Saturated Zone Radionuclide Transport Predictions and Abstractions for Total System Performance Assessment

Presented to:
U.S. Nuclear Waste Technical Review Board Panel on the Natural System

Presented by:
Bill W. Arnold
Principal Member of Technical Staff
Sandia National Laboratories

March 9-10, 2004
Las Vegas, Nevada
Outline

• Overview of Total System Performance Assessment-License Application (TSPA-LA) Modeling Approach and Abstraction for Saturated Zone Flow and Transport

• Assumptions in Saturated Zone (SZ) Modeling Approach

• Uncertainty in SZ Flow and Transport in TSPA-LA Analyses

• SZ Flow and Transport Modeling Results

• Sensitivity Analysis of SZ Flow and Transport Modeling Results
Radionuclide Migration in the Saturated Zone

Repository

Water Table

Unsaturated Zone Flow and Transport

Saturated Zone Flow and Transport

Biosphere

Contaminated Soil and Water

North

South
General Approach to Saturated Zone Flow and Transport Abstraction in Total System Performance Assessment-License Application

- 3-D SZ site-scale flow and transport model used to simulate radionuclide mass transport to the accessible environment from a point mass source (four source regions below the repository)

- Convolution integral method used to couple radionuclide source term from the Unsaturated Zone (UZ) with the SZ transport in the TSPA-LA calculations

- Radionuclide concentration in groundwater source to the biosphere calculated by dividing radionuclide mass crossing the boundary of the accessible environment by the representative groundwater volume of 3000 acre-ft/year

- Climate change incorporated by scaling radionuclide mass breakthrough curves in proportion to SZ flux changes

- Abstracted 1-D transport model used for radioactive decay chains
Saturated Zone Site-Scale Flow and Transport Model

- Particle tracking method includes radionuclide transport processes of advection, dispersion, matrix diffusion in fractured volcanic units, and sorption
- Simulated flow paths from the repository occur in the upper few hundred meters of the SZ
- Simulated flow paths cross the boundary of the accessible environment approximately 5 km west-northwest of the highway intersection at Amargosa Valley
Convolution Integral Method
1-D Radionuclide Transport Model

- Four simplified decay chains modeled
- 1-D SZ transport model implemented directly in TSPA-LA model using GoldSim software with the “pipe” module
- Radionuclide transport processes in the 1-D model, including matrix diffusion, sorption, and colloid-facilitated transport, are consistent with the 3-D SZ site-scale model

Actinide Radioactive Decay Chains

<table>
<thead>
<tr>
<th>Fission Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>14 C (5.7x10^7)</td>
</tr>
<tr>
<td>10 Sr (29)</td>
</tr>
<tr>
<td>99 Tc (2.1x10^7)</td>
</tr>
<tr>
<td>129 I (1.7x10^7)</td>
</tr>
<tr>
<td>135 Cs (2.2x10^7)</td>
</tr>
<tr>
<td>137 Cs (30)</td>
</tr>
<tr>
<td>232 U (70)</td>
</tr>
</tbody>
</table>

Actinium Series: 241 Am (7x10^7) → 241 Am (432) → 240 Pu (6.5x10^7) → 239 Pu (3.8x10^6)

Neptunium Series: 239 Pu (2.4x10^7) → 239 Np (2.1x10^7) → 239 U (2.3x10^7) → 238 U (4.8x10^7) → 238 Pu (68)

Thorium Series: 235 U (7x10^7) → 235 U (1.6x10^7) → 232 Th (1.4x10^7)

Uranium Series: 232 Th (7x10^7) → 232 Pa (3.3x10^7) → 238 Th (7.3x10^7) → 226 Ra (5.8) → 226 Ra (1.6x10^7)

* Calculated by assuming secular equilibrium
1-D Radionuclide Transport Model
(Continued)

- Comparison between the 3-D SZ Site-Scale Transport Model and the SZ 1-D Transport Model indicates that the 1-D model is accurate for a wide range of parameter uncertainty.

