U.S. Department of Energy
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Sorption, Matrix Diffusion and Colloid-Facilitated Transport in Saturated Zone Radionuclide Transport Models

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Presented by:
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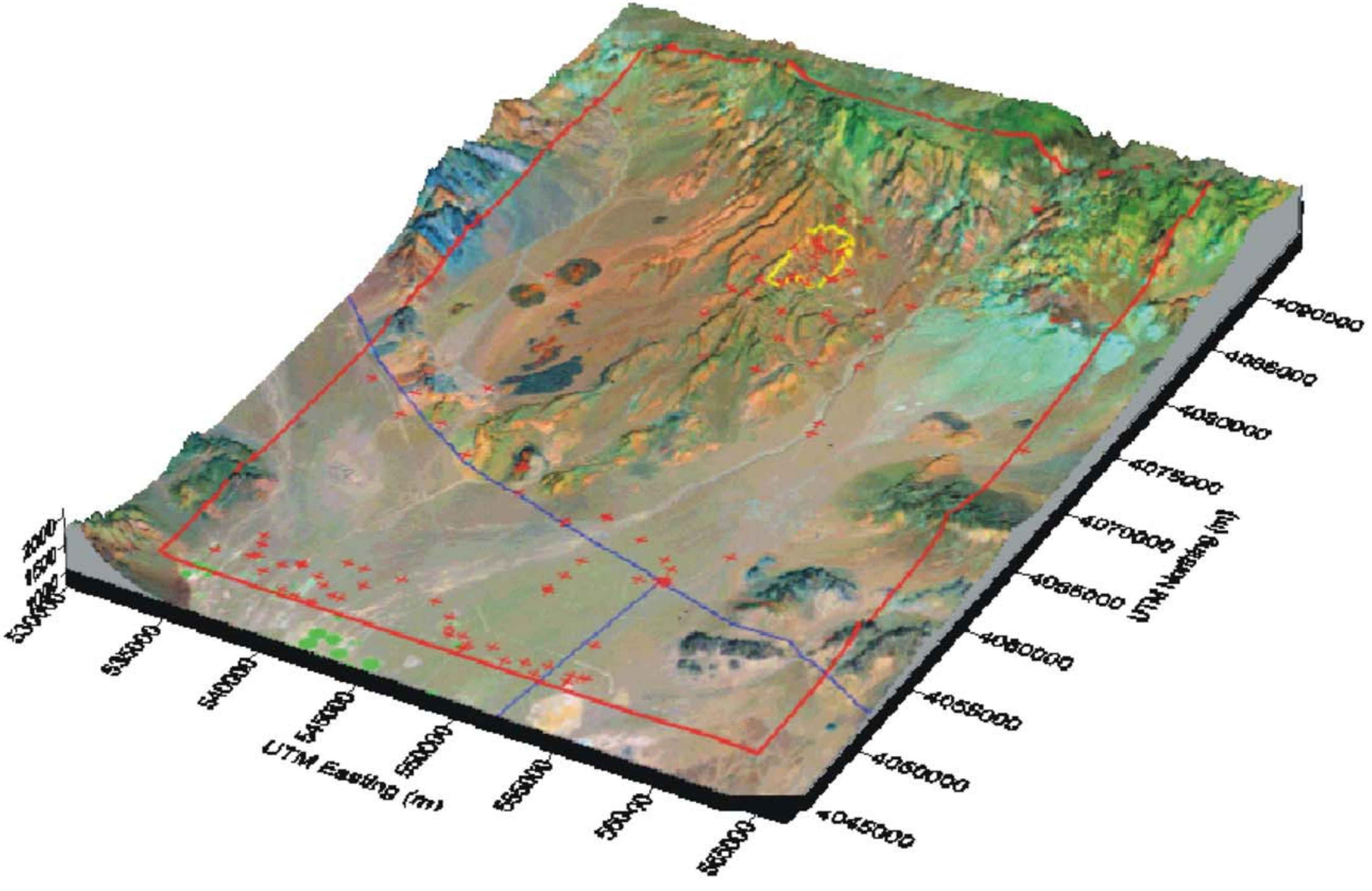
Outline

- Introduction to Saturated Zone (SZ) Radionuclide Transport Modeling at Yucca Mountain
- For each key transport process, discuss: conceptual model/approach and barrier capability
  - Matrix diffusion
  - Sorption and
  - Colloid-facilitated transport
- Conclusions

