Multi-Region Reactive Transport Due To Strong Anisotropy In Unsaturated Soils With Evolving Scales of Heterogeneity

Project 86952

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Collaborators and Co-investigators

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- PNNL
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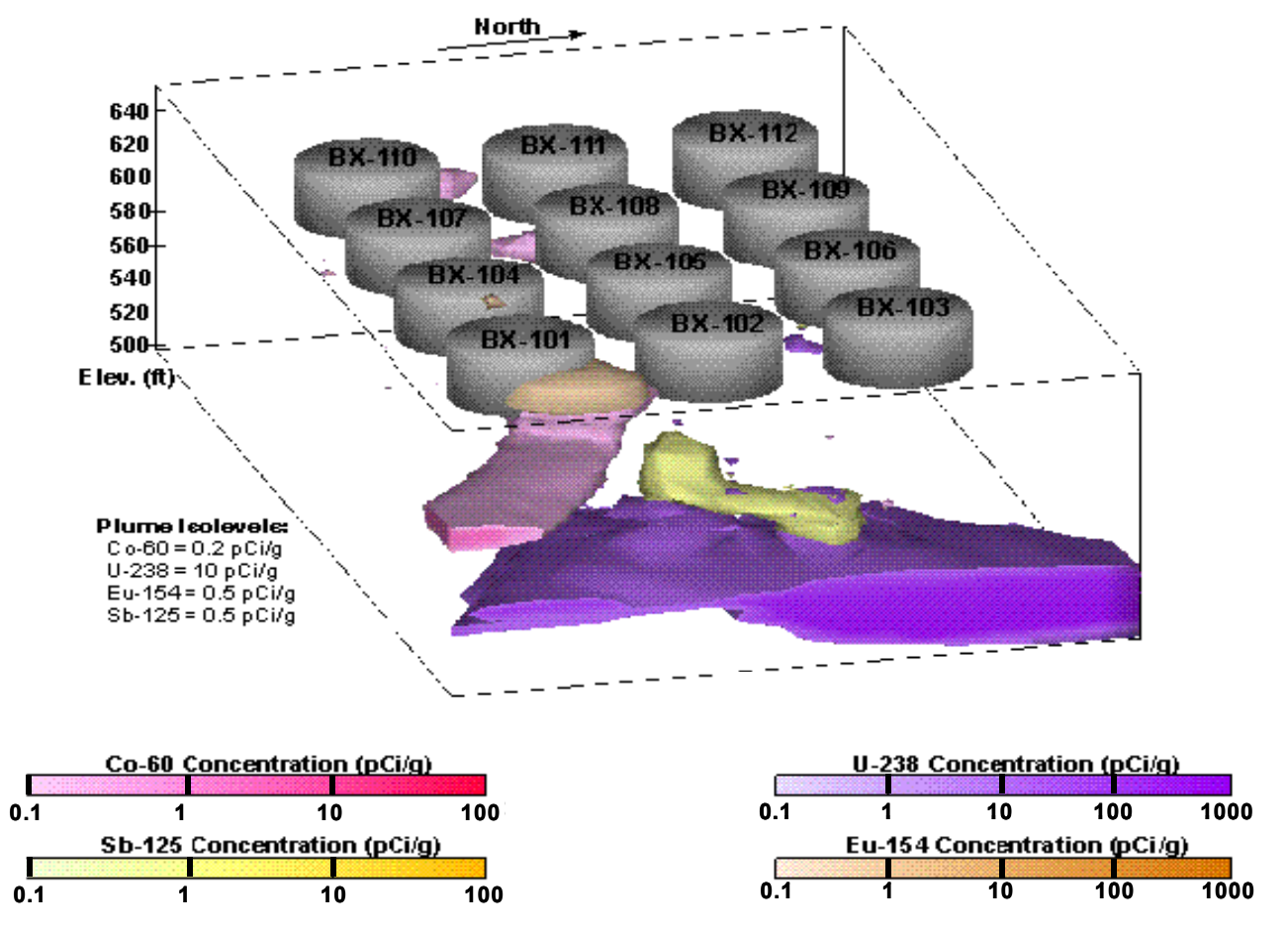
Background

- Well recognized discrepancy between predictions and observations of contaminant distributions at Hanford
  - early arrival and high concentrations of mobile contaminants
  - Late or non arrival of sorbing contaminants
- Discrepancy is due primarily to
  - inappropriate choice of model parameters
  - inappropriate conceptual models
- Conceptual Errors
  - Lateral flow due to anisotropy

