Permeameters for *in situ* Characterization of Unsaturated Heterogeneous Permeability

Project Participants: J. Wilson[1], R. Glass[2], R. Holt[1,2], E. Aronson[1]
[1]New Mexico Institute of Mining and Technology
[2]Sandia National Laboratories

Summary of EMSP Research

Research Objectives

Thick unsaturated zones underlie many Department of Energy (DOE) landfills, industrial areas, and waste storage sites in the western United States and are the primary pathway for contaminants to migrate into underlying aquifers. The spatial variability of unsaturated hydraulic properties in these heterogeneous geologic materials directly influences the movement of water and non-aqueous phase liquids (NAPL's). Poor characterization of heterogeneity may lead to ineffective remedial designs and increased risk, requiring subsequent additional remedial actions at increased cost and time. Remedial design can be improved using probabilistic risk-based decision analysis, which requires a large number of hydraulic property observations. Laboratory methods for estimating the unsaturated permeability are expensive, time-consuming, and may not yield results representative of heterogeneous field conditions. Simple and rapid field methods for estimating *in situ* unsaturated permeability are appealing and potentially cost-effective.

The primary objective of our EMSP research is to design, develop, and test new permeameters for use in spatial variability studies. We have established a series of permeameter design criteria, including: 1) measurements should be relatively rapid, 2) the total cost per data point should be low, 3) results would accurately reflect the variation of unsaturated hydraulic properties between sampled locations, 4) the volume sampled (measurement support) would be small, and 5) useful range would be relevant to the range of soil moisture conditions encountered at DOE sites.

Research Progress and Implications

Analytical Inversion Techniques We evaluated, developed, and verified parameter estimation methods for inverting steady-state permeameter data, including a variety of boundary conditions and source geometries. Several analytical and quasi-analytical techniques for inverting steady-state permeameter data yield estimates of unsaturated hydraulic conductivity at specific tensions that are independent of parametric models. This represents an advantage over numerical estimation techniques, because numerical estimation yields parametric-model-specific parameter values. Because the time-scales required to reach steady state are large, however, steady-state permeameter methods are inconsistent with our first design criterion.

Numerical Simulations Numerical simulations of permeameter performance are an integral part of our approach to permeameter design. We evaluated a variety of unsaturated flow codes, but found that they were computationally inefficient, did not preserve the required precision, did not implement necessary iterative schemes, or lacked other required options (e.g., types of source). Because modification of these codes was not practical, we developed and verified a flexible multi-application code (MAPP). MAPP is a two dimensional, steady-state finite element code for solving horizontal plane, vertical cross-section, and axisymmetric variably-saturated flow problems. It utilizes triangular elements with linear basis functions. Other options include: simultaneous solution of adjoint state equations; Gardner exponential, van Genuchten, and piecewise exponential unsaturated flow models; multiple pre- and post-processors to allow easy preparation and operation, as well as ease of use; choice of Picard or Newton-Raphson schemes for non-linear iteration; and extensive documentation for easy modification.

Error Evaluation We are evaluating the effect of error on the uncertainty of estimated spatial statistics to improve permeameter designs. Elsewhere in this poster, we present in detail some of the results of these efforts.

Effect of Measurement Scale Heterogeneity We hypothesize that measurement-scale heterogeneity will introduce additional uncertainty in estimated spatial statistics for unsaturated hydraulic properties. As a result, we are developing adjoint sensitivity analysis techniques to quantify the impact of measurement scale heterogeneity on hydraulic parameters estimated with various permeameter designs. This approach yields a quantitative measure of the sensitivity of a measured effective property to the heterogeneities present within the measurement support. We have successfully applied this approach to the air permeameter, an instrument that measures saturated hydraulic conductivity in air dry sediments.

Independent Estimates of Scaling Variables We believe that independent estimates of scaling variables, saturated hydraulic conductivity and the air entry value, may be subject to less error, therefore, providing better estimates of spatial statistics. Both of these variables can be estimated with a modification of the air mini-permeameter device. We are currently validating this approach.