General Approach to Saturated Zone Transport Modeling

- **Key radionuclide transport processes in the SZ at Yucca Mountain include sorption, matrix diffusion and colloidal transport**
- **Matrix diffusion of dissolved radionuclides is implemented in fractured volcanic units. The valley-fill (alluvium) units are simulated as a porous medium using the effective porosity approach**
- **Particle tracking with the FEHM code is used to simulate radionuclide mass migration in the saturated zone**
- **A linear sorption approach is used in the matrix of the volcanic and alluvium units**
- **Colloid-facilitated transport of radionuclides is simulated to occur by two modes (reversible attachment to colloids and irreversible attachment)**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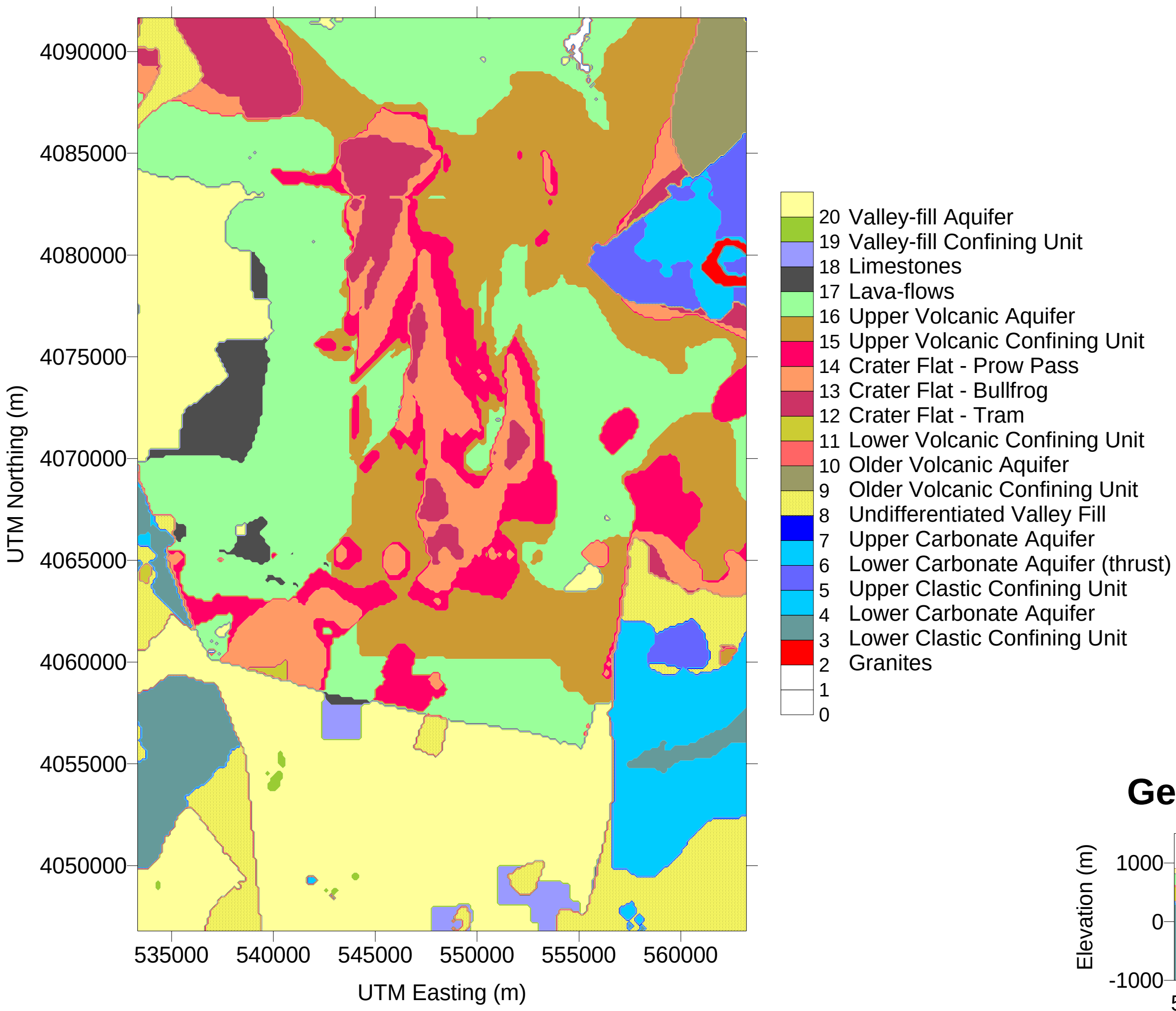
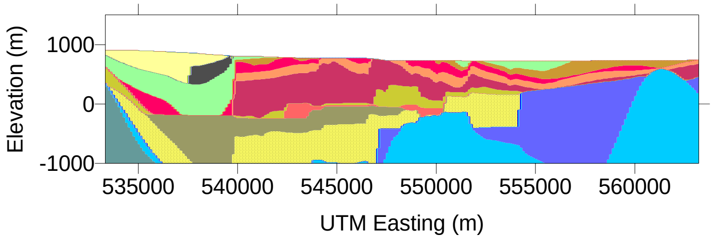
Hydrogeologic Framework Model

