Quantifying Vadose Zone Flow and Transport Uncertainties Using a Unified, Hierarchical Approach

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Significance

- Vadose zone heterogeneity
  - can have a significant effect on flow and transport
  - is often conceptualized realistically but is given a simplified representation in models
- Remediation and waste management decisions
  - require estimates of future impacts (predictions)
  - require estimates of prediction uncertainty
- Characterization
  - No systematic, proven strategy for effectively allocating limited funds

Project Objectives

- Apply indirect methods for estimating hydraulic and transport parameters to conditional simulation of water flow and solute transport in the vadose zone
- Evaluate relationships between data type, quantity, and measurement scale on accuracy and uncertainty of simulation results
- Develop guidance for application of novel parameterization methods for predictive modeling of vadose zone contamination and remediation problems

Methods

- Geophysical measurements as a source of hard and soft data
- Neural network methods to derive pedotransfer functions relating physical and hydraulic properties
- Similar media scaling and conditional geostatistical simulation to parameterize models
- Infiltration/tracer field experimental data to evaluate methods and develop guidance

Neural Network Pedotransfer Functions (Schaap et al., 1998)

- Hierarchical prediction of hydraulic parameter values and uncertainty using readily available and less expensive physical property data, such as:
  - bulk density
  - sand, silt, and clay contents
  - water content at specified pressure heads
  - organic matter content

Similar Media Scaling and Conditional Simulation (Rockhold et al., 1996)

- A generalized scaling analysis is used
  - extension of Miller & Miller approach for scaling constitutive permeability-saturation-pressure relationships
- Conditional geostatistical simulation
  - using auto- and cross-correlation structures
- Novel parameterization methods
  - using hard and soft data (i.e., directly and indirectly measured)
  - upscaling where necessary

