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:
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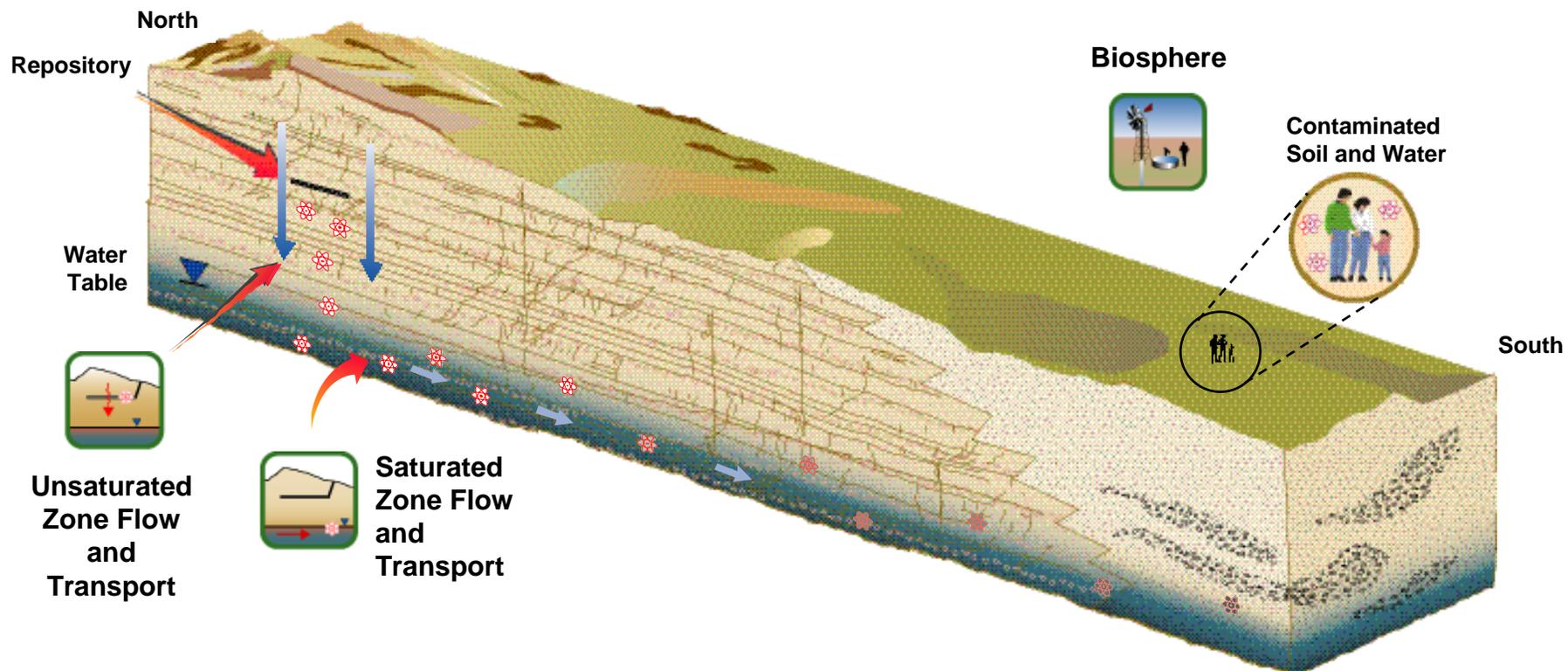**Sandia National Laboratories**

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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