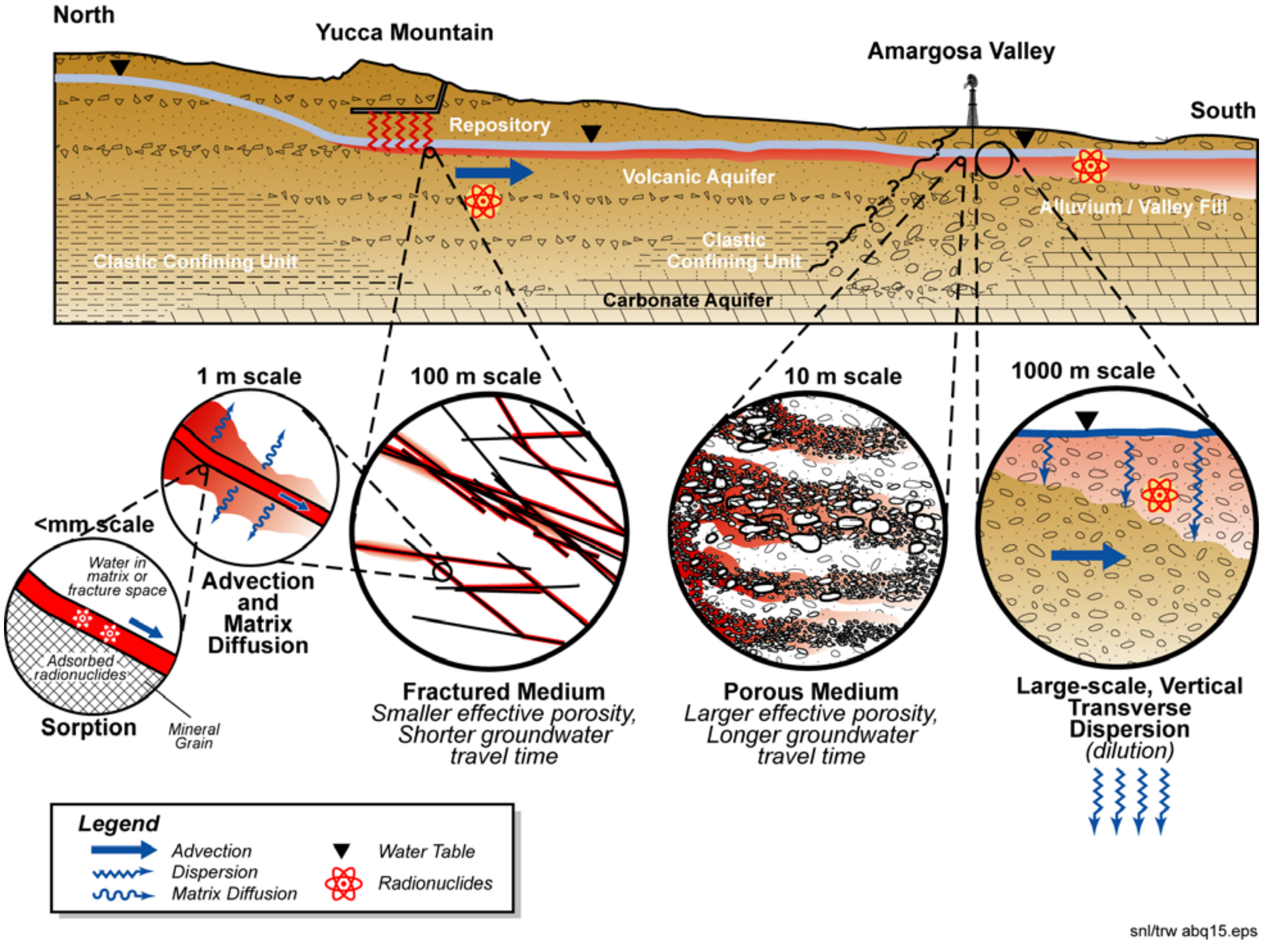


- **3-D model has domain 30 km x 45 km x 2750 m below water table**
- **Orthogonal grid with 500 m horizontal spacing and variable resolution in the vertical direction**