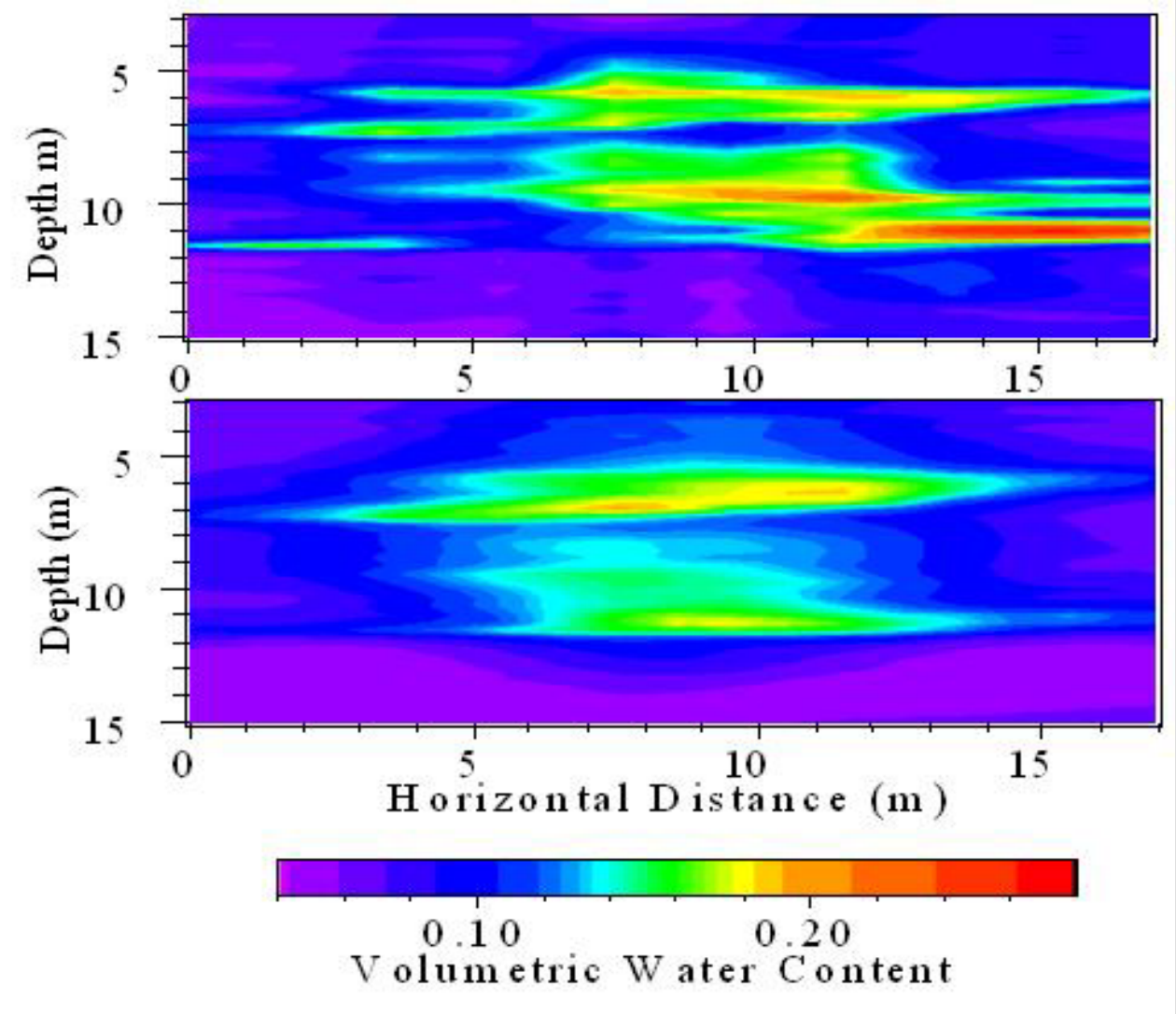
Typical Hydrogeological Assumptions

- Flow in the vadose zone is predominantly downward
  - Predictions- pervasive early arrival and high concentrations of mobile contaminants
  - Observations- lateral flow due to anisotropy has dominated every experiment, planned and unplanned at Hanford