Schedule: Currently in Year 1 of 3-yr Project

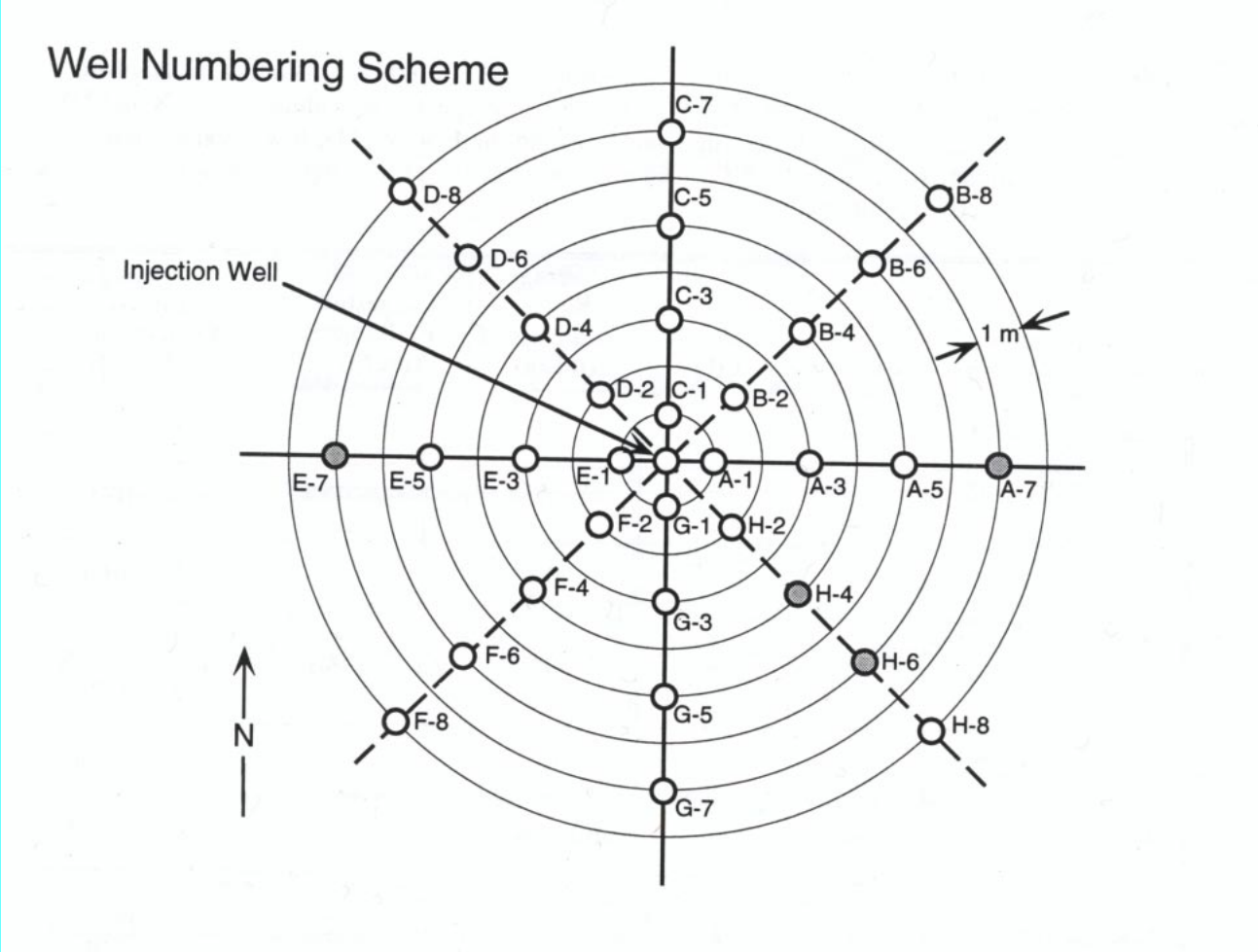
- Year 1 Activities
  - Collaboration with Hanford Site Vadose Zone Transport Field Study Project for collection of cores and geophysical measurements from the field site
  - Physical and hydraulic property measurements on core samples obtained at the field site
  - Neural network pedotransfer function analysis of field site data and other relevant Hanford Site data
  - Scaling and geostatistical analyses of field site data
  - Best-case simulation analysis using all available data

Field Site

- Relatively large scale
- Experiment conducted in 1980-81 using radioactive tracers
  - Data includes water content and tracer activities
- Additional geophysical logging in 1995
  - Data includes water content, bulk density, and spectral gamma measurements
- Site of Hanford Vadose Zone Transport Field Study Project infiltration/tracer experiment in May-July, 2000