Geologic Cross Section, N=4076000

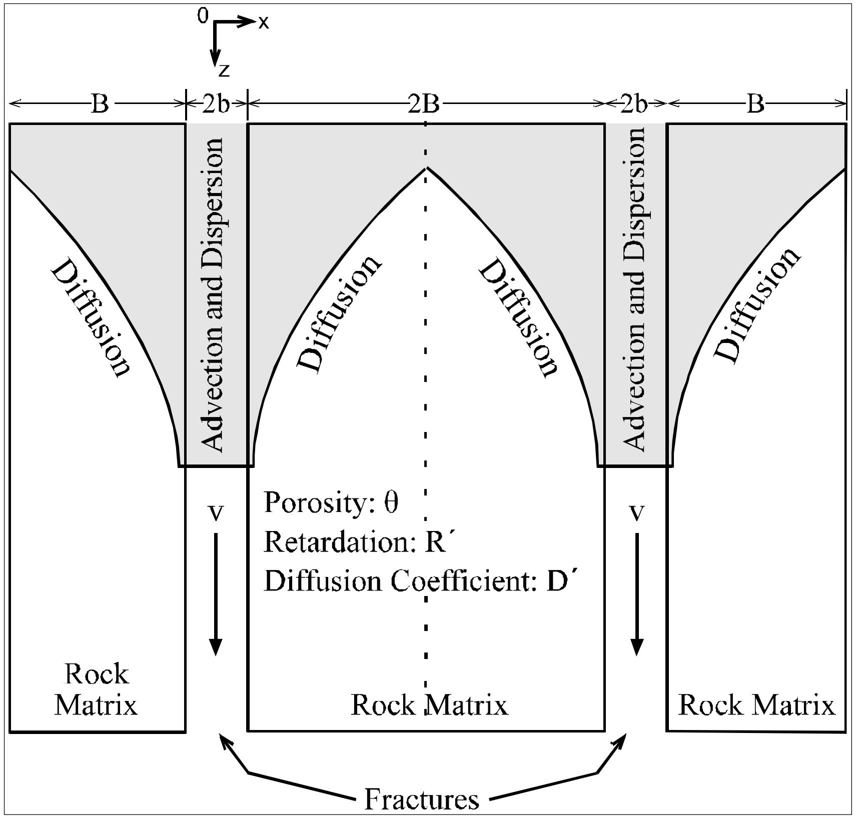


Conceptual Model of Radionuclide Transport Processes in the Saturated Zone

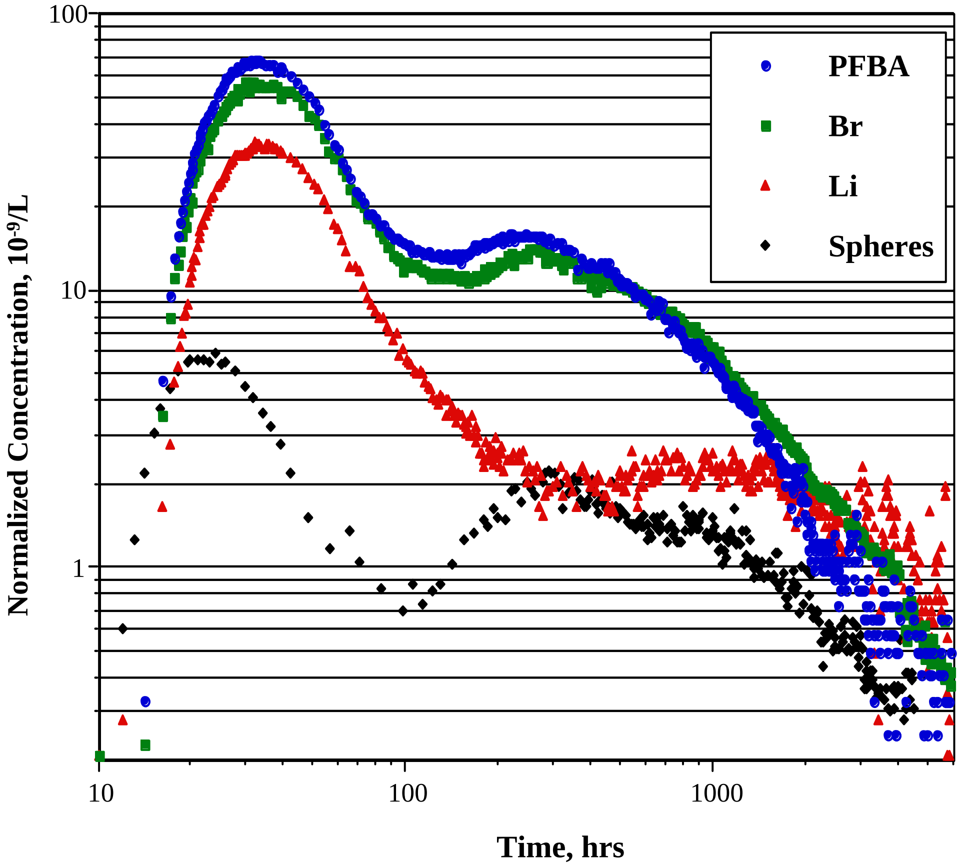


Conceptual Model of Matrix Diffusion

- Schematic diagram of the matrix diffusion submodel geometry and assumptions