Device Design We have completed preliminary permeameter component designs. The basic permeameter design is modular consisting of a water-source package, a hybrid air mini-permeameter, and an instrument package. Development of each package is proceeding independently, allowing for flexibility in specific permeameter configuration.

Planned Activities

We believe that measurement error and bias, caused by systematic errors and measurement-scale heterogeneity, can substantially increase the uncertainty in estimated spatial statistics for unsaturated hydraulic properties. We will, therefore, continue to investigate the effects of these errors and biases with emphasis on minimizing their effect in final permeameter designs. We will specifically examine: boundary condition and flow geometry errors, the effects of improper model specification, data inversion error, and the influence of measurement-scale heterogeneity on effective property bias.

Based upon these results, we will continue to refine and finalize permeameter component designs. Prototype components will be constructed, and their performance verified in the laboratory before field testing. Our final activity will be a field test of the final permeameter design. A field test site has already been selected, and permeameter testing will be performed at a U.S. DOE EMSP project site (project: A Hybrid Hydrogeologic - Geophysical Inverse Technique for the Characterization, Monitoring, and Risk Assessment of Leachates in the Vadose Zone) in Socorro, New Mexico.

Effect of Measurement Error on Estimated Spatial Statistics of Unsaturated Hydraulic Conductivity

Motivation

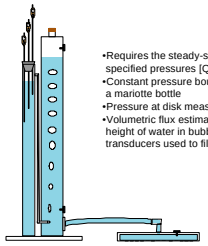
The primary motivation of our EMSP research is to develop permeameters for estimating the spatial variability of *in situ* unsaturated hydraulic conductivity. Measurement errors may significantly limit our ability to recognize spatial variations. We have chosen to illustrate the effect of measurement error on spatial statistics of unsaturated hydraulic parameters determined with a tension infiltrometer. The tension infiltrometer is frequently used for estimating spatial statistics related to unsaturated hydraulic conductivity, because of ease of use, rapid measurements, and low cost. Previous workers, however, have seen very little evidence of spatial correlation, and measurement error may be responsible.

We examine the influence of very small measurement errors on spatial statistics estimated with the tension infiltrometer. We set this work in the context of site characterization for Monte Carlo Simulation of flow and transport. It is important to recognize that we have neglected other more serious errors in this analysis. We feel that the results of this work bear on all aspects of hydraulic property measurement for spatial variability studies.

Suppose We Wanted to Characterize the Spatial Variability of Unsaturated Hydraulic Properties in These Deposits for use in Monte Carlo Simulations of Flow and Transport

Once Sample Locations are Prepared, We Could use a Tension Infiltrometer to Estimate the Hydraulic Properties

Tension Infiltrometer is Designed to Establish Steady, Unsaturated Flow with a Constant Pressure Disk Source



- Requires the steady-state flux-rates at two specified pressures [$Q_1(\Psi_1)$ and $Q_2(\Psi_2)$]
- Constant pressure boundary maintained with a mariotte bottle
- Pressure at disk measured with transducer
- Volumetric flux estimated by measuring height of water in bubbling tower (two transducers used to filter bubbling errors)

We Know that Variogram Estimates, in General, are Subject To Error

- Structural Errors (e.g., sample location)
- Measurement Errors (e.g., pressure transducer error and drift)
- Boundary Condition and Flow Geometry Errors (e.g., pressure or flux not uniformly distributed across flow boundary
- Improper Parametric Model (e.g., $K(\psi)$ not exponential)
- Data Inversion Errors (systematic bias due to inversion)
- Unresolved Physics (e.g., non-isothermal flow)

Interpretation of Results Requires a Simplifying Assumption

- Unsaturated hydraulic conductivity is exponential

$$K(y) = K_s \exp(a\,y)$$

- Inverse solution for α

$$\hat{a} = \frac{\ln(\hat{Q}_1/\hat{Q}_2)}{y_1 - y_2} \quad \text{Samples are Rejected if } \hat{Q}_1 \le \hat{Q}_2$$