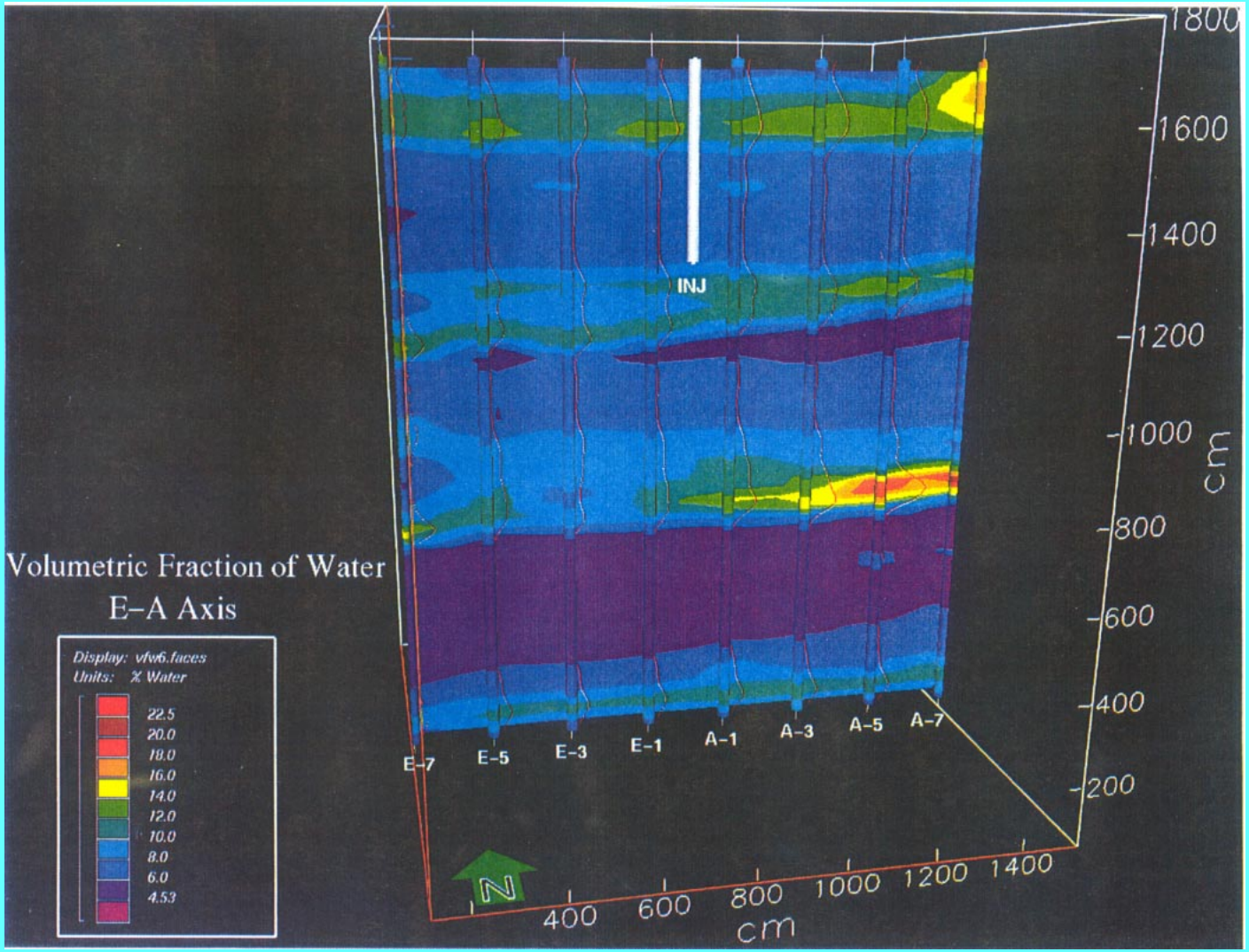
Original Field Site

- Array of 18-m deep steel-cased boreholes
- Injection well is about 5-m deep



Data from the 1995 Geophysical Logging (15-cm resolution)