- Dual-porosity model with equally spaced, parallel fractures
- C-wells reactive tracer test demonstrated that models incorporating matrix diffusion provide more reasonable fits to the tracer experiment data than those that use a single continuum



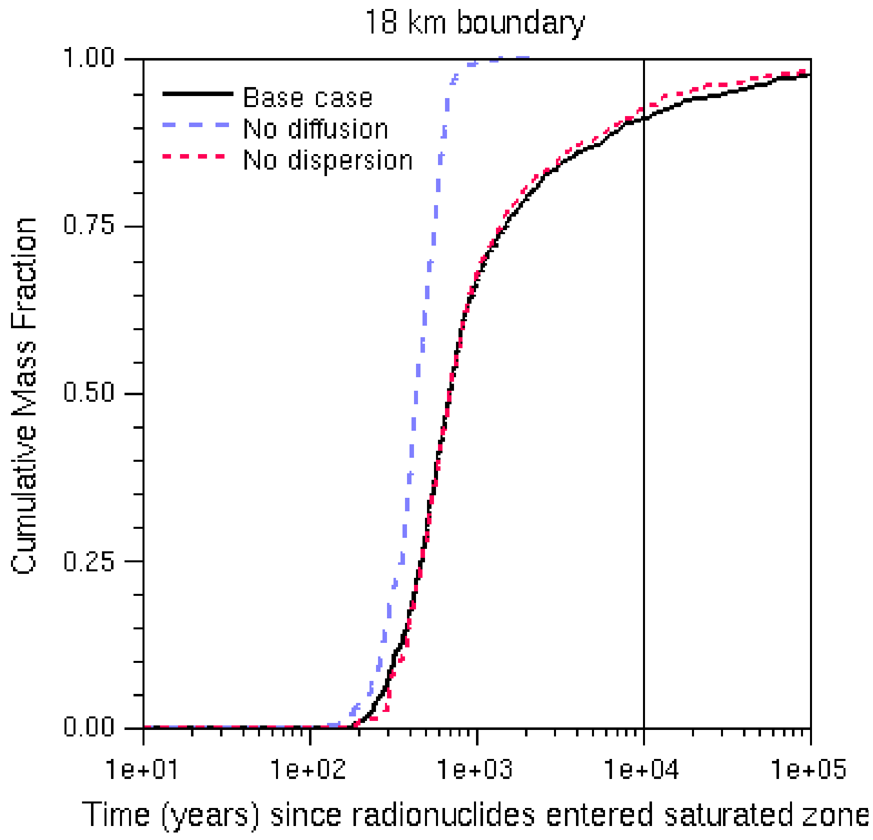
Saturated Zone Tracer Testing in Volcanic Units and Alluvium