- Figure shows the results of the 3-D model (symbols) compared to the 1-D model (lines) for three cases (fast, median, and slow) of simulated neptunium transport.

The data shown in this figure are based on a model that is appropriately conservative for TSPA analyses and not intended to represent expected breakthrough of radionuclides or groundwater travel time for saturated zone portion of the Yucca Mountain flow system.
Key Assumptions in Abstraction for Total System Performance Assessment - License Application

- Steady-state groundwater flow simulated in the SZ
- Instantaneous change in SZ groundwater flux with climate change; no change in flow paths
- Matrix diffusion from uniformly spaced, parallel fractures in the fractured volcanic units, as implemented in the Sudicky and Frind (1982) analytical solution
- All radionuclide mass at the boundary of the accessible environment is contained in the representative groundwater volume annual usage (3000 acre-ft/year) and the average concentration in this volume is released by pumping to the reasonably maximally exposed individual in the biosphere
Key Assumptions in Abstraction for Total System Performance Assessment - License Application
(Continued)

- Equilibrium, linear sorption occurs in tuff matrix and alluvium

- For transport of radionuclides reversibly attached to colloids, local equilibrium is assumed among the colloids, the aqueous phase, and the aquifer material

- For radionuclides irreversibly attached to colloids, it is assumed there will be no desorption of radionuclides from the colloids

- Colloids are subject to attachment and detachment from the mineral grains, but no permanent filtration of colloids occurs
Uncertainty in Saturated Zone Flow and Transport

- **Groundwater flow and geological uncertainty:**
  - Groundwater specific discharge
  - Horizontal anisotropy in permeability (fractured tuff)
  - Alluvium – tuff contact in the subsurface

- **Radionuclide transport uncertainty:**
  - Matrix diffusion in fractured tuff
    - Flowing interval spacing
    - Effective diffusion coefficient in tuff matrix
    - Flow porosity in tuff
  - Sorption coefficients (tuff matrix and alluvium)
  - Dispersivity (longitudinal, transverse horizontal and vertical)
  - Effective porosity of alluvium
  - Source location
  - Colloid retardation factor (tuff and alluvium)
  - Sorption coefficients onto colloids
  - Groundwater colloid concentration
Uncertainty in Specific Discharge

- Uncertainty in specific discharge is based on results of the SZ expert elicitation and more recent well testing at the alluvial tracer complex.

- The discrete CDF used for uncertainty has 80 percent of probability between 1/3 and 3 times the best estimate of specific discharge.

- The tails of the distribution are taken from the SZ expert elicitation.
Uncertainty Analysis

- Monte Carlo analysis is conducted by sampling uncertain parameters using the Latin Hypercube sampling method.
- Multiple simulations (200 equally likely realizations) of radionuclide transport in the SZ are produced using these uncertain parameter vectors in the 3-D SZ Site-Scale Transport Model.
- Radionuclide transport simulation results consist of radionuclide mass breakthrough curves.
- The resulting “library” of breakthrough curves is used in the TSPA model for probabilistic risk assessment analyses via the convolution integral method.
Transport times for stochastic realizations vary over several orders of magnitude.

Many breakthrough curves exhibit a long “tail” characteristic of diffusive mass transfer in the rock matrix of volcanic units.

Note that breakthrough curves do not include radioactive decay.

The data shown in this figure are based on a model that is appropriately conservative for TSPA analyses and not intended to represent expected breakthrough of radionuclides or groundwater travel time for saturated zone portion of the Yucca Mountain flow system.
Variability in transport times among realizations for $^{237}$Np extends from less than 1000 years to greater than 100,000 years.

Sorption and retardation for $^{237}$Np is generally moderate in alluvium and minor in the matrix of fractured volcanic units.

Approximately half of the realizations exhibit median transport times of greater than 20,000 years in the SZ under present climatic conditions.

Note that breakthrough curves do not include radioactive decay.