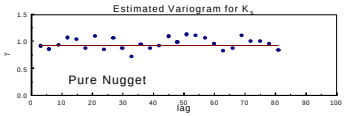
- Inverse solution for K_s

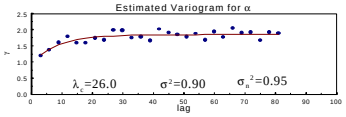
$$\hat{K}_s = \frac{\hat{Q}_1}{p\,r_d^2} e^{-\hat{a}y_1} \left(1 + \frac{4}{p\,r_d \hat{a}}\right)^{-1}$$

Characterizing Our Site Would be Expensive

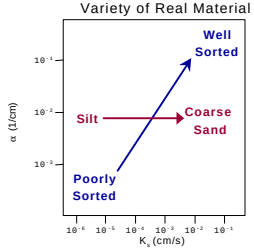
- Pre-characterization activities (~ 200 MH) ~$20K
- Field activities (~500 MH) ~$50K
- Data reduction/reporting (~100 MH) ~$10K
- Equipment costs ~$20K
- Primary product: 200 data points and two variograms (K_s and α)
- Total cost ~$100K

How Much Confidence do We Have in These Results?





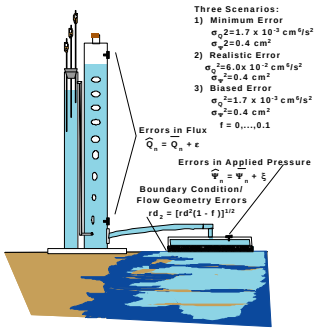
How do These Errors affect Spatial Statistics Estimated from Tension Infiltrometer Data for a Variety of Real Material Types?



How can we characterize the effects of errors on estimated spatial statistics?

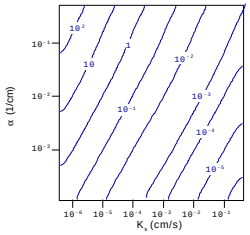
1) Define errors that can be treated
2) Determine how well the device performs through-out its parameter space
3) Examine the effect of errors on estimated spatial statistics

We Evaluate the Effect of Simple Errors on Estimated Spatial Statistics



Over the Material Types of Interest, These Errors are Small

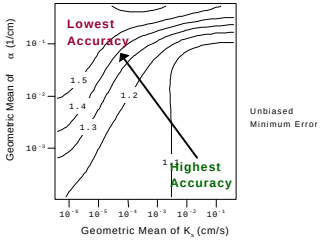
Coefficient of Variation - Minimum Error - Q_1



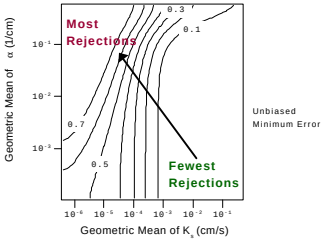
Examine Effect of Geometric Mean of α and K_s on Instrument Behavior using Monte Carlo Simulations

- Fix var[ln(K_s)] and var[ln(α)]
- Generate 16,000 values of α and K_s
- If biased, then change change disk radius for $\bar{Q}_2$ calculation
- Calculate "true" instrument response ($\bar{Q}_1$, $\bar{Q}_2$, $\bar{\Psi}_1$, and $\bar{\Psi}_2$)
- Add instrument noise calculate $\hat{Q}_1$, $\hat{Q}_2$, $\hat{\Psi}_1$, and $\hat{\Psi}_2$)
- Reject sample if $\hat{Q}_1 \le \hat{Q}_2$
- Invert $\hat{Q}_1$, $\hat{Q}_2$, $\hat{\Psi}_1$, and $\hat{\Psi}_2$ for $\hat{\alpha}$ and $\hat{K}_s$
- Calculate geometric mean of $\hat{\alpha}$ and $\hat{K}_s$ and the variance of ln($\hat{K}_s$) and ln($\hat{\alpha}$)
- Set new value of geometric mean of α and K_s
- Repeat 1,600 times

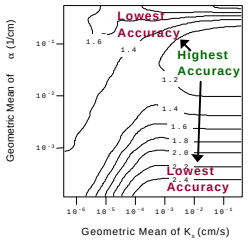
Variance of K_s is More Accurately Estimated at High K_s