- Conceptual model of fracture flow and matrix diffusion in volcanic rocks at the C-Wells site is consistent with the data
- Sorbing tracer (Li) breakthrough curve is consistent with combined matrix diffusion/sorption model
- Microspheres break through slightly earlier than solutes, but are attenuated
- Preliminary single-well tracer testing in alluvium confirms porous medium behavior

Saturated Zone Transport Barrier Capability: Matrix Diffusion

- **Breakthrough Curves Comparing the Base Case, Nondispersive, and Nondiffusive Cases**
- **Base-case simulation (solid black curve) is the breakthrough curve for a conservative, nonsorbing radionuclide in the absence of radioactive decay**
- **Matrix diffusion delays transport times and spreads the distribution of the arrival times of radionuclides**



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 Transport Sorption Approach

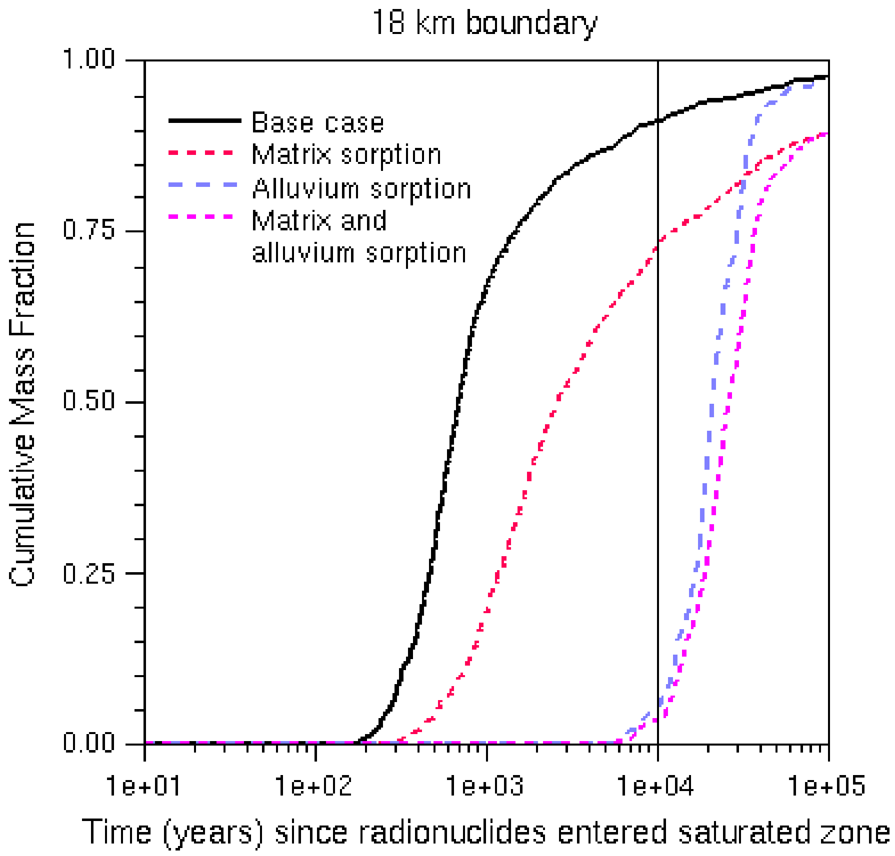
- **Linear sorption approach is used in the matrix of the volcanic and alluvium hydrogeologic units (as a component of the matrix diffusion model)**
- **No sorption on fracture surfaces is simulated in the fractured volcanic units**
- **Geochemical conditions along the entire flow path assumed to be oxidizing**
- **Uncertainty in sorption coefficients captured in probability distributions**
- **Single sorption coefficient value for each transport simulation**

Saturated Zone Transport Sorption Approach
(Continued)

- Sorption coefficient probability distributions incorporate:
  - Water chemistry
  - Variations in rock surface properties
  - Mineralogical composition
- Probability distributions based on:
  - Experimental data
  - Professional judgment regarding the impact of variables not considered in the experimental program
  - Study to compare variability of sorption coefficients at the scale of model grid blocks to variability at the lab scale

