Modeling Working Group Update

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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
Model Domain and Bedrock Geology

Pine Ridge

NT-2

NT-1

S3 Ponds

A-3

A-2

A-1

Chestnut Ridge

“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

Observed Plume

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

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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 $5 \times 10^{-5}$ d$^{-1}$
- Field-scale results are insensitive to magnitude of local MTCs
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Model formulation and/or parameter sensitivities may change with scale!