North

Repository

Water Table

Biosphere

Contaminated Soil and Water

South

Unsaturated Zone Flow and Transport

Saturated Zone Flow and Transport

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**

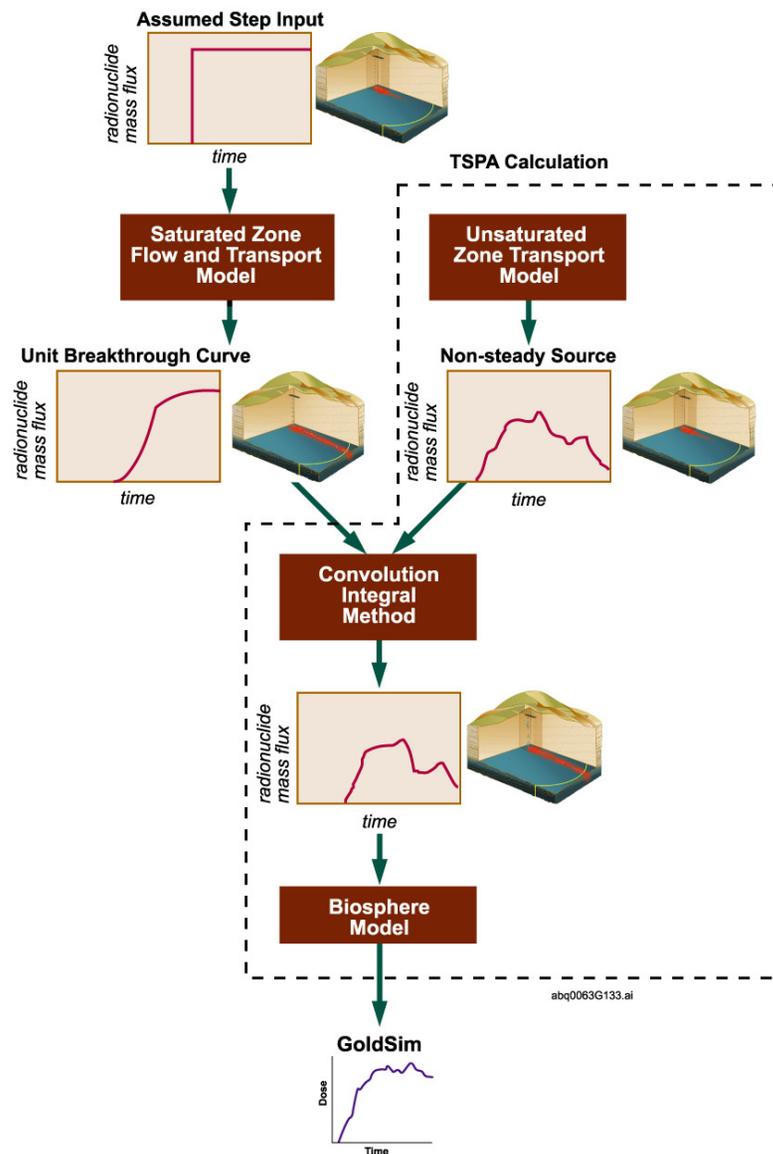- **Abstracted 1-D transport model used for radioactive decay chains**

Saturated Zone Site-Scale Flow and Transport Model
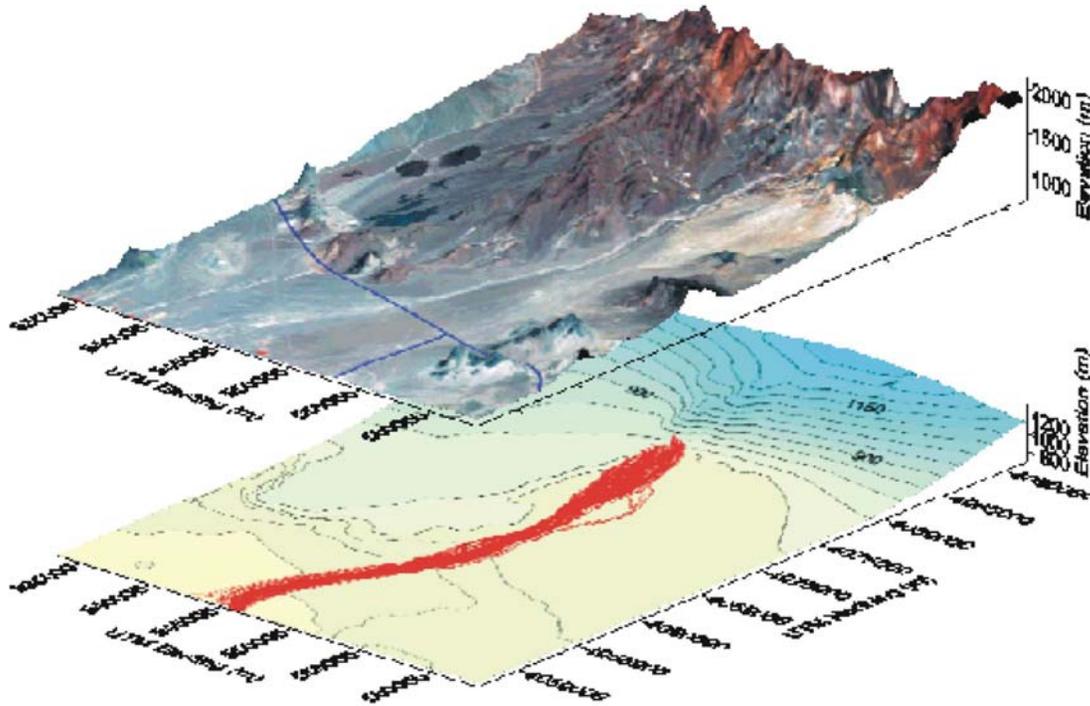
- **Particle tracking method includes radionuclide transport processes of advection, dispersion, matrix diffusion in fractured volcanic units, and sorption**