- Water content along the E-A cross-section



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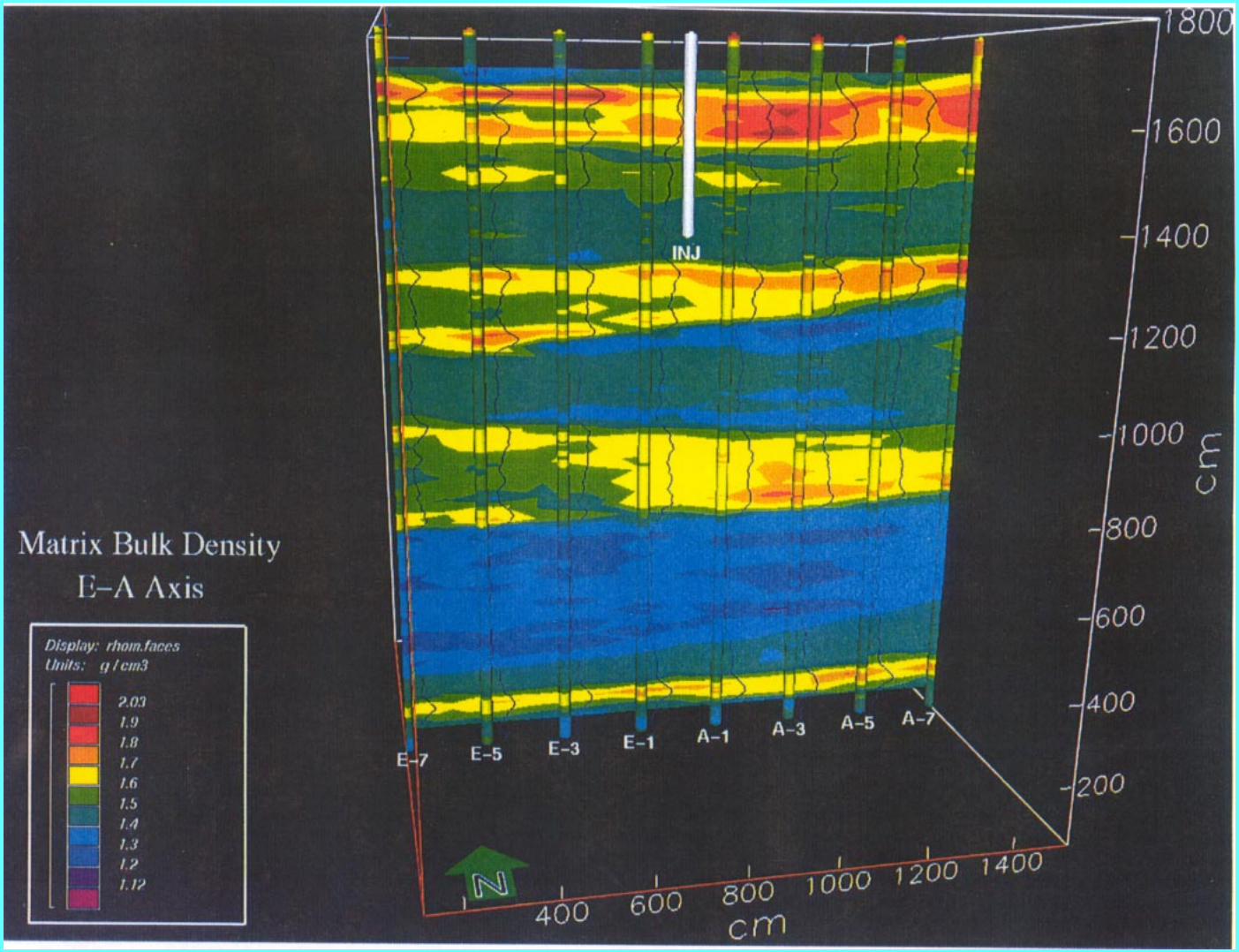
Data from the 1995 Geophysical Logging (15-cm resolution)

- Bulk density along the E-A cross-section



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New Data to be Collected from the Field Site

