Unsaturated Zone Flow and Transport at Yucca Mountain

- George Zyvoloski
- Los Alamos National Laboratory
- NWTRB Board Meeting
- July 11-13, 1994
Los Alamos Radionuclide Migration Program

- Mineral Stability
- Mineralogy/Petrology
- Groundwater Chemistry
- Solubility
- Speciation
- Radiocolloids
- Natural Colloids
- Sorption
  - Biological Term
  - Radionuclide Migration (RSA)
  - Site Performance
- Flow Conditions
- Pathways
- Dispersion
- Diffusion

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Retardation Sensitivity Analysis

- **Flow**
  - Fractures
  - Faults
  - Infiltration
  - Thermal Load

- **Sorption**
  - Min/Pet
  - Geochemistry

- **Numerical**
  - Geometric Realization
  - Numerical Diffusion
Outline of Talk

- Technical Challenges
- Solution Approaches
- Applications
- Concerns
- Future Developments
Technical Challenges

- Very Long Time Frame
- Complex Geologic Setting
- Complex Flow and Transport Mechanisms
Complex Geologic Setting

- 20 Defined Hydrogeologic Units
- More Units needed for Transport (Zeolite Zones)
- Topography Affects Infiltration and Gas Flow
20 Defined Hydrogeologic Units

- Stratigraphy/Topography Data from Project Databases
  - Sandia
  - USGS/LBL

- Other Data Includes
  - Intrinsic Permeability
  - Relative Permeability and Capillary Data
  - Fracture Volumes and Spacing
  - Faulting
Complex Flow and Transport Mechanisms

- Air/Water Vapor/Water/Heat
- Fracture Flow
- Dry Unsaturated Media
- Complicated Sorption and Diffusion
- Coupled Flow and Geochemistry
Complicated Sorption and Diffusion

- Retardation Factors Vary with Unit Type and Zeolitization
  - Data Obtained from Los Alamos Studies
  - Validation Studies are Planned
  - Fracture Data will be Provided

- Diffusion Can Be Important in Fracture Flow
  - Competition Between Fracture Flow and Matrix Diffusion
  - Data Obtained from Los Alamos Studies
Solution Approaches: FEHM Numerical Model

- Fully Coupled Fully Implicit Numerics
- Grid Generation
- Finite Element/Finite Volume Numerics
- Nonisothermal Multiphase
- Dual Porosity/Dual Permeability Module
- Comprehensive Transport/Geochemistry Module
Applications

- Grids
- Transport Studies
- 3-d Flow and Transport (Conservative Tracer)
High and Low Resolution Structured and Unstructured Mesh
Transport Studies

- $^{36}$Cl - Residence Time Indicator
- Np
- Dissolution/Precipitation with Repository Heat
Antler Ridge Cross Section, Yucca Mountain

Colors Denote Different Stratigraphic Units
Cl-36 Distribution, Low Infiltration Rate

Distance, m

Elevation, m

Normalized Cl-36 Concentration
Cl-36 Distribution, High Infiltration Rate

Distance, m

Elevation, m

Normalized Cl-36 Concentration
**FEHM Np Transport Time Simulations**  
*(Continuum Model)*

<table>
<thead>
<tr>
<th></th>
<th>Np Transport Time* (million yr)</th>
<th>Infil. Rate = 0.0365 mm/yr</th>
<th>Infil. Rate = 0.365 mm/yr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom</td>
<td>2.3</td>
<td>0.25</td>
<td></td>
</tr>
<tr>
<td>Middle</td>
<td>6.4</td>
<td>1.1</td>
<td></td>
</tr>
<tr>
<td>Top</td>
<td>∞</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>Entire Repository</td>
<td>4.8</td>
<td>0.45</td>
<td></td>
</tr>
</tbody>
</table>

* time for 1% of Np to reach the water table

\[ ^{237}\text{Np: } t_{1/2} = 2.14 \times 10^6 \text{ yr} \]

\[ K_d: 4 \text{ g/cc in CHn1 and CHn2, 0.5 g/cc elsewhere} \]
FEHM Np Transport Time Simulations
(Dual Porosity/Dual Permeability Model)

Assumptions
- Total repository breach
- Fracture spacing = 10 m
- Infiltration rate = 0.0225 mm/yr
- \( K_{d,frac} = 0; \ K_{d,\text{matrix}} = 0.5 - 4 \ \text{g/cc} \)

Case 1: \( D_{mol} = 0 \)
Transport time = 25,000 yr

Case 2: \( D_{mol} = 1 \times 10^{-11} \ \text{m}^2/\text{s} \)
Transport time = 240,000 yr

Conclusion: Transport time increases significantly if credit can be taken for matrix diffusion and/or sorption on fracture surfaces.

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Dissolution/ Precipitation with Repository Heat

- Explore Reactions with EQ3/6
- Download Small Set (5-10 Reactions) to FEHM
- Simulate Coupled Flow and Geochemistry

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Temperature at 10000 Years

Elevation, m

Distance, m

Temperature, deg. C
Saturation at 10000 Years Long Geochemical Effect on Permeability

Saturation at 10000 Years

Distance, m

Elevation, m

Distance, m
Distribution of Reacting Solid at 10000 Years

Distribution of Reacting Solid at 10000 Years, Strong Geochemical Effects on Permeability

Fraction of Reacting Solid
Concerns

- Availability of Data
  - Geology
  - Flow Parameters
- Computing Power for Fine Grid Simulations
- Geostatistics (Multiple Realizations)
- Validation or Confidence Building
Where we need to be

- 1,000,000 nodes
- Air/Water/Water Vapor/Heat Physics
- Dual Permeability
- Geochemistry
Future Work

- Fine Grid-Minimum $K_d$
- Parallel Computation
- GUI Interfaces
- Stratigraphic Interfaces (Faults)
- Particle Tracking
Summary

- **Transport**
  - Complex Flow Requires 3-d Models
  - Need to Incorporate Min/Pet Studies

- **Coupled Flow and Geochemistry**
  - Is Important Near the Repository
  - Technically Feasable

- **$^{36}$Cl**
  - Useful in Residence Time Studies
  - Can Indicate Fast Flow Paths Where More Resolution Is Required

- **Np**
  - Significant retardation of Np in Calico Hills Units
  - If significant fracture flow exists, matrix diffusion or fracture sorption will be required to increase travel times