The data shown in this figure are based on a model that is appropriately conservative for TSPA analyses and not intended to represent expected breakthrough of radionuclides or groundwater travel time for saturated zone portion of the Yucca Mountain flow system.
Saturated Zone Site-Scale Transport Results (Continued)

- Colloid-facilitated transport of $^{137}\text{Cs}$ occurs by reversible sorption onto colloids
- Sorption of cesium is very strong in the matrix of the volcanic units and in the alluvium
- Given the relatively short half life of $^{137}\text{Cs}$ (30 years), there is essentially zero probability of breakthrough from the SZ predicted
- Note that breakthrough curves do not include radioactive decay

The data shown in this figure are based on a model that is appropriately conservative for TSPA analyses and not intended to represent expected breakthrough of radionuclides or groundwater travel time for saturated zone portion of the Yucca Mountain flow system.
Sensitivity Analysis of Saturated Zone Transport Simulation Results

- Sensitivity analysis provides information on the relationships between uncertainty in individual input parameters (independent variables) and uncertainty in model predictions (dependent variable)

- Median transport time from the simulated mass breakthrough curves is taken as the dependent variable

- Sensitivity analysis results provide:
  - Enhanced understanding of model behavior
  - Valuable information for strategies to reduce uncertainty in model predictions
Stepwise Linear Regression Results

## Uncertain Parameters with Significant Impact on Saturated Zone Transport Simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Parameter Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>GWSPD</td>
<td>Groundwater specific discharge</td>
</tr>
<tr>
<td>FISVO</td>
<td>Flowing interval spacing in volcanic units (effective fracture spacing)</td>
</tr>
<tr>
<td>HAVO</td>
<td>Horizontal anisotropy in permeability in volcanic units</td>
</tr>
<tr>
<td>DCVO</td>
<td>Effective diffusion coefficient in volcanic matrix</td>
</tr>
<tr>
<td>CONC_COL</td>
<td>Concentration of colloids in groundwater</td>
</tr>
<tr>
<td>NVF19</td>
<td>Effective porosity in alluvium</td>
</tr>
<tr>
<td>KDNPAL</td>
<td>Sorption coefficient of neptunium in alluvium</td>
</tr>
<tr>
<td>KDUVO</td>
<td>Sorption coefficient of neptunium in volcanic units</td>
</tr>
<tr>
<td>SRCX1</td>
<td>X location of the point source below the repository (zone 1)</td>
</tr>
<tr>
<td>CORAL</td>
<td>Retardation factor for colloids in alluvium</td>
</tr>
<tr>
<td>CORVO</td>
<td>Retardation factor for colloids in volcanic units</td>
</tr>
<tr>
<td>FPVO</td>
<td>Flowing interval porosity in volcanic units (effective fracture porosity)</td>
</tr>
<tr>
<td>KD_AM_COL</td>
<td>Sorption coefficient of americium onto colloids</td>
</tr>
<tr>
<td>KDRAAL</td>
<td>Sorption coefficient of radium in alluvium</td>
</tr>
<tr>
<td>KDRAVO</td>
<td>Sorption coefficient of radium in volcanic units</td>
</tr>
<tr>
<td>KDSRAL</td>
<td>Sorption coefficient of strontium in alluvium</td>
</tr>
<tr>
<td>KDSRVO</td>
<td>Sorption coefficient of strontium in volcanic units</td>
</tr>
</tbody>
</table>
Summary

- 3-D SZ site-scale flow and transport model is used for radionuclide mass transport simulations in TSPA-LA
- Matrix diffusion is explicitly simulated by the particle tracking method in the SZ site-scale model
- SZ site-scale transport modeling results are abstracted for TSPA calculations using the convolution integral method
- 1-D radionuclide transport model is used to simulate SZ transport for decay chains
- Uncertainty in key groundwater flow and radionuclide transport parameters is incorporated into multiple realizations of the SZ system
- Sensitivity analysis indicates that uncertainties in specific discharge and flowing interval spacing have the greatest impact on uncertainty in transport predictions for most radionuclides