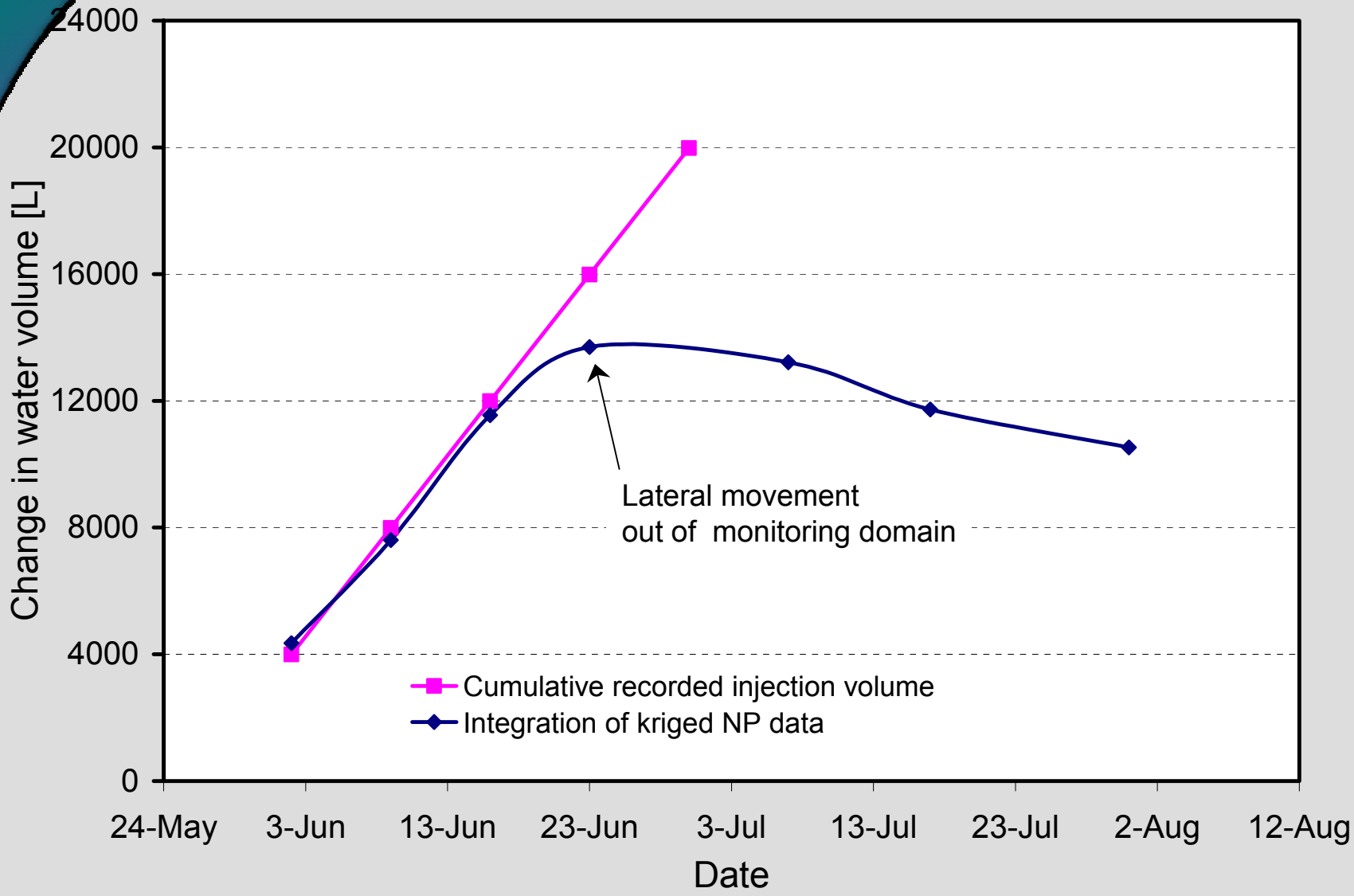
Anisotropy at Hanford's BX Tank Farm



Anisotropy at Sisson and Lu (VZTFS) Test Site



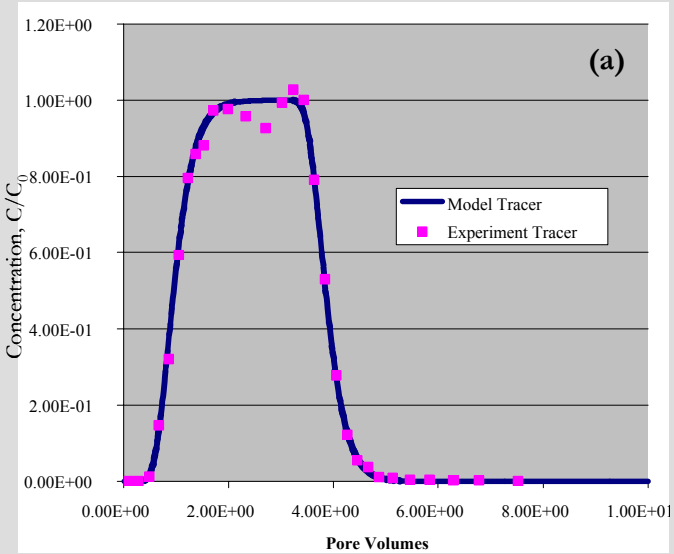
Mass Balance Comparison at VZTFS

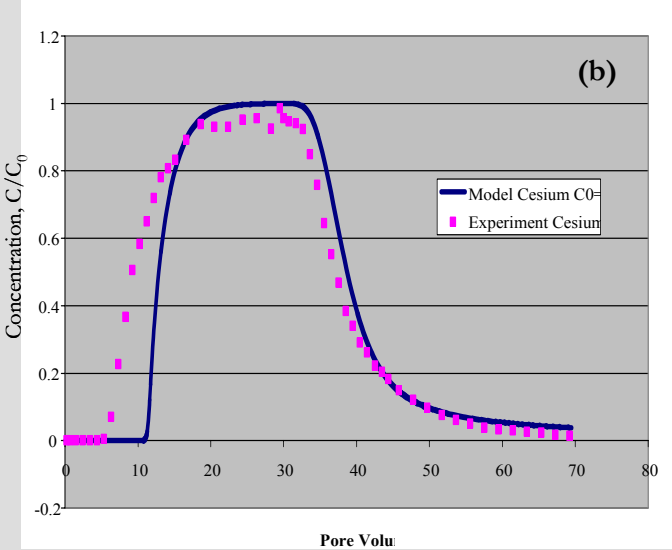


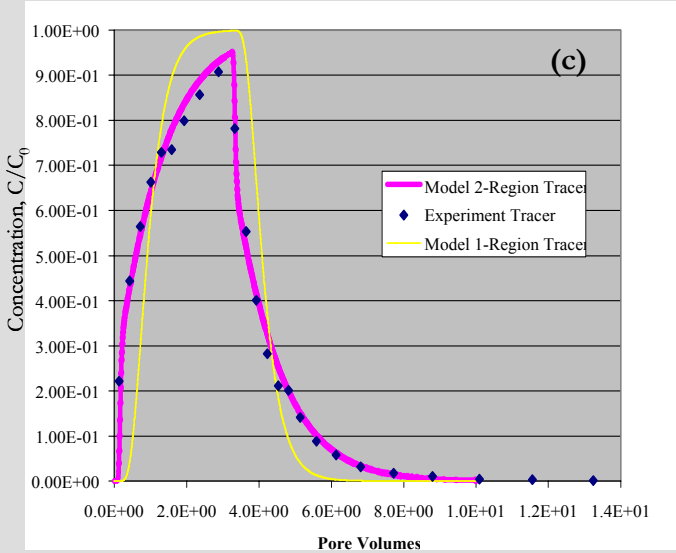
Typical Geochemical Assumptions

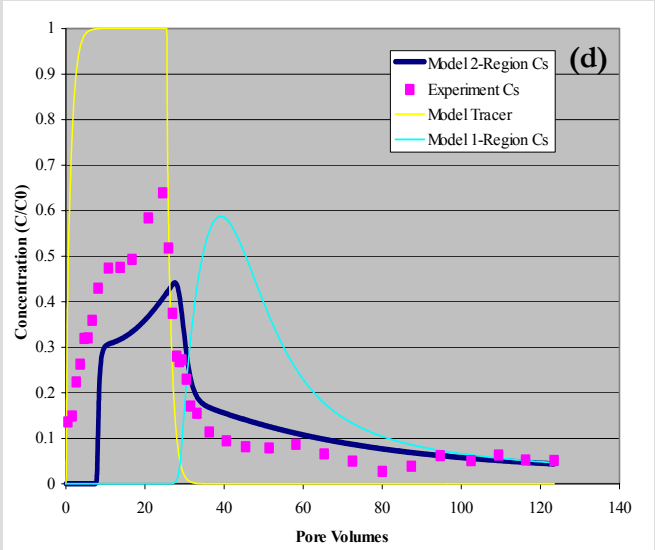
- All reactive sites are assessable to contaminants
  - Predictions- strong retardation and long delays in arrival time for reactive contaminants
  - Observations- significant bypass due to immobile regions and anisotropy