- **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**
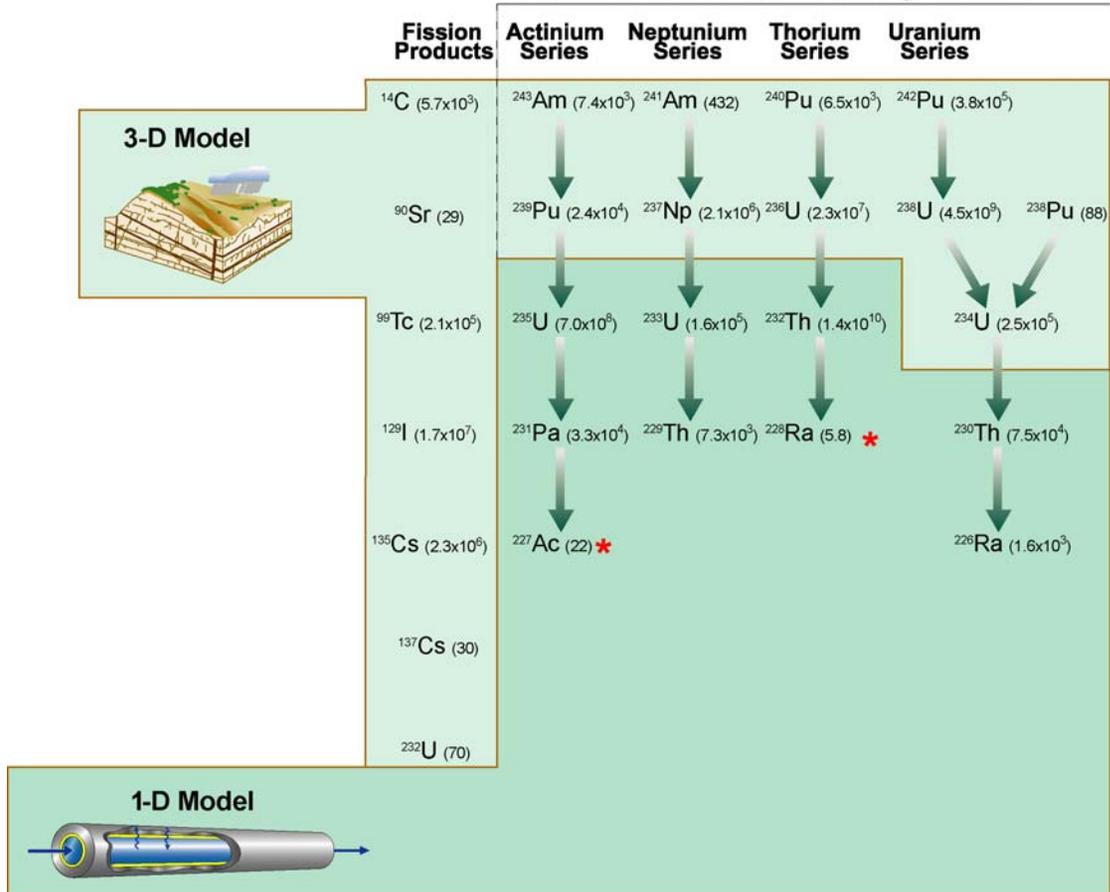
Convolution Integral Method

