Characterizing Flow and Transport in highly heterogeneous media - A theoretical study

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Talk Focus

- Strongly heterogeneous media -> spatial variability of point measurements
  - manifested in flow channeling and fast paths
- How uncertainties inherent in site characterization will influence performance predictions
- How site specific data should be assimilated into performance assessment process
  - reduce uncertainty of prediction
  - finite amount of data
- A site specific example
Outline

- Stochastic Continuum Model of a fracture medium
  - Site specific hydrological data from SKB's Aspo Hard Rock Laboratory

- Transport Predictions Sensitive to the Structures of Heterogeneity
  - Sensitivity depends on choice of predictive quantity/performance measure

- Calculations to Quantify Uncertainties in Transport from Single Canister Sources

- Fickian Limit Not Reached
  - Implication to inference from small scale testing to large scale prediction

- Concluding Remarks
SKI SITE-94 Project

- Part of Swedish Nuclear Power Inspectorate's strategy for developing integrated Performance Assessment as a licensing tool for nuclear waste repositories.
  - Alternative geological, hydrological, transport, geochemical conceptual models
  - Dress rehearsal: from site characterization to performance assessment

- Based on surface and borehole data (1986-1990) from SKB's Aspo Hard Rock Laboratory
  - Geological
  - geophysical
  - hydrological
  - geochemical
Figure 3.15  Location map of boreholes on Åspö
Figure 12. Map of extensive fractures which are identified in boreholes by means of fracture logs and borehole radar measurements. A 3D model is presented below in Figures 13-15.
Class 0

\[ \gamma(h) \times 10^{-21} \]

\[ \sigma^2 = 1.1 \times 10^{-19} \]

Class 1

\[ \gamma(h) \times 10^{-21} \]

\[ \sigma^2 = 1.95 \times 10^{-19} \]

Class 2

\[ \gamma(h) \times 10^{-18} \]

\[ \sigma^2 = 2.15 \times 10^{-17} \]
Stochastic Continuum Hydrological Model

◆ Geostatistical generation of 3D hydraulic conductivity field conditioned on “point” data of injection test in 3m packed sections
  – Variograms of “point” data display only short range correlation
  – Clustered nature of data cannot discriminate presence or absence of long range correlation structure

◆ Option of incorporating geological information of major fracture zones
  – Very transmissive structures with long correlation lengths
  – Used as “soft” data

◆ Single continuum representation of both the fractures and the rock matrix

◆ Flow results calibrated by interference pumping test

◆ Stochastic transport calculations by particle tracking
Conditioned Sequential Indicator Simulation

- Non-parametric technique (Gomez-Hernandez) - no particular distribution model is assumed; data are divided into classes bounded by indicators.
- Indicator covariance defined in terms of joint probability of two values in space.
- Classes of extreme values may have covariance different from the rest.
- If the extreme values of hydraulic conductivity are given a large correlation length, the generated field can have long range connectivity for only the extreme values.
- Allows concentration of large conductivities in specified planes of orientations - fractures in the stochastic continuum representation.
Stochastic Continuum Model

Fracture Network Model
Pumping KAS 02, 03, 06 and HAS 13, All Sections

- Packed Sections
- Good Hydraulic Contacts

Distance (m) From Pumped to Observed Section

LPT2 All Hydraulic Communication

- Observed Sections
- All Hydr. Comm.

Distance (m) from Pumped to Observed Section

Pumping All Sections, KAS 02, 03, 06 and HAS 13

- Packed Sections
- Good Hydraulic Contacts

Distance (m) From Pumped to Observed Section
Appropriate Performance Measure
(What are the feasible predictive quantities for management decisions?)

Solute breakthrough in small areas $A_{ij}$ has strong spatial dependence (Flow Channeling)
Remarks on Tracer Breakthrough Results

- Discrimination of fracture-dominated systems versus heterogeneous continuum requires extensive measurements.

- Spatially integrated solute arrivals much less sensitive to alternative heterogeneous systems - similar order of magnitude in solute arrival and concentration.

- Implication on choice of performance measure - quantities to be predicted:
  - "point quantities" - large variations
  - spatially integrated parameter, more stable, more commensurate with our ignorance of the heterogeneous medium.
Tracer breakthrough from single canister sources

- Quantify uncertainties due to spatial variability
- Repeat calculations for hundreds of randomly selected sites of tracer source
- Obtain transport parameters for each breakthrough curve (v and D)
- Distributions of transport parameters are measures of the uncertainty
Fit of 3D Breakthrough Curves by 1D Advective-Dispersive Equation Solution
Distribution of Fitted U(m/yr, left graphs) and D (m²/yr, right graphs), in Logarithm Scale

Reference Case, dip angle 80°
Distribution of Fitted U(m/yr, left graphs) and D (m²/yr, right graphs), in Logarithm Scale

- Isotropic case with only short correlation structure
<table>
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<th>Nomenclature (°)</th>
<th>no. of peaks fitted</th>
<th>$\bar{V} \pm \sigma$ (m/yr)</th>
<th>$\bar{D} \pm \sigma$ (m*m/yr)</th>
<th>no. of peaks fitted</th>
<th>$\bar{V} \pm \sigma$ (m/yr)</th>
<th>$\bar{D} \pm \sigma$ (m*m/yr)</th>
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<td>0.045±0.061</td>
<td>5.9±44.</td>
<td>680</td>
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<td>427</td>
<td>0.014±0.0062</td>
<td>0.43±0.56</td>
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Inference from small scale measurement to large scale predictions

- Compute tracer breakthrough curves from single canister sources for transport distances of 100m, 200m..... up to 600m
- Fitted transport parameters $v$ and $D$ as function of transport distance
Combine full recovery canisters into a single breakthrough curve; one fit at each distance.
Summary

- **Stochastic continuum model**
  - Non-parametric sequential indicator simulation conditioned to data
  - Long range correlation structures to account for fractures
  - Different heterogeneity structures, all consistent with data, to evaluate model uncertainty

- **Choice of Performance Measure**
  - Large uncertainty if "point" quantities are chosen as predictive quantity/performance measure - probably will never have enough data
  - Spatially integrated solute arrivals less sensitive to heterogeneity structures - more commensurate with our ignorance of the heterogeneous medium
Transport from Single Canister Sources Releases
- Fit of 3D flow and transport results by 1D advective-dispersive equation
- $v$ and $D$ for hundreds of calculations to quantify associated variability

Demonstrate an approach to go from site characterization data to performance assessment
- Fickian limit not reached - cannot infer from small scale measurement to large scale predictions

Caution in using the Predictions - inherent ignorance of a strongly heterogeneous system
- spatial variability
- model uncertainty