Saturated Zone Transport Barrier Capability: Sorption

- **Breakthrough Curves for the Base Case and Sorbing Radionuclide**
  - **Matrix sorption: Np K_d of 1.3 mL/g**
  - **Alluvium and matrix sorption: Np K_d of 6.3 mL/g in volcanics and 1.3 mL/g in the volcanics**
- **Sorption delays transport times and spreads the distribution of the arrival times of radionuclides**



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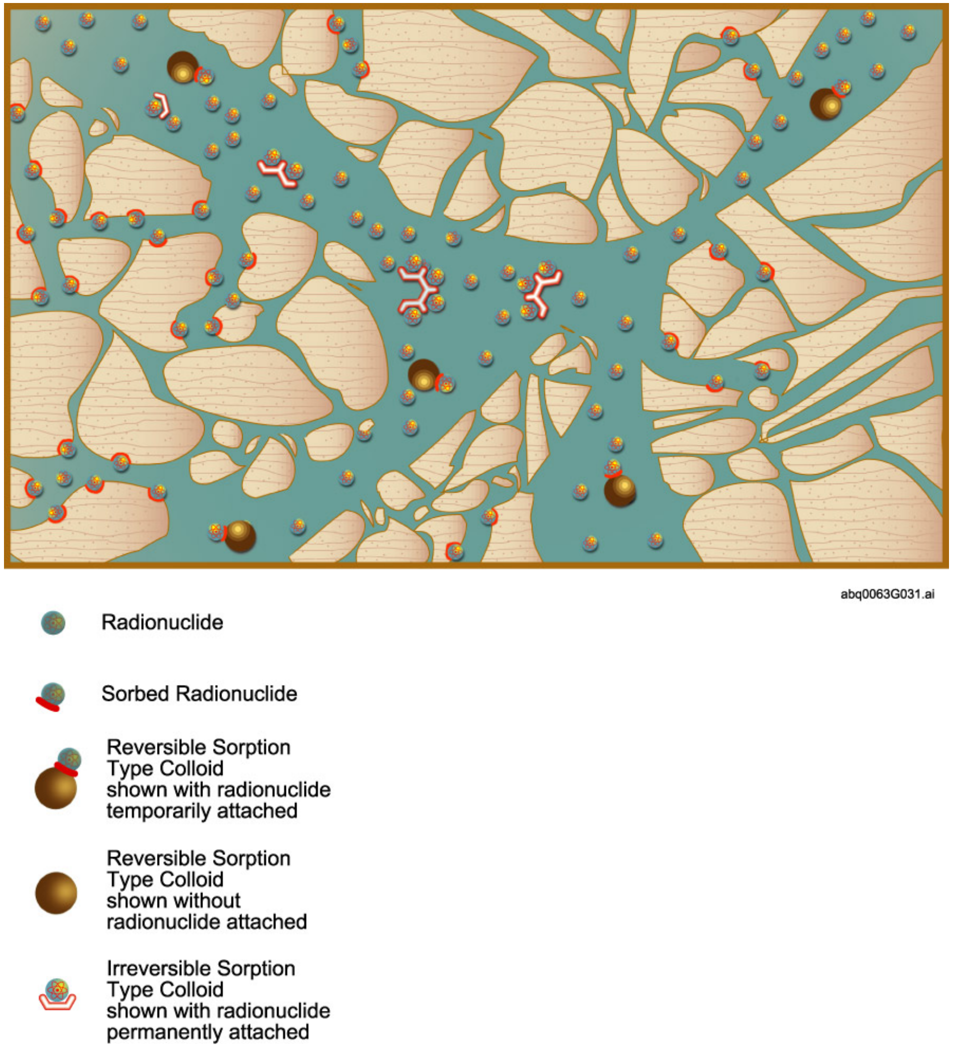
Saturated Zone Colloidal Transport



Saturated Zone Transport
Colloidal Approach

- **Colloid-facilitated transport of radionuclides is simulated to occur by two modes (reversible attachment to colloids and irreversible attachment)**
- **Reversibly attached colloids:**
  - **Are in equilibrium with the aqueous phase and the aquifer material**
  - **In this mode of transport the effective retardation of these radionuclides during transport in the SZ is dependent on:**
    - **The sorption coefficient of the radionuclide onto colloids**
    - **The concentration of groundwater colloids**
    - **The sorption coefficient of the radionuclide onto the aquifer material**

Saturated Zone Transport Colloidal Approach
(Continued)