1-D Radionuclide Transport Model

Actinide Radioactive Decay Chains

| Fission Products	Actinium Series	Neptunium Series	Thorium Series	Uranium Series
^{14}C (5.7x10³)	^{243}Am (7.4x10³)	^{241}Am (432)	^{240}Pu (6.5x10³)	^{242}Pu (3.8x10⁵)
^{90}Sr (29)	^{239}Pu (2.4x10⁴)	^{237}Np (2.1x10⁶)	^{236}U (2.3x10⁷)	^{238}U (4.5x10⁹) ^{238}Pu (88)
^{99}Tc (2.1x10⁵)	^{235}U (7.0x10⁸)	^{233}U (1.6x10⁵)	^{232}Th (1.4x10¹⁰)	^{234}U (2.5x10⁵)
^{129}I (1.7x10⁷)	^{231}Pa (3.3x10⁴)	^{229}Th (7.3x10³)	^{228}Ra (5.8) *	^{230}Th (7.5x10⁴)
^{135}Cs (2.3x10⁶)	^{227}Ac (22) *			^{226}Ra (1.6x10³)
^{137}Cs (30)				
^{232}U (70)				

3-D Model

1-D Model

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* Calculated by assuming secular equilibrium

- **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**

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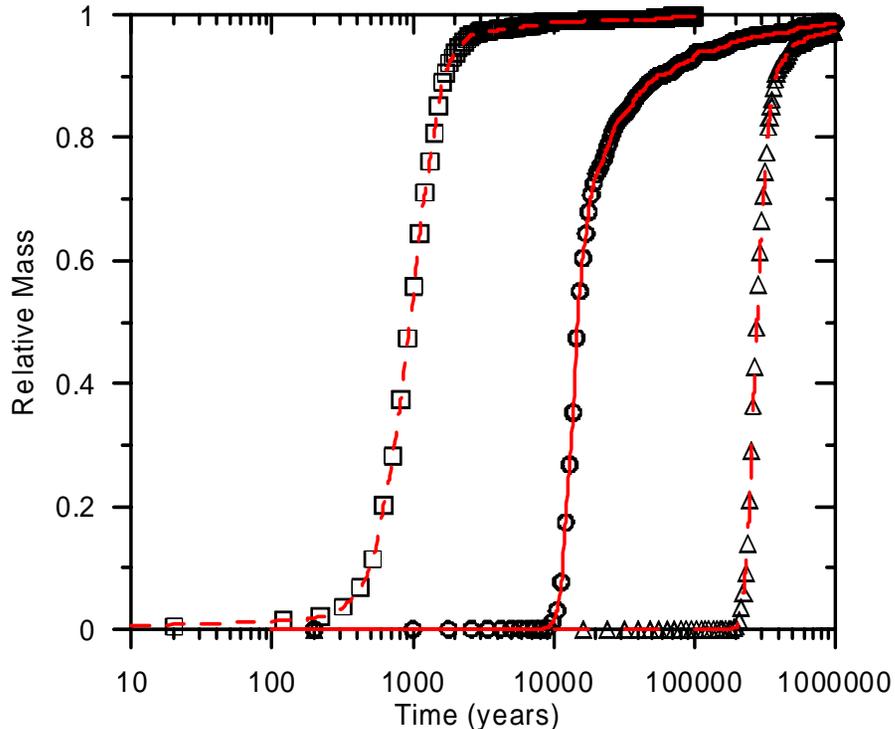
- **Comparison between the 3-D SZ Site-Scale Transport Model and the SZ 1-D Transport Model indicates that the 1-D model is accurate for a wide range of parameter uncertainty**