Two-region Transport and Ion Exchange

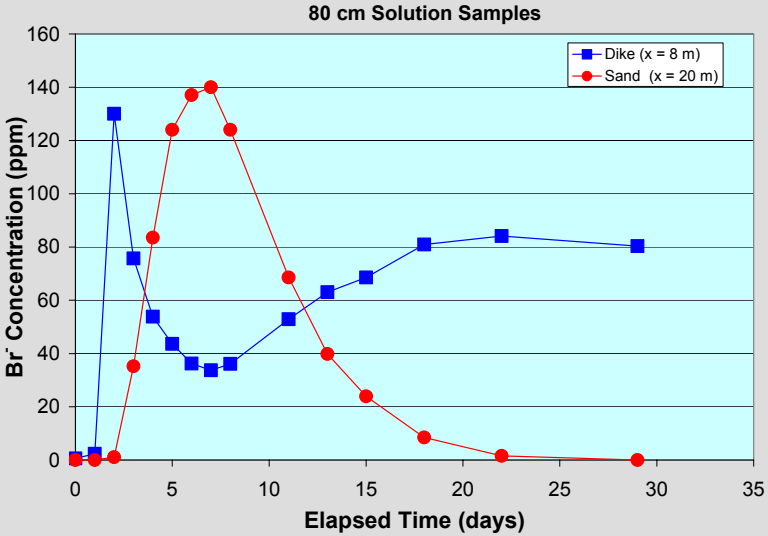








Multi-region Flow at Army Loop Road Dike



Challenge:

Develop rigorous method represent unsaturated flow and transport in typical heterogeneous, porous media

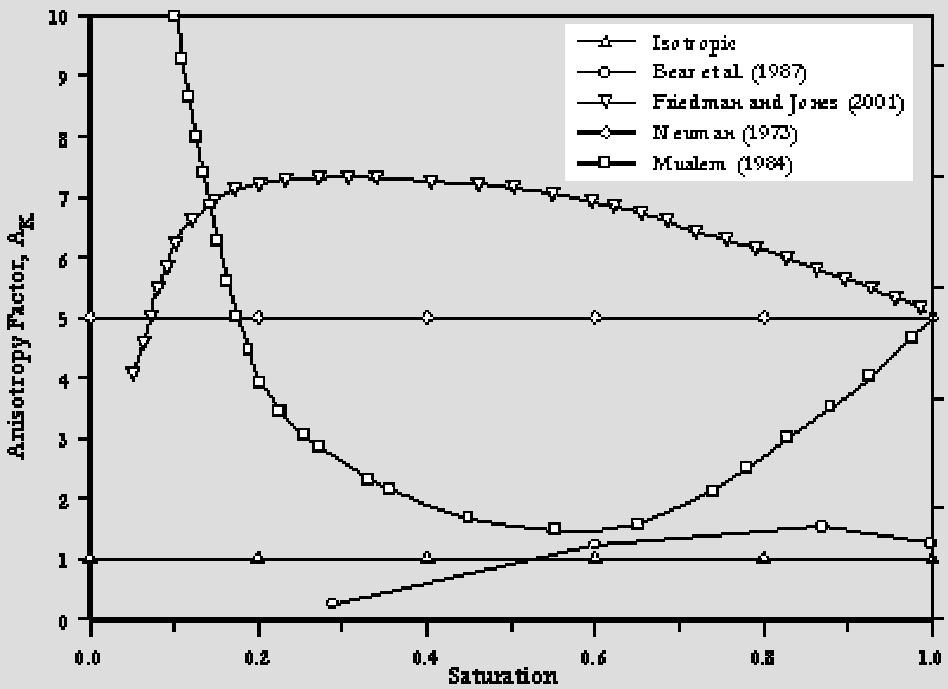
Battelle

Project Goals and Objectives

- Determine the scale of applicability and the limitations of the small perturbation (stochastic) approach for predicting flow and transport at arid sites with strong heterogeneity.
- Develop an appropriately rigorous averaging approach to better quantify local-scale behavior in anisotropic soils.
- Develop a multi-region transfer method to bridge the gap between pore-scale fluid migration and macro-scale displacement behavior under strong anisotropy

Approaches to Modeling Anisotropy

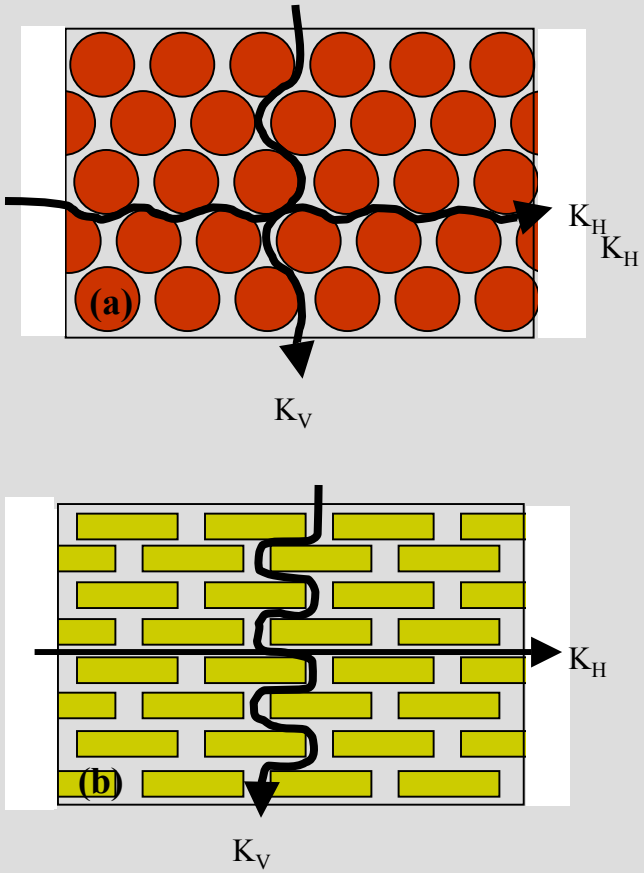
- Evidence to suggest anisotropy is state-dependent
- Stochastic approach assumes that flow can be linearized and treated as a small perturbation of unsaturated dynamics
- Assumes an exponential relationship between K and ψ.
- Requires small variance in ln K
- Horizontal K is always larger than vertical K



