Modeling Working Group Update

NABIR Fall Meeting
March 2003

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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?

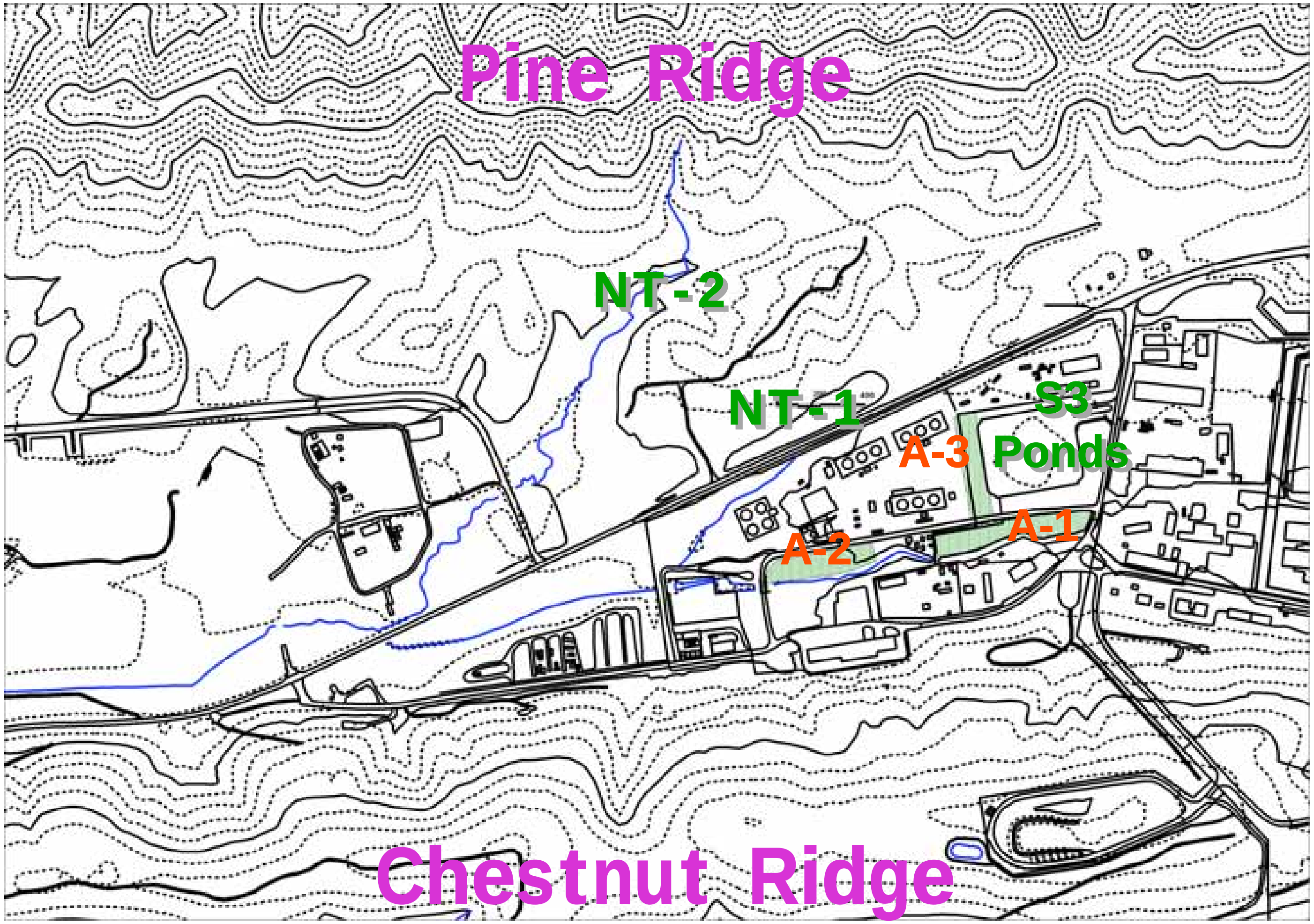
Site-Wide Modeling Effort Objectives

- 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

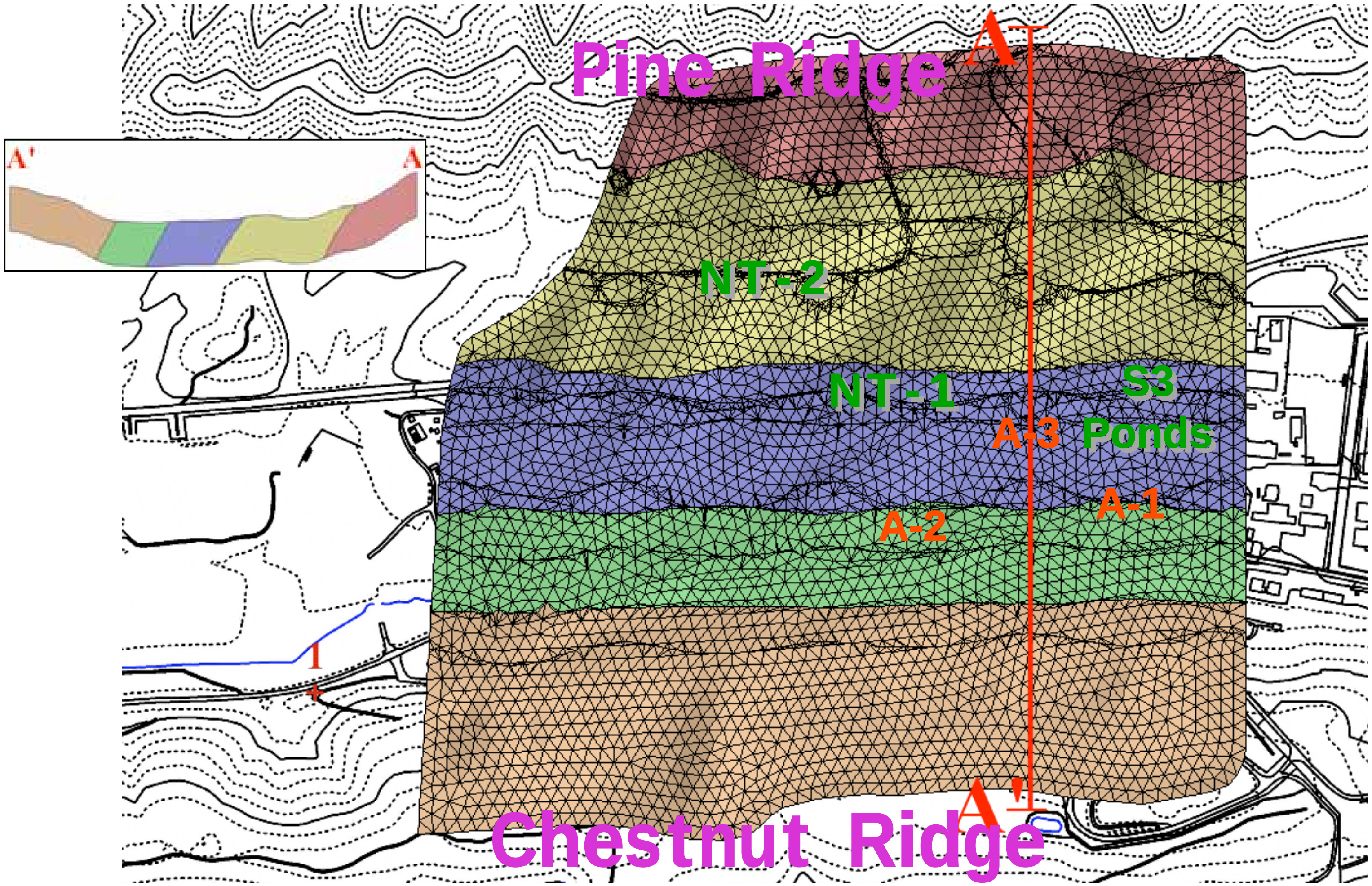
- Using HYDROGEOCHEM version 5 which is an enhancement of HBGC123D
- Models 3D transient sat/unsat flow, heat transport, dissolved transport, and complex biogeochemical reactions
- Allows user-definable kinetic functions, which provides flexibility to adapt to new formulations as our understanding improves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

