. 1953-1996



Preliminary Transport Model Results for Nitrate Plume from S3 Ponds ca. 1953-1996



Simulated Plume



Observed Plume

Findings, Issues and Questions

- ❖ Geochemical mobile-immobile model successful for describing column and field tracer tests at/near WAG5
- ❖ Uncertainty in anisotropic permeability and porosity with depth and areally within geologic units
- ❖ Delineation and permeability of fill material near Area 2
- ❖ Uncertainty in biogeochemical rate functions and parameters (and effects of scaling up to field)
- ❖ Uncertainty in effects of physical mass transfer limitations at field scale

Upscaling Issues - Shifting Priorities?

- ❖ A great deal of information has been gleaned by NABIR program on lab and near-field processes
- ❖ Time to take step back and assess sensitivity of field-scale plume behavior to various processes and parameters at different scales
- ❖ Studies of large scale heterogeneous systems suggest processes found to dominate lab-scale behavior may become much less important
- ❖ e.g., petroleum reservoir engineering, remediation design, etc.

Illustration - Field Scale DNAPL Dissolution Kinetics

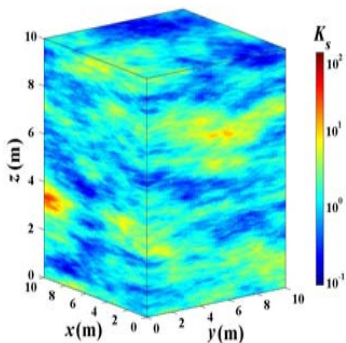
Laboratory Scale

- ❖ Lab-scale first-order mass transfer kinetics is well defined
- ❖ For conditions of interest for illustration, the lab-scale mass transfer coefficient (MTC) is 10^{-3} d^{-1}
- ❖ Predicted field-scale effluent concentration in a uniform aquifer is equal to DNAPL solubility



Field Scale

- ❖ Simulate heterogeneous permeability and DNAPL distribution in $10 \times 10 \times 10 \text{ m}$ source zone
- ❖ Predict mean mass flux using lab mass transfer functions locally within the heterogeneous velocity field
- ❖ The mean effluent concentration is only 5% of solubility and the apparent field-scale MTC is only $5 \times 10^{-5} \text{ d}^{-1}$
- ❖ Field-scale results are *insensitive* to magnitude of local MTCs



Model formulation and/or parameter sensitivities may change with scale!