Conceptualization

(a) Spherical particles (e.g. sand) could be isotropic due to the small difference in tortuosity and connectivity in the horizontal and vertical directions and KH ≅ KV

(b) Flat particles (e.g. mica), leads to major differences in tortuosity and connectivity in the horizontal and vertical directions and KH >> KV.

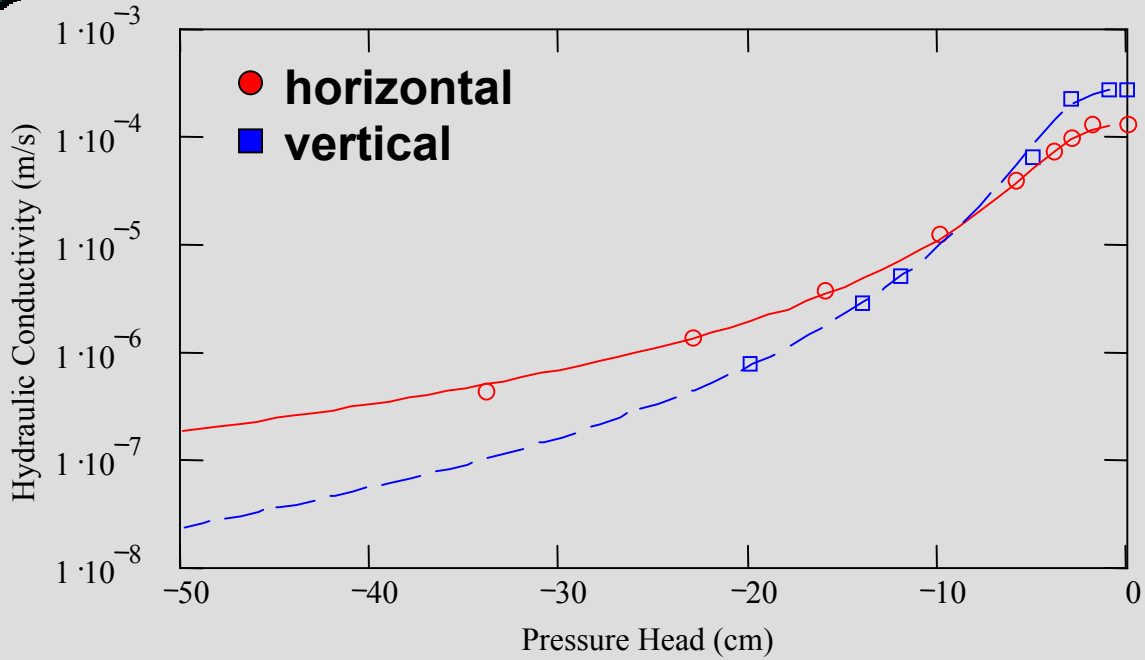


Research Design and Methodologies

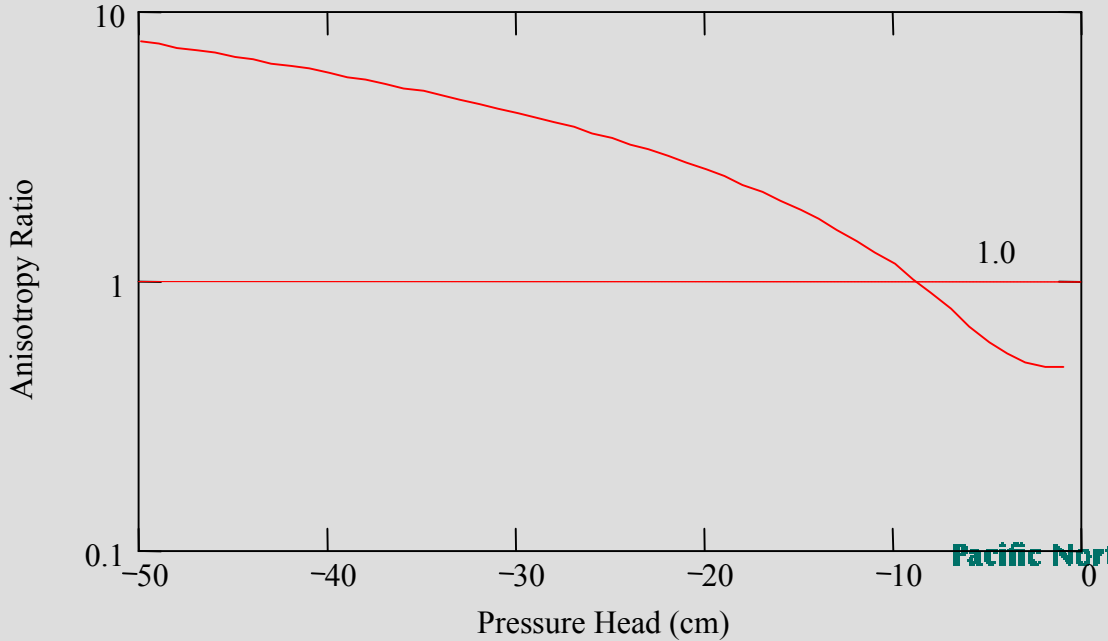
- Controlled Laboratory Studies
- Controlled Field Experiments
- Numerical Simulations