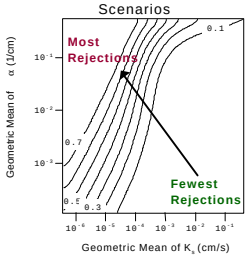
Fraction Points Rejected Decreases as the Geometric Mean of K_s Increases



When the Error is Biased, the Variance of K_s is Poorly Estimated at High K_s



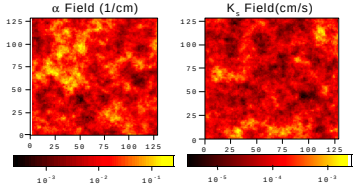
For Biased Error, the Fraction of Points Rejected is Smaller than that for the Unbiased Scenarios



Examine the Effect of Measurement Error on Estimated Spatial Statistics using Monte Carlo Simulations of Correlated Random Fields

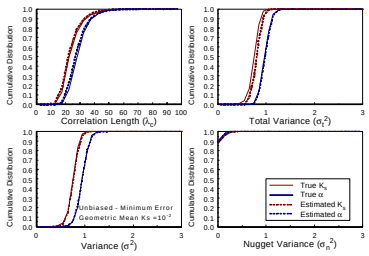
- Fix geometric mean of α and K_s
- Generate correlated random fields (128 x 128) with an exponential variogram: λ_c=30 and var[ln(K_s)]=var[ln(α)]=1.0
- If biased, then change change disk radius for Q_2 calculation
- Calculate "true" instrument response (Q_1, Q_2, Ψ_1, and Ψ_2)
- Add instrument noise, calculate Q_1, Q_2, Ψ_1, and Ψ_2)
- Reject sample if $Q_1 \le Q_2$
- Invert Q_1, Q_2, Ψ_1, and Ψ_2 for α and K_s
- Select 200 points, calculate variogram for α, K_s, α, and K_s
- Fit exponential variogram, calculate λ_c, σ^2, and σ_n^2
- Repeat variogram calculations and fits 500 times
- Calculate distributions of λ_c, σ^2, and σ_n^2

Random Fields used in Study

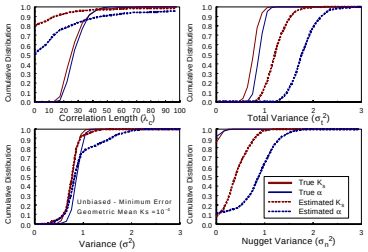


Model Variogram $g = s^2\left[1 - \exp\left(-\frac{3h}{l_c}\right)\right]$ $l_c = 30.0$ $s^2 = 1.0$

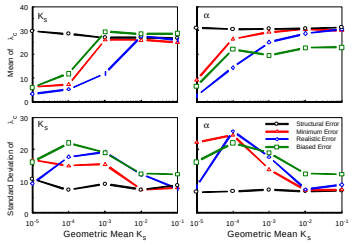
For High Geometric Mean of K_s, Variogram Parameters show "Only" Structural Error



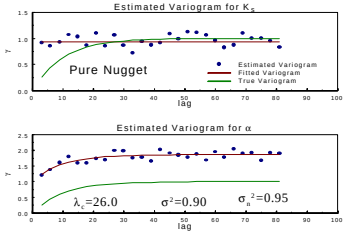
For Smaller Geometric Mean of K_s, Variogram Parameters with Measurement Error show Bias and Noise



Estimated Correlation Lengths are Very Uncertain when the Geometric Mean of Ks is Low



We have Spent $100K but have Very Little Confidence in these Results



What Have We Learned?

- The errors depend upon the sampled field - they cannot be modeled as homogeneous white noise
- Very small amounts of measurement error can translate into huge uncertainties in estimated spatial statistics - Not all sources of error were considered here
- Estimated spatial statistics are biased by to the fraction of points rejected and non-homogeneous forms of measurement error
- Small measurement errors may preclude satisfactory estimation of parameters for Monte Carlo simulations of flow and transport

What can We do?

- Characterize the effect of device-specific measurement errors on estimated spatial statistics - define parameter regions where device works
- Develop highly accurate devices for measuring unsaturated hydraulic properties
- Develop alternative models that use easily measured parameters
- Other (e.g., Geological process modeling)