2007

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Geostatistical and Stochastic Study of Radionuclide Transport in the Unsaturated Zone at Yucca Mountain

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Motivation: Why Study of Unsaturated Zone?

- The unsaturated zone (UZ), where the proposed repository would be located, acts as a critical natural barrier by delaying the arrival of radionuclides at the saturated zone and by reducing radionuclide concentrations in groundwater through dispersion and dilution.

- Quantitative prediction of radionuclide transport in the unsaturated zone becomes critical for performance assessment and design of the proposed repository of the Yucca Mountain Project.
Motivation: Why Geostatistical and Stochastic Methods?

- Previous study (e.g., numerical simulations conducted by LBNL) assumes that hydraulic parameters within each model layer of the unsaturated zone are constant and deterministic.

- Field measurements show that hydraulic parameters vary significantly within and between the layers. Hydraulic parameters are inherently uncertain.

- Few investigation has been conducted to study the uncertainty, especially in a three-dimensional, mountain-scale modeling domain.

- Geostatistical and stochastic methods are used to assess the parametric uncertainty, conditioned on site measurements and model calibration results.
Project Duration and Task Completion

Project duration:

Project Tasks:
• Data collection (100%)
• Geostatistical study of heterogeneity (100%)
• Monte Carlo simulation of groundwater flow and solute transport (95%)
• Develop and apply a numerical method of moments for a sensitivity study of how various random parameters affect flow and transport (70%)

This task generates none-quality-affecting results for information only, and was subcontracted to Dr. Bill Hu at the Florida State University since the project started in 10/2004.
Task 1: Data Collection
(100% Completed)

• Compile Q and none-Q data from TDMS database for scope study.

• Measurements of state variables
  – Water saturation
  – Water potential

• Core-scale rock properties
  – Porosity
  – Permeability
  – Capillary parameters for rock matrix
  – Sorption coefficient of the rock matrix
Task 2: Geostatistical Study of Heterogeneity (100% Completed)

Geostatistical methods are used to generate random fields of hydraulic parameters to incorporate parameter uncertainty.

Random fields are generated in two related ways:

- Hydraulic parameters are random, and homogeneous within each model layer (layer-scale heterogeneity is addressed)
- Hydraulic parameters are random, and heterogeneous within each layer (layer-scale and local-scale heterogeneity is addressed)
Task 3: Stochastic Simulations (95% Completed)

- Monte Carlo method is used to assess radionuclide transport uncertainty.
- Random fields generated in Task 2 are used in the Monte Carlo simulations.
- Simulated matrix saturations are compared with field measurements.
- Uncertainty in travel time of radionuclide is assessed.
Task 3: Future Work

- Complete all the Monte Carlo realizations.
- Analyze simulation results to investigate parametric uncertainty of radionuclide transport at the unsaturated zone.
- Determine sensitivity of travel time uncertainty to parametric uncertainty, and provide guideline of uncertainty reduction.
Task 4: Development of Numerical Moment Method (70% Completed)

- Moment equations have been derived and numerical codes of solving the equations are developed.

- Numerical simulations have been conducted for synthetic cases.
Task 4: Future Work

- Apply the numerical moment method to this project.
- Develop a software of NMM3 based on previous work of Hu conducted for saturated zone of Yucca Mountain.
Numerical Grid

From Wu et al. (2004)
A typical cross section of unsaturated zone at Yucca Mountain (Wu et al., 2004)
Distribution Identification

• Data transformation
  - Saturated hydraulic conductivity, porosity, and sorption coefficient
  - Lognormal (LN), Log ratio (SB), Hyperbolic
  - arcsine (SU), $1/X$, $X^{1/2}$, $X^{1/3}$, $X^2$

• Lillifors Test
Distribution Identification

Empirical and theoretical CDF for transformed hydraulic parameters (Ye et al. 2007)
Homogeneous Random Field Generation

- Latin Hypercube sampling (LHS) method
- 200-realization random fields of hydraulic parameters
- Spearman Rank correlation
Results

Histograms of measured and generated hydraulic parameters (Ye et al. 2007).
Heterogeneous Random Field Generation

Procedure of heterogeneous random field generation:

1. **START**
2. Transform measurements following Ye et al. (2007)
3. Conduct GSLIB normal score transformation
4. Determine correlation length
5. Generate random fields using SGSIM in 3-D regular domain
6. Conduct GSLIB normal score back transformation
7. Interpolate random fields to the 3-D irregular Yucca Mountain UZ domain
8. Transform random fields back to original scale based on Ye et al. (2007)
9. Shift the generated random fields if calibrated inputs in Wu et al. (2004) beyond the range of generated data
10. **STOP**
Correlation Length Determination

Sample and fitted variograms of transformed measurements in matrix permeability and porosity for Layer TLL.
Results

Mean and variance of generated random Log permeability at east-west cross section through borehole UZ-14.
Uncertainty Assessment of Flow and Transport

- Monte Carlo simulation
- TOUGH2 Code
- Homogeneous case: layer-scale heterogeneity of hydraulic parameters
- Heterogeneous case: layer-scale and local-scale heterogeneity of hydraulic parameters
Flow Results: Homogeneous Case

Comparison of observed and 3-D model simulated matrix liquid saturation for borehole SD-12 (Ye et al., 2007)
(a) Mean (b) variance, (c) 5th percentile, and (d) 95th percentile of simulated percolation fluxes at the water table (Ye et al., 2007).
Comparison of observed and 3-D model simulated matrix liquid saturation for borehole SD-12.
(a) Mean (b) variance, (c) 5\textsuperscript{th} percentile, and (d) 95\textsuperscript{th} percentile of simulated percolation fluxes at the water table.
Comparison

Variance of percolation flux (a) heterogeneous case at water table, (b) homogeneous case at water table, (c) heterogeneous case at repository layer, (d) homogeneous case at repository layer.
Simulated breakthrough curves of cumulative mass arriving at the water table for (a) the conservative tracer ($^{99}$Tc).
Simulated breakthrough curves of cumulative mass arriving at the water table for (b) the reactive tracer (237Np).
Variance after 1,000,000 years, (a) $N_p$ for heterogeneous case; (b) $N_p$ for homogeneous case; (c) $T_c$ for heterogeneous case; (d) $T_c$ for homogeneous case.
Summary

- Generated random fields agree well with the measurements, to represent probabilistic distributions of random hydraulic parameters.
- The uncertainty bounds of saturation include a large portion of the measurements, suggesting that data variability can be partially explained by parametric uncertainty and heterogeneity.
- The uncertainty of flow and transport is significantly reduced by conditioning field measurements of hydraulic parameters.
Publications


- Effect of matrix retention parameters in radionuclide transport uncertainty in the unsaturated zone of Yucca Mountain (In preparation).