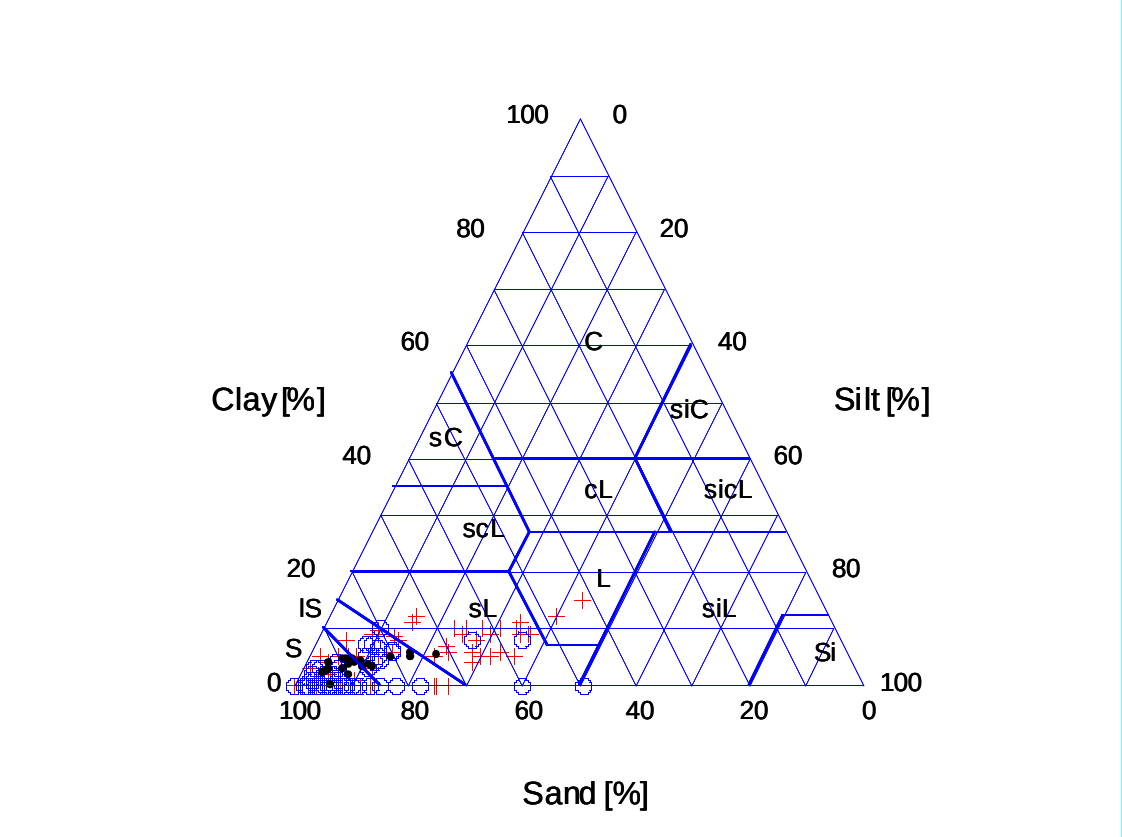
- By this project: particle size distribution, bulk density, porosity, water retention, and hydraulic conductivity on 50-60 core samples
- Methods used by the Hanford Site Vadose Zone Transport Field Study project and its collaborators
  - Neutron probe and advanced tensiometers
  - Electrical resistance tomography
  - Cross-borehole ground-penetrating radar
  - High resolution resistivity and electromagnetic induction
  - Tracer measurements

Neural Network Pedotransfer Function (PTF) Analysis of Existing Hanford Site Data

- Two sets of PTFs were evaluated:
  - "Generic" PTFs derived from measurements on soil samples distributed across the U.S. and covering all soil textures (Schaap and Leij, 1998)
  - Hanford PTFs derived from measurements on soil samples obtained from the 200 East and 200 West Areas of the Hanford Site (Khaleel and Freeman, 1995)
- These PTFs were evaluated using a set of 20 sample measurements obtained from a borehole near the field site [an Immobilized Low-Activity Waste (ILAW) Site borehole] (Fayer et al., 1998)

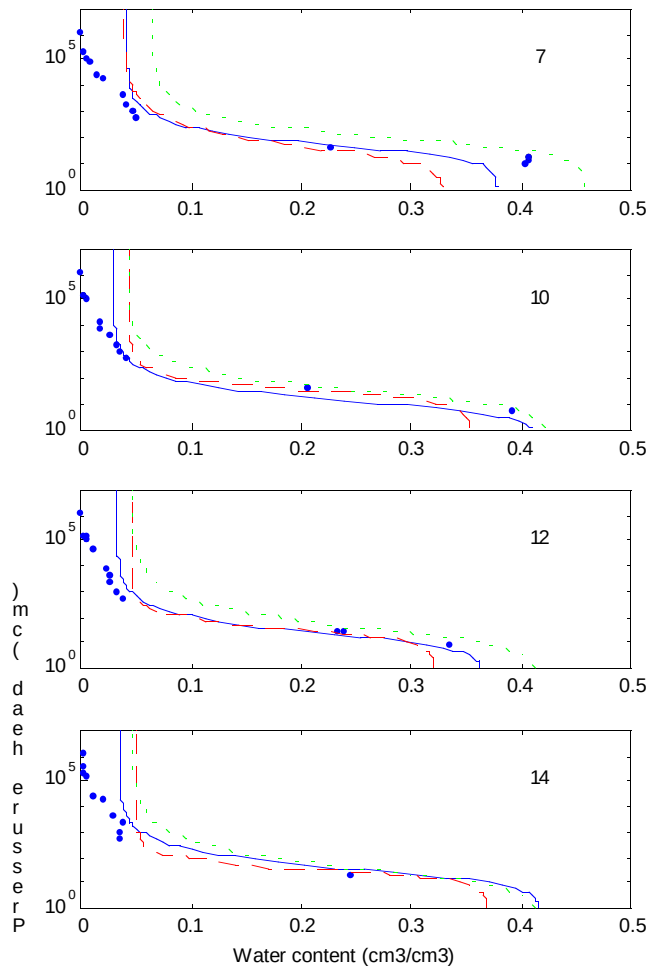
Textural Distribution of Hanford Samples