- **Irreversible colloids:**
  - Radionuclides that are irreversibly attached to colloids are transported at the same rate as the colloids
  - Colloids with irreversibly attached radionuclides are themselves delayed by interaction with the aquifer material
  - For the SZ transport simulations a small (uncertain) fraction of the radionuclide mass irreversibly attached to colloids is transported without retardation and the remaining fraction of the radionuclide mass is delayed

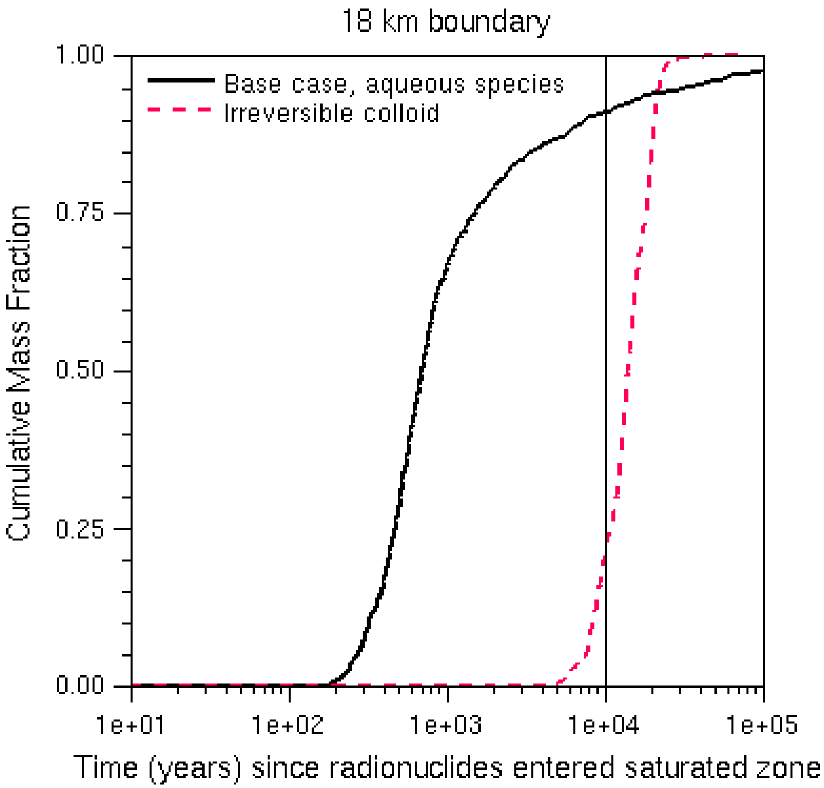
Saturated Zone Transport Colloidal Approach

(Continued)

- **Pu and Am are transported as irreversible colloids for the SZ transport simulations**
- **Pu, Am, Th, Pa, and Cs are transported as reversible colloids for the SZ transport simulations**
  - **For these transport simulations radioisotopes of Pu are transported as one group,**
  - **Radioisotopes of Am, Th and Pa are transported as a second group and**
  - **Cs is transported as a third species**

Saturated Zone Transport Barrier Capability: Colloidal Transport

- Breakthrough Curves for the Base Case and Radionuclides Irreversibly Attached to Colloids
- Colloids irreversibly sorbed onto radionuclides have delayed transport times



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Summary

- Radionuclide transport in the saturated zone for Total System Performance Assessment for the License Application is simulated considering the key processes of matrix diffusion, sorption, and colloid-facilitated transport
- Matrix diffusion delays transport times and spreads the distribution of the arrival times of radionuclides
- Sorption in the alluvium can increase the transport times by orders of magnitude for even weakly sorbing radionuclides such as neptunium
- Colloids irreversibly and reversibly bound to radionuclides may be delayed by several thousand years

Backup

Implementation of Reversible Colloid Model for the Saturated Zone

- **In the volcanics...**

$$D_e^{adusted} = \frac{D_e}{(1 + K_c)^2}$$

- **In the alluvium**

$$K_d^{new} = \frac{K_d^{orig}}{1 + K_c}$$

Implementation of Irreversible Colloid Model for the Saturated Zone

(Continued)

Alluvium Units:

$$K_d^{eff} = \frac{(R_f - 1)\Phi_{eff}}{\rho_b}$$

Volcanic Units:

Retardation factor is applied directly as an input parameter in the SZ Transport Abstraction Model