- **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

Cumulative Probability vs. Log Groundwater Specific Discharge Multiplier
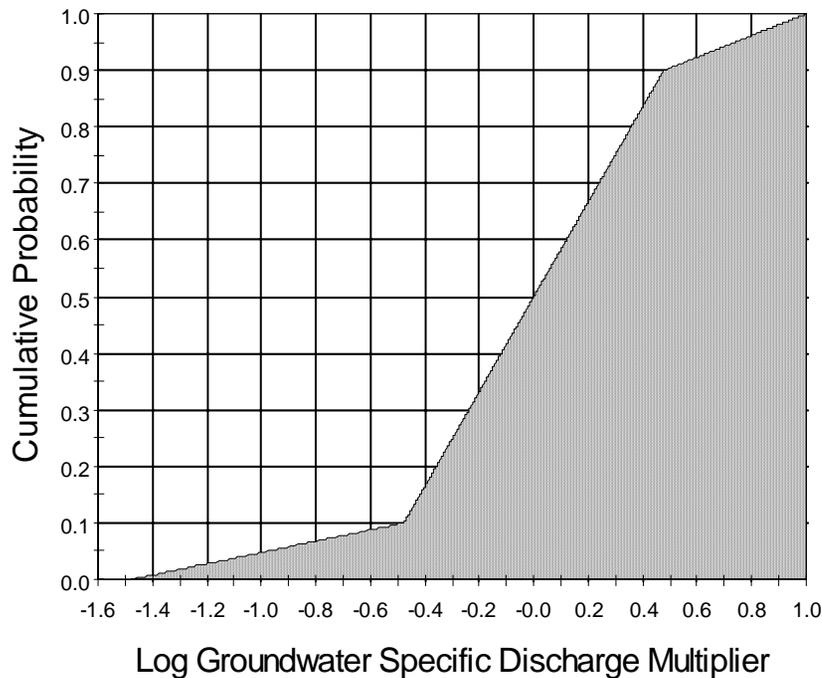
- **Uncertainty in specific discharge is based on results of the SZ expert elicitation and more recent well testing at the alluvial tracer complex**

- **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**

Saturated Zone Site-Scale Transport Results

Simulated Unit Breakthrough Curves and Histogram of Median Travel Times of Mass Flux for Non-Sorbing Species, Present Climate
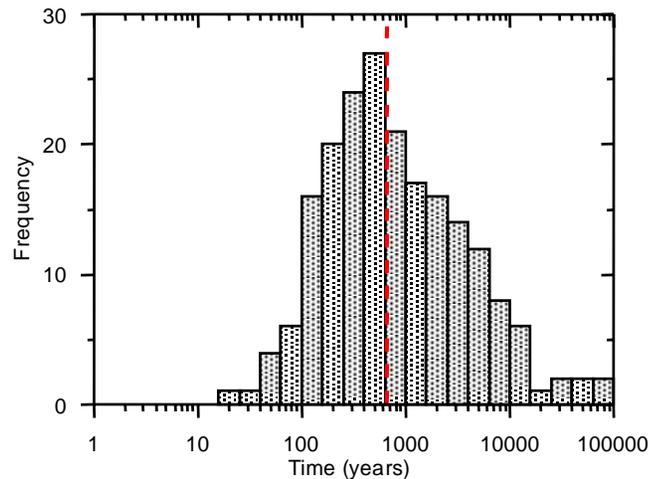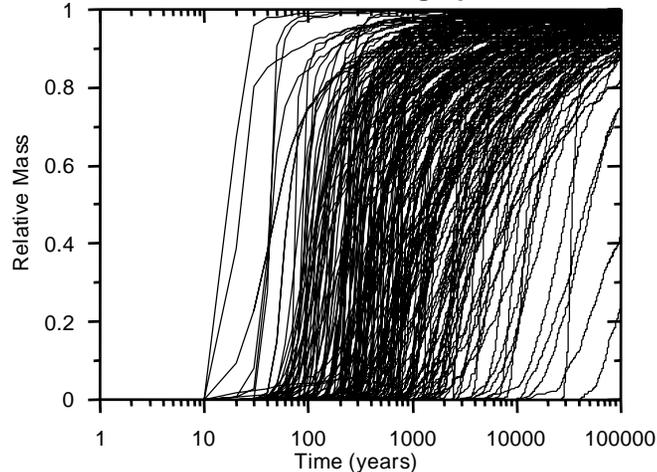
- **Transport times for stochastic realizations vary over several orders of magnitude**