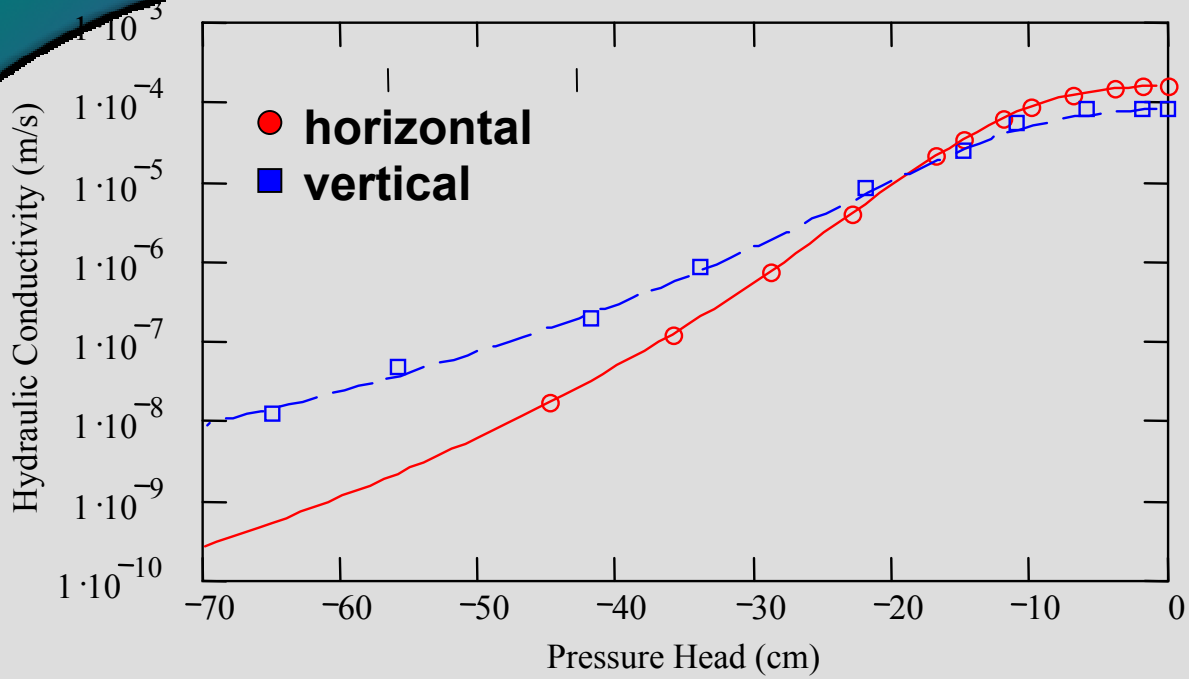
Controlled Laboratory Studies

- Quantitative Pore Morphology
  - Map pore morphology and connectivity of samples representative of facies in Upper Hanford Formation
  - Quantify pore-induced anisotropy and connectivity for each facies
- Pore-scale Anisotropy
  - Measure directional K
  - Determine water entry pressures and connectivity tensor
  - Develop dataset to verify pore-scale modeling
- Centrifuge Modeling
  - Centrifuge scaling relationships for anisotropic flow and transport
  - Investigate effect of flow regime on multi-region processes

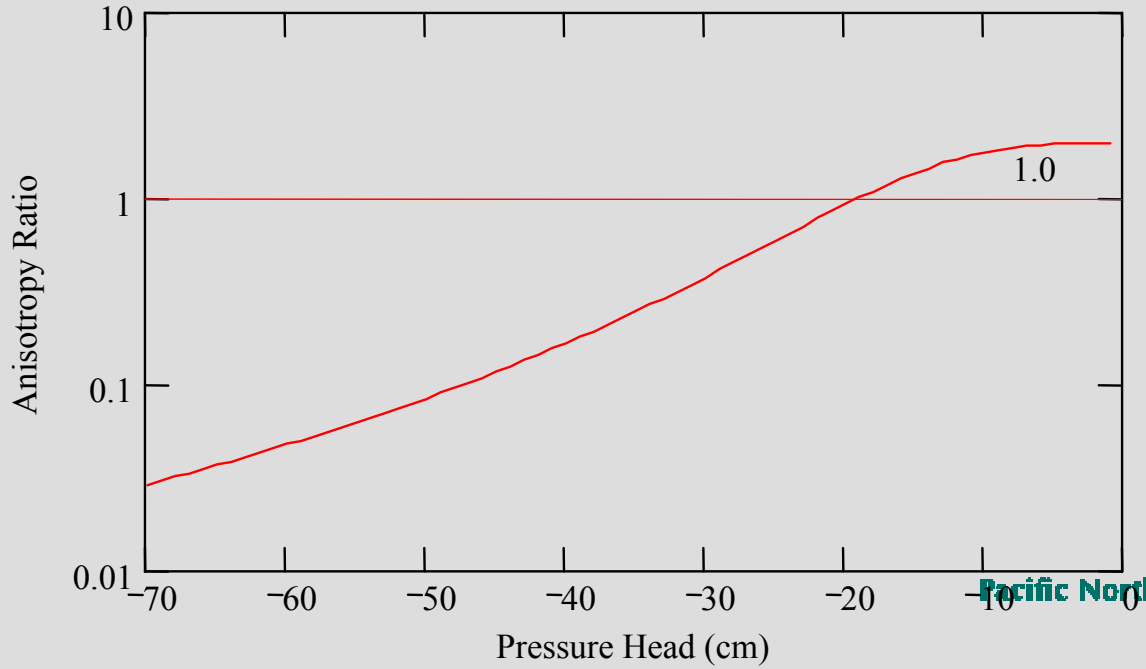


Fort Colins Soil (Laliberte, 1966)