Overview of FRC Area



"Plant" North

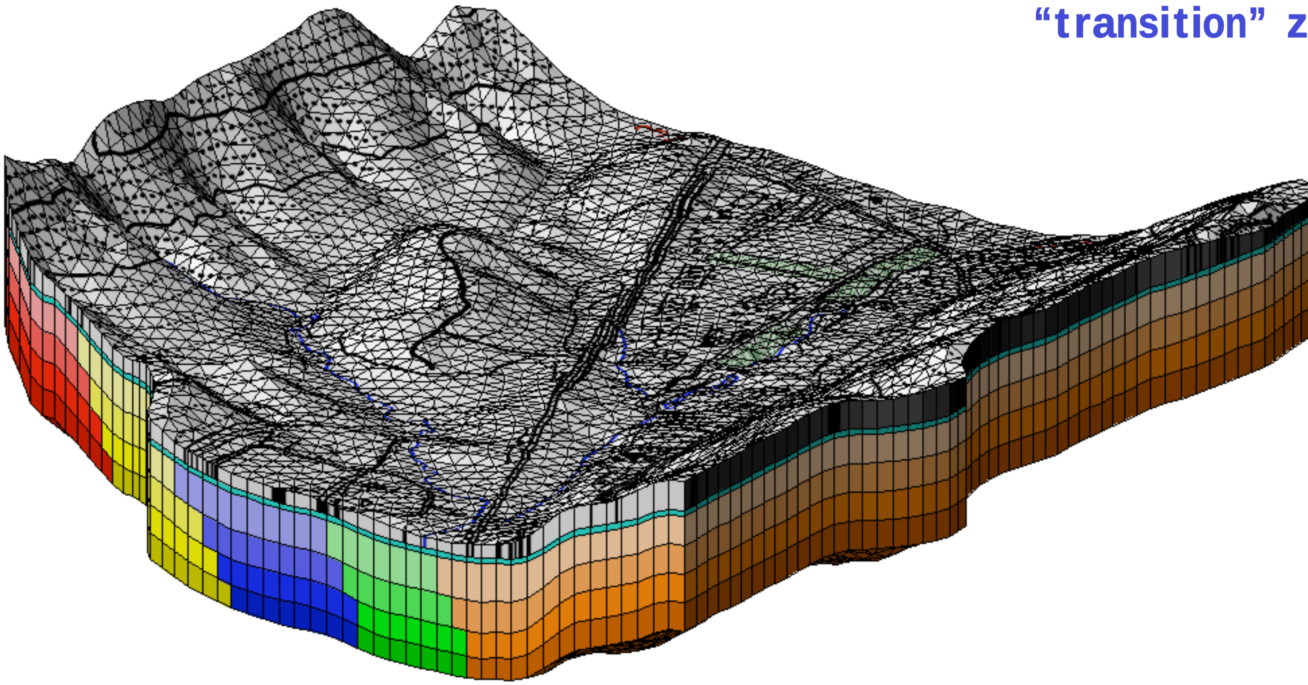
Model Domain and Bedrock Geology



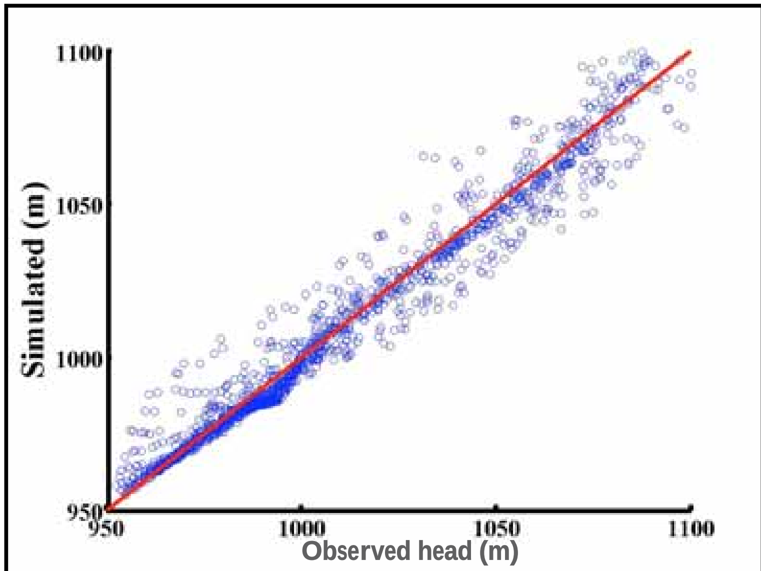
"Plant" North

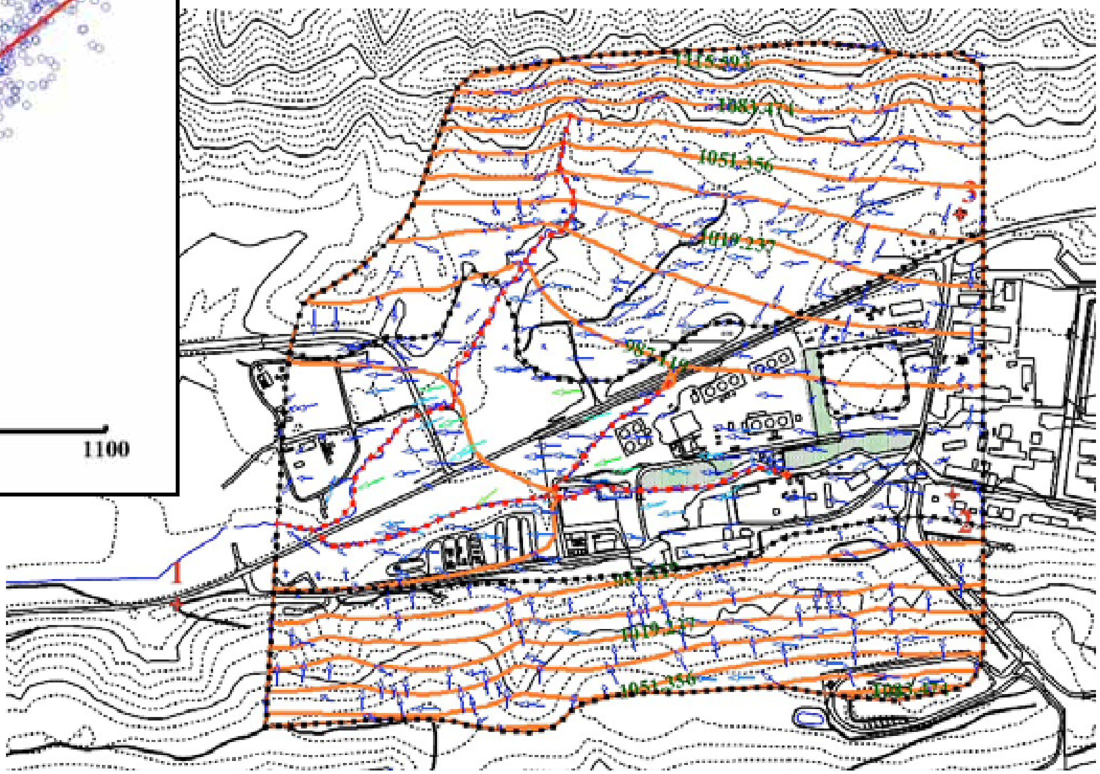
Discretized Model Domain

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

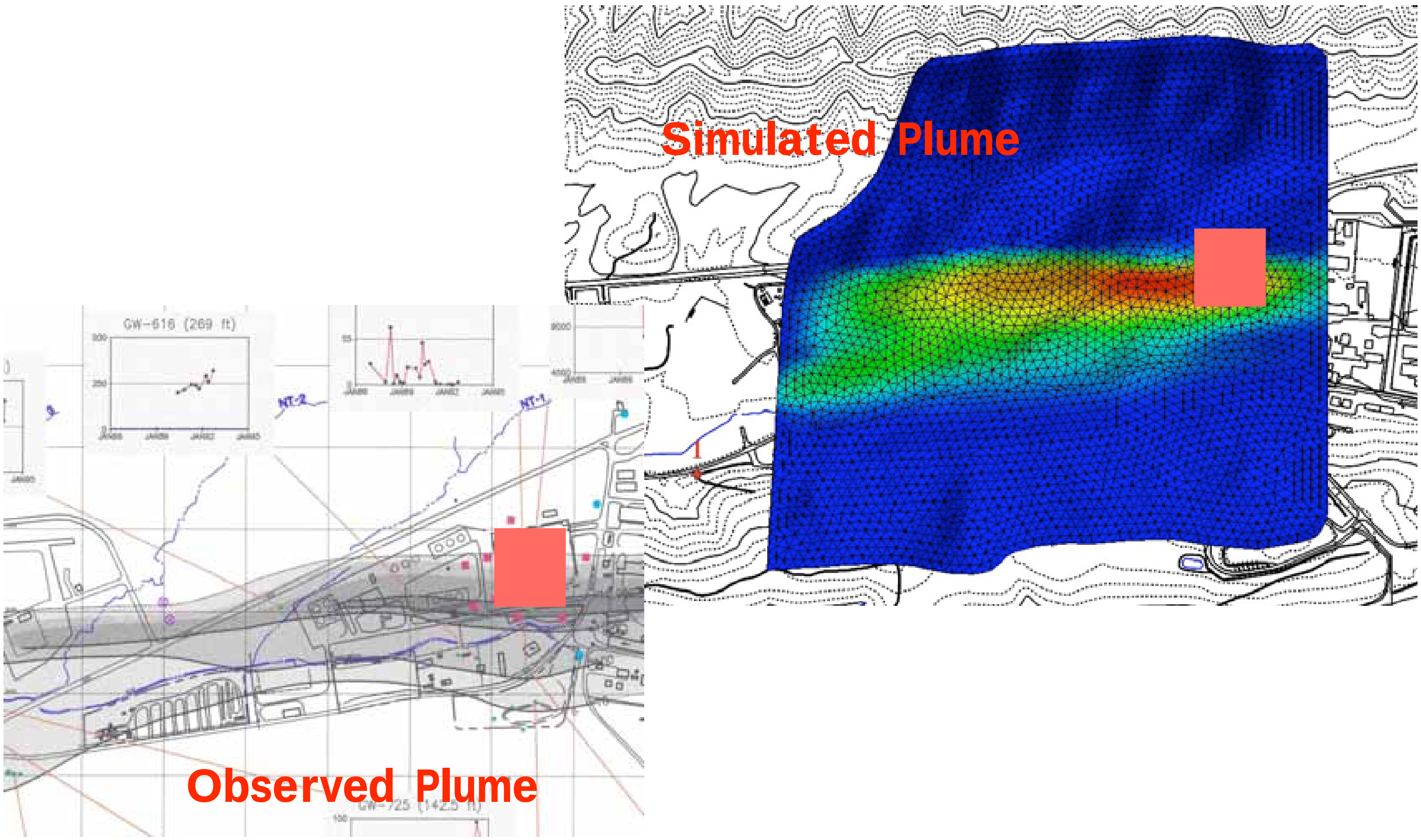