- 200 West Samples: Red Crosses
- 200 East Samples: Blue Circles
- ILAW Site Samples: Black Dots



Water Retention Results from 4 ILAW Samples (van Genuchten model)

- Measured data: Blue Dots
- “Measured” parameters (from Fayer et al., 1998): Solid Blue Line
- Predictions using “Generic” PTF (sand, silt, clay, bulk density model): Dashed Red Line
- Predictions using Hanford PTF (gravel, coarse sand, fine sand, silt, clay model): Dashed Green Line



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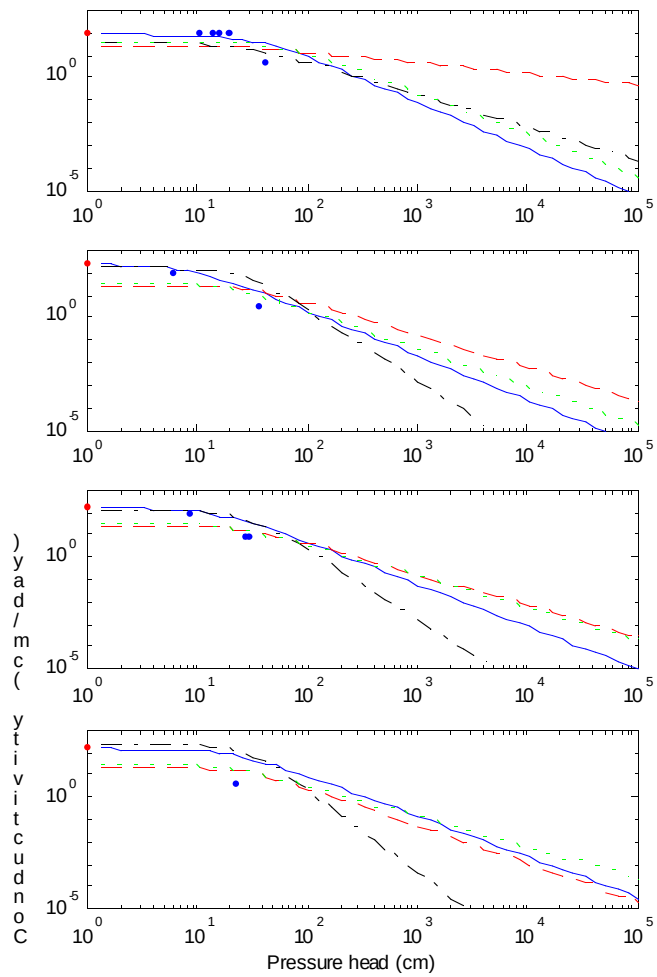
Hydraulic Conductivity Results from 4 ILAW Samples (van Genuchten-Mualem model)