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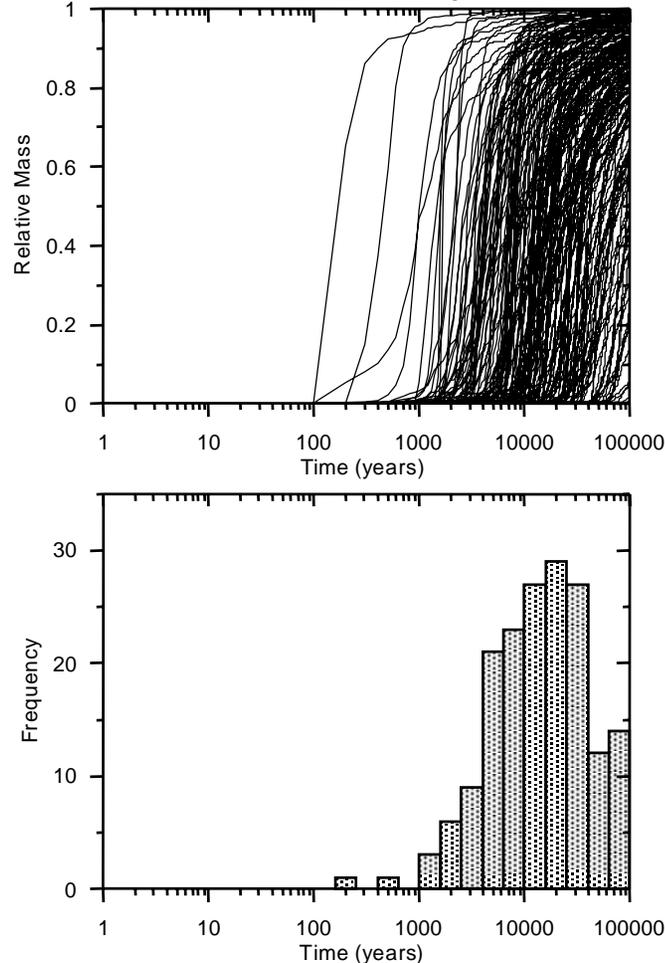
The data shown in this figure are based on a model that is appropriately conservative for TSPA analyses and not intended to represent expected breakthrough of radionuclides or groundwater travel time for saturated zone portion of the Yucca Mountain flow system.

Saturated Zone Site-Scale Transport Results
(Continued)

Simulated Unit Breakthrough Curves and Histogram of
Median Travel Times of Mass Flux for Neptunium, Present Climate

- **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**

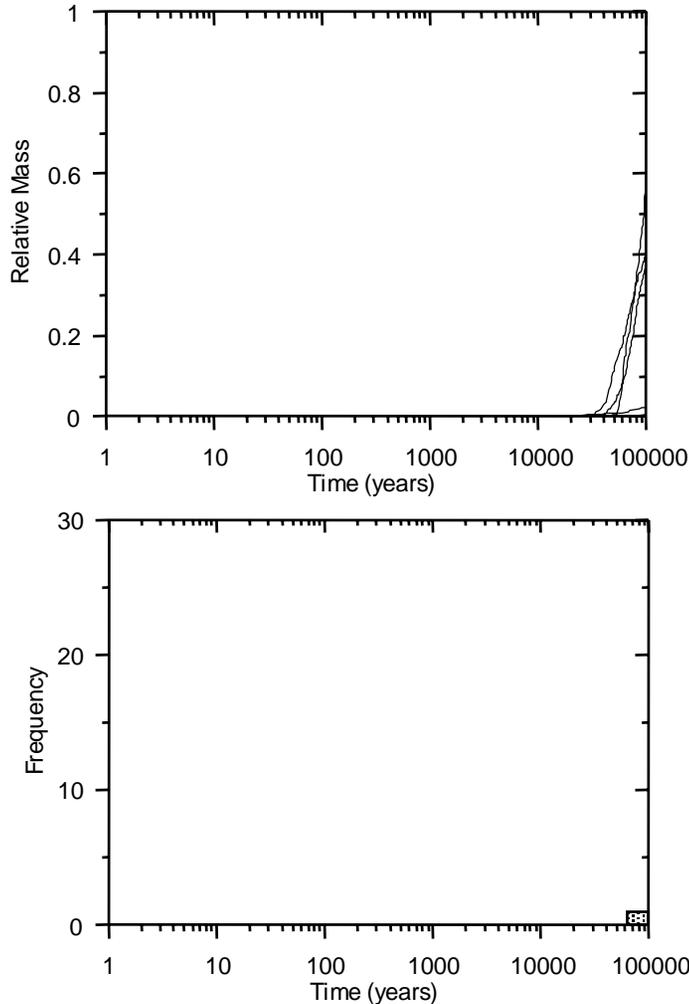- **Note that breakthrough curves do not include radioactive decay**