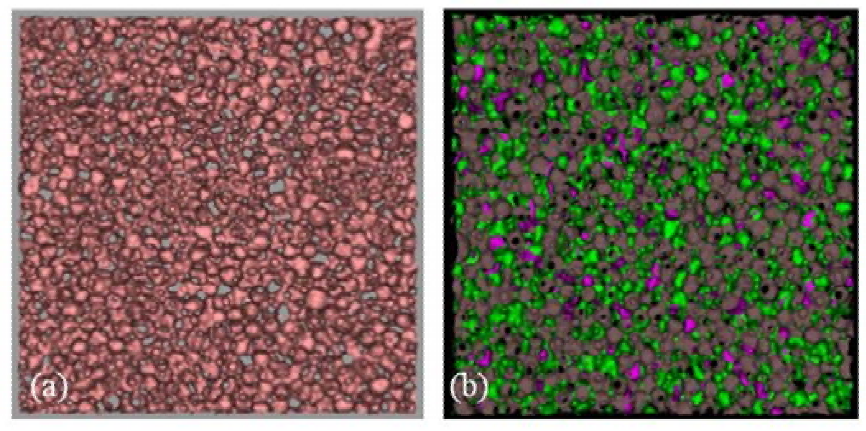


Cass Soil (Laliberte, 1966)



Improved Conceptual and Numerical Models

- Pore-scale Modeling (Lattice Boltzmann)
  - generate 3-D pore scale model representative of each facies
  - Develop an understanding of pore-scale anisotropy in relation to particle shape and pore characteristics
  - quantify effects of flow regime and fluid properties on relative permeabilities, anisotropy, and non-equilibrium transfer



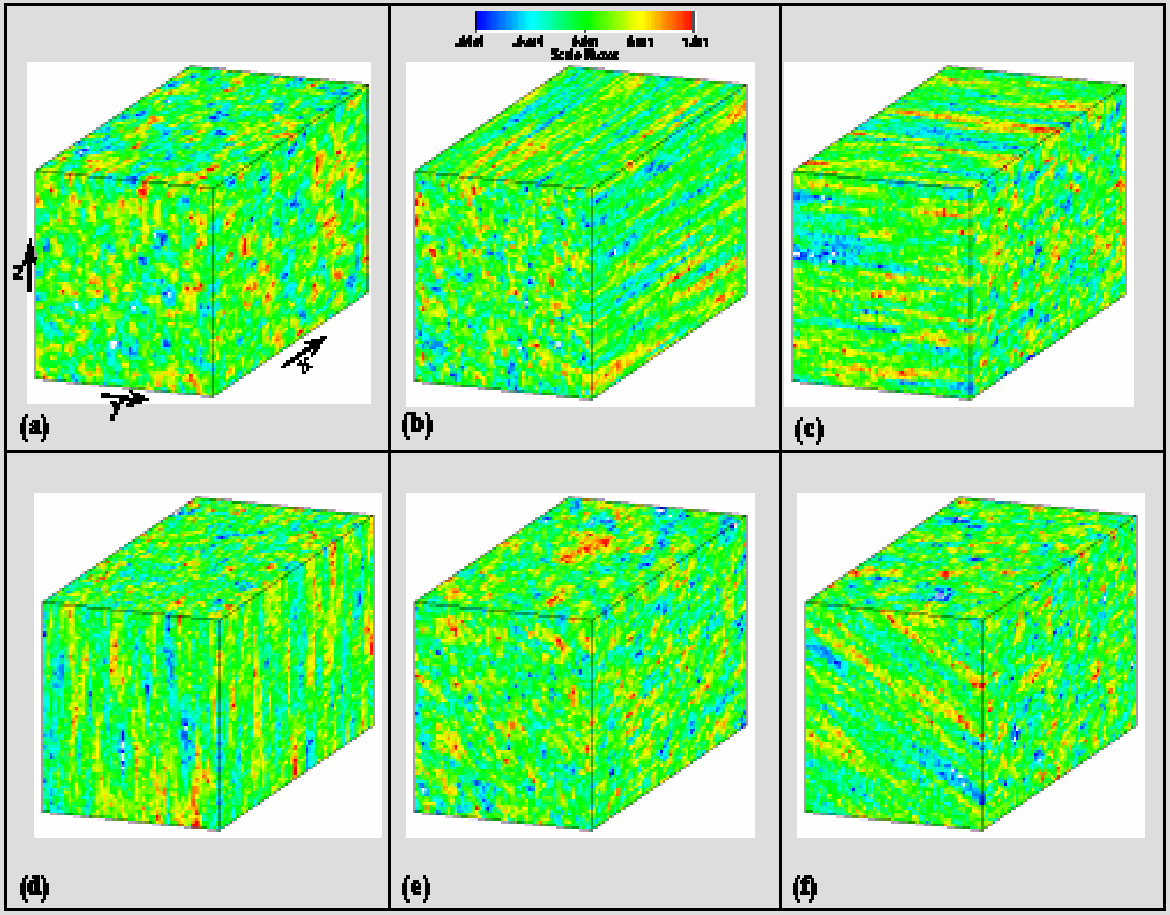
Controlled Field Experiments

- Establish an hierarchical description of heterogeneity
- Collect quantitative dataset for validating macroscale continuum model and for identifying effective parameters

Significance to EM Mission

- Most subsurface remediation problems require predictions over large temporal (≥ 10^3 yr) and spatial (≥ 1 km) scales
  - small scale observations => relevant scales
- Improved conceptual models (NAS)
  - Improved understanding of long-term fate and transport
  - Selection and design of remediation technologies
  - Reduced incidence of over-engineered solutions
- Results will bridge gap between local scale measurements and field scale observations