- Measured data: Red and Blue Dots
- Predicted from measured water retention and K_s (from Fayer et al., 1998): Solid Blue Line
- Predictions using “Generic” PTF (sand, silt, clay, bulk density model) and L=0.5: Dashed Black Line
- Predictions using “Generic” PTF (sand, silt, clay, bulk density model) and L fitted: Dashed Red Line
- Predictions using Hanford PTF (gravel, coarse sand, fine sand, silt, clay model) and L=0.5: Dashed Green Line



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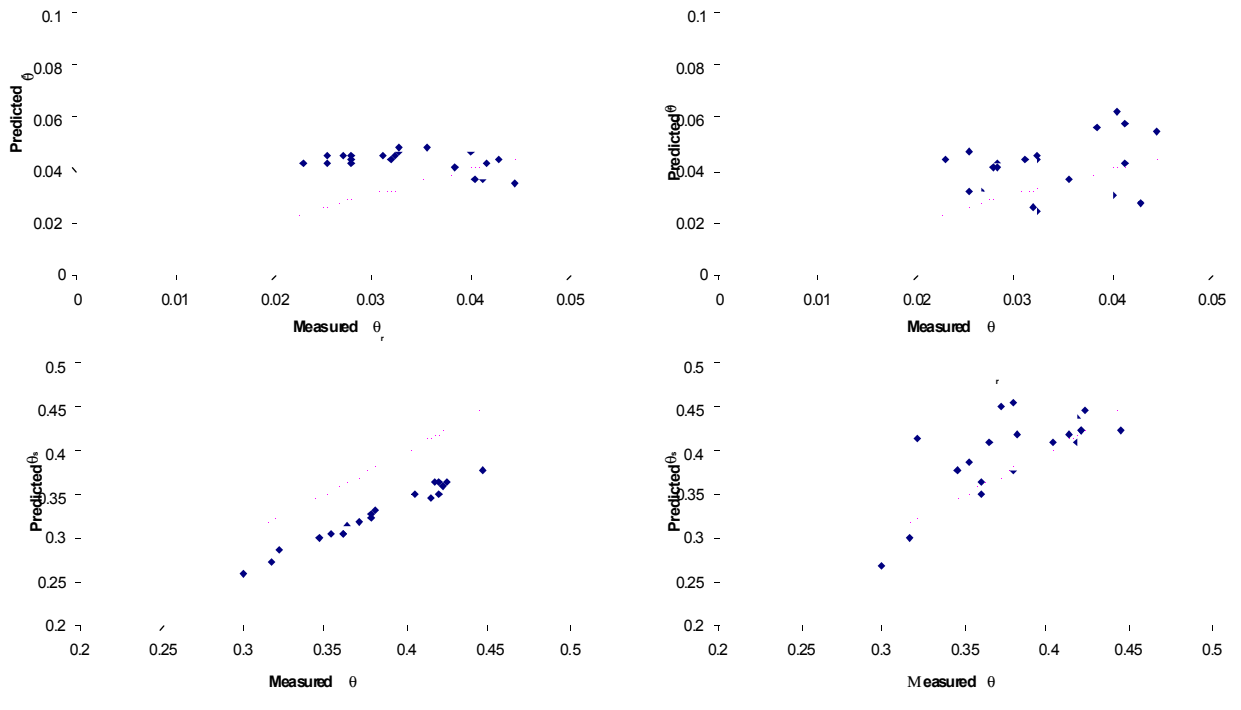
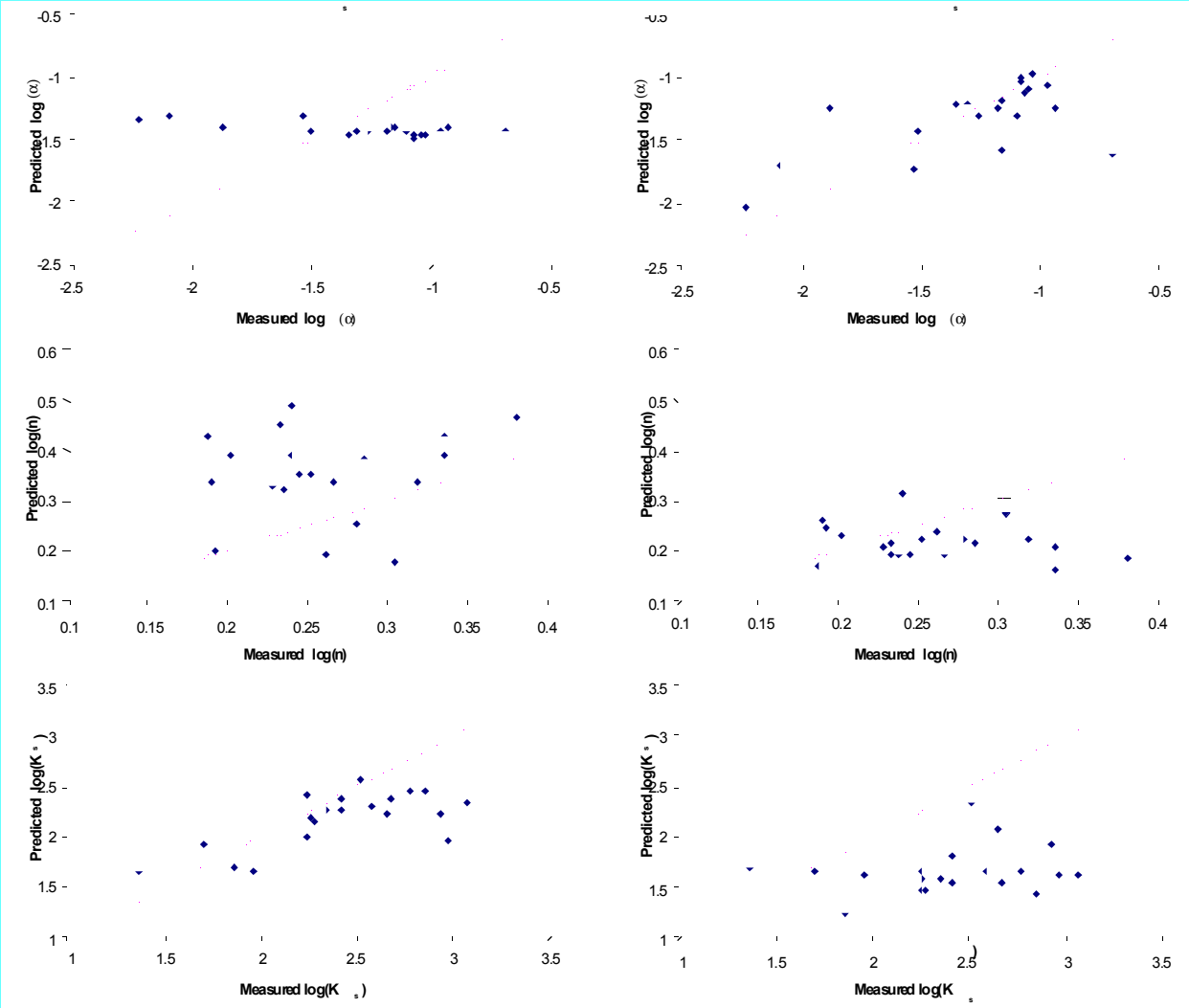
L: pore interaction parameter

Parameter Correlations for 20 ILAW Samples

- Predicted parameter values (from the Generic PTF on the left and the Hanford PTF on the right) vs measured parameter values (from Fayer et al., 1998)



Parameter Correlations for 20 ILAW Samples (continued)



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Preliminary Neural Network PTF Observations

- No clear and compelling differences between the "Generic" and Hanford PTFs when evaluated on the ILAW borehole data
- Evaluation data is limited. Site-specific data to be collected on core samples later this year will be necessary for a better evaluation.
- Van Genuchten water retention model does not reflect the data on the dry end (> 10,000 cm pressure head). Alternative models may be needed.

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