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)

Simulated Unit Breakthrough Curves and Histogram of Median Travel Times of Mass Flux for Cesium, Present Climate

- **Colloid-facilitated transport of ^{137}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}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
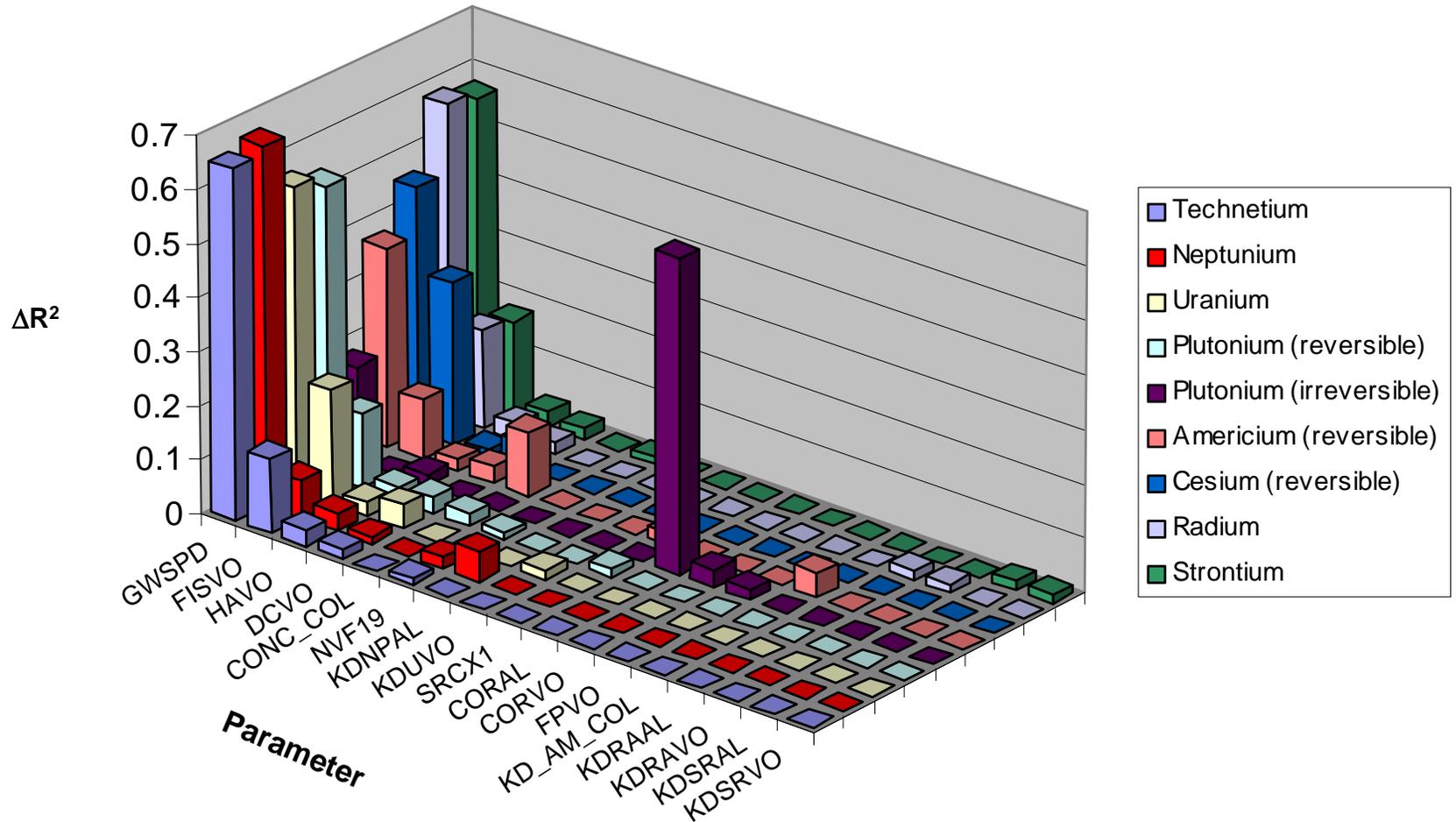
from Arnold and Kuzio (2004)

Uncertain Parameters with Significant Impact on Saturated Zone Transport Simulations

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

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**