Preliminary Steady State Groundwater Flow Model Calibration





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



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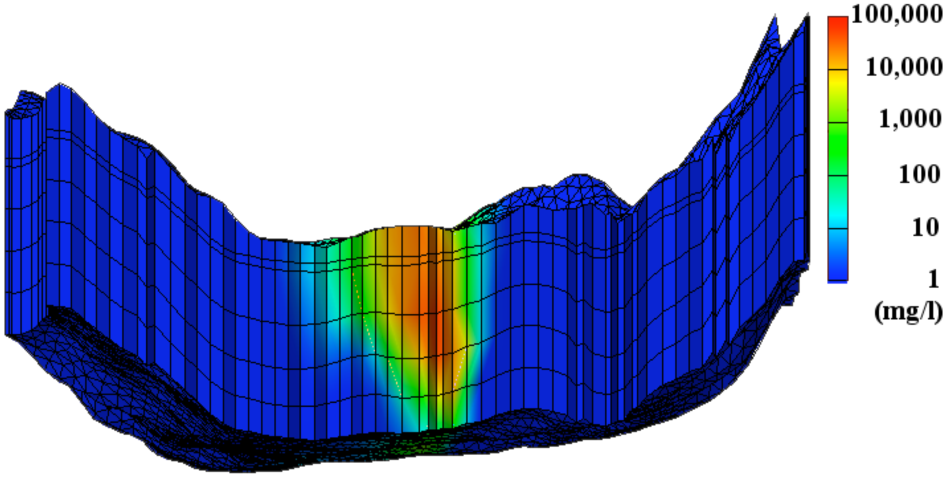
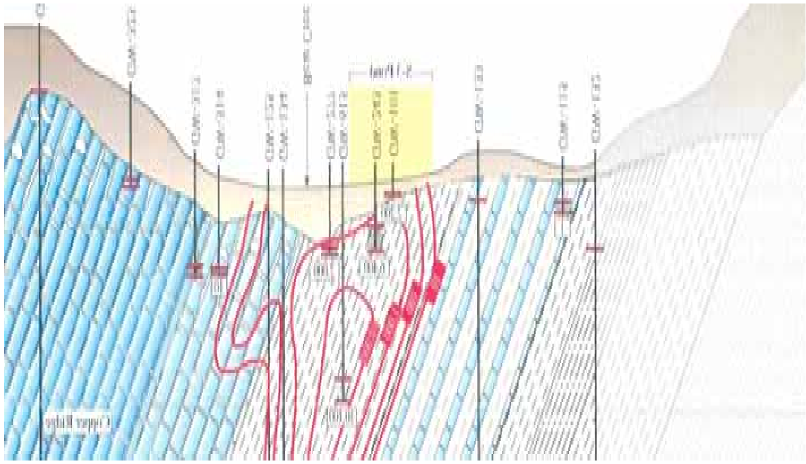


Simulated Plume



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?

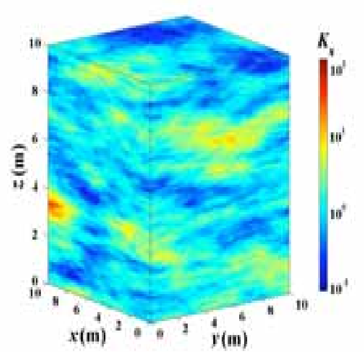
- A great deal of information has been gleaned by NABIR program on lab and near-field processes
- Time to take step back and assess sensitivity of field-scale plume behavior to various processes and parameters at different scales
- Studies of large scale heterogeneous systems suggest processes found 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 x 10 x 10 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 x 10^{-5} d^{-1}
- Field-scale results are *insensitive* to magnitude of local MTCs

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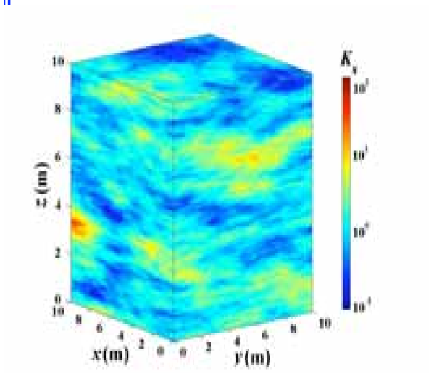

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Model formulation and/or parameter sensitivities may change with scale!