Preliminary Results



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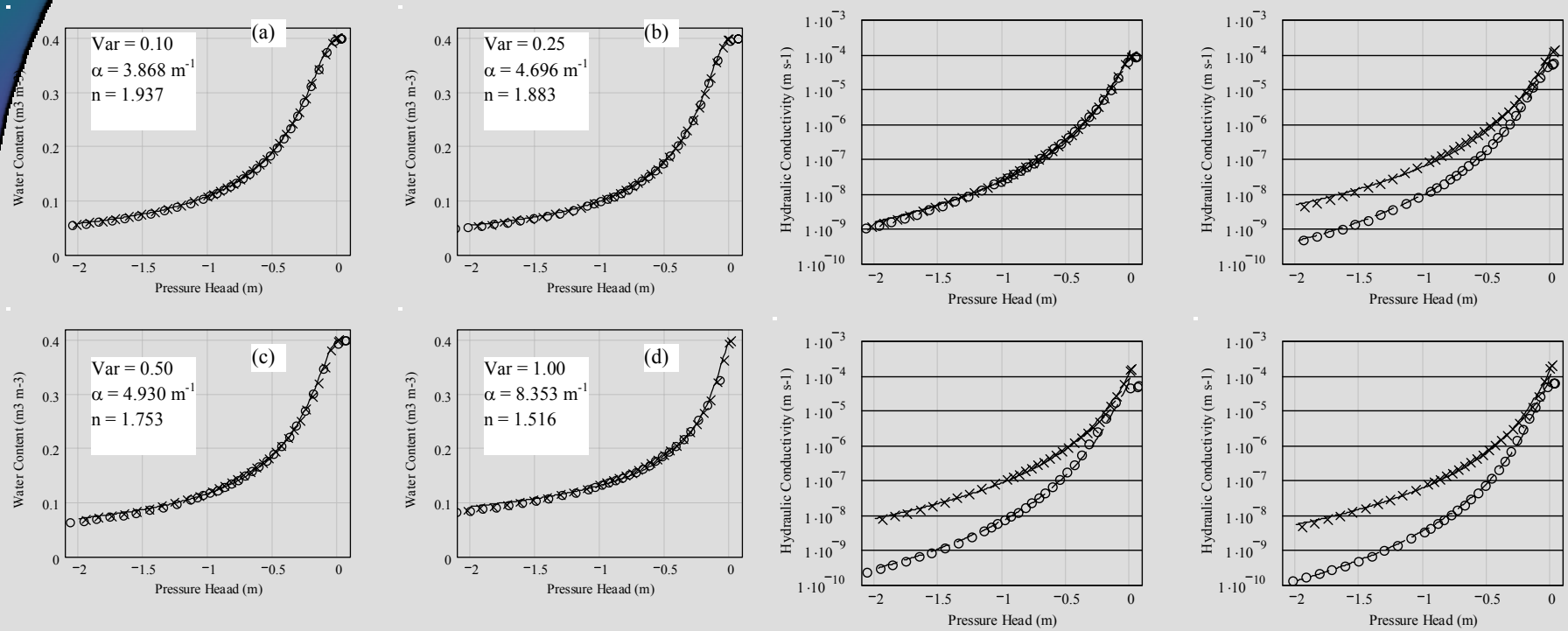
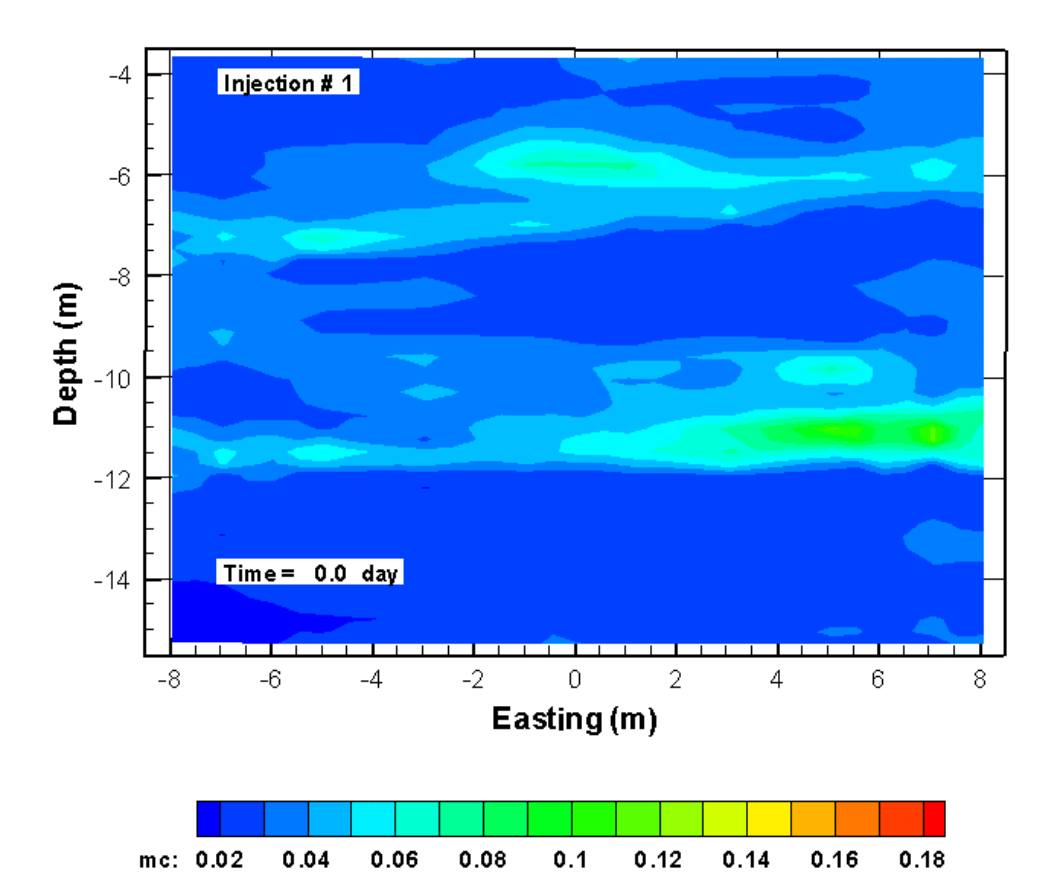
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