Unsaturated 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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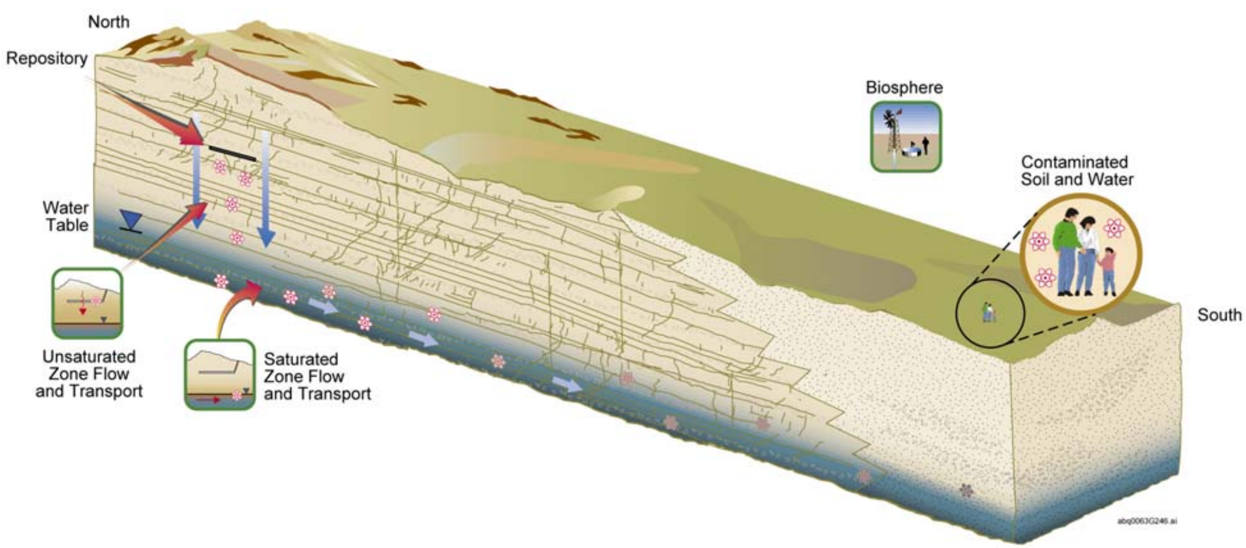
Topics of Discussion

- Goals and requirements of Unsaturated Zone (UZ) transport abstraction model
- Model Formulation
- Relationship to other Total System Performance Assessment (TSPA) Submodels
- Validation of Abstraction Model
- Transport Processes and Parameters
- Conclusions

Primary Information Source: Particle Tracking Model and Abstraction of Transport Processes, MDL-NBS-HS-000020 REV00

Goals and Requirements of Unsaturated Zone Transport Abstraction Model

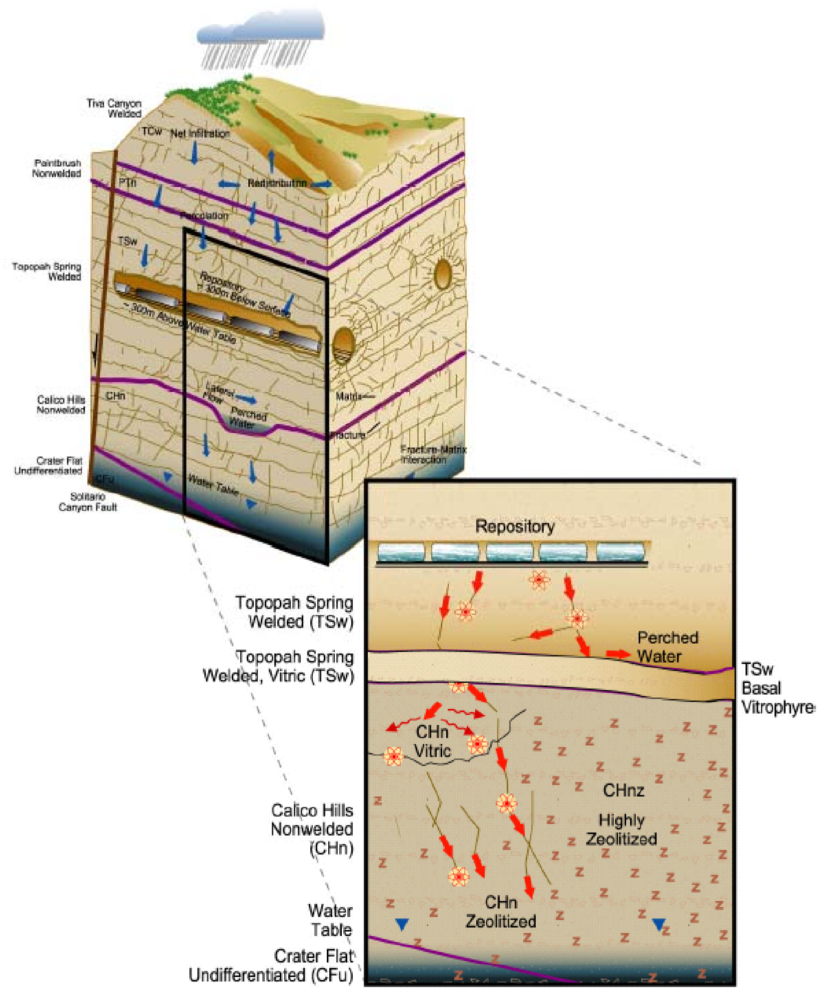
- **TSPA model simulates the concentration in the plume at the compliance boundary for a fixed pumping rate q of 3000 acre-ft/yr**
- **Concentration = m/q, where m is the radionuclide mass flux (grams Rn/yr) arriving at the compliance boundary, where q is 3000 acre-ft/yr**
- **The mass flux released from repository will eventually arrive at the well unless it decays or is retarded**



Goals and Requirements of Unsaturated Zone Transport Abstraction Model

(Continued)

- **UZ transport abstraction model must predict <u>travel times</u> of radionuclides through the UZ as a function of flow and transport parameters**
  - **In situ concentration (simulation of the plume) within the UZ is not directly required**
  - **Prediction of dilution of radionuclides in UZ waters is not directly required**
- **For determining the distribution of travel times, a particle tracking model is an effective approach**



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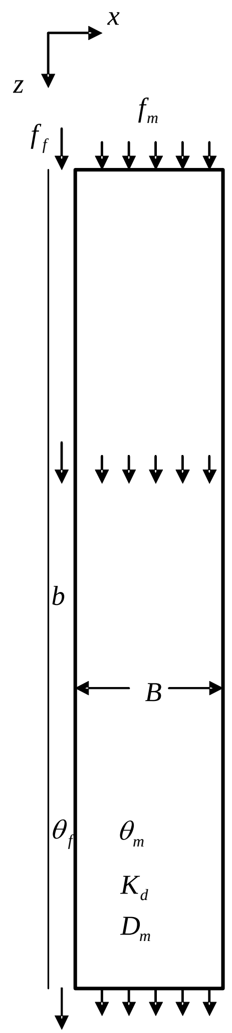
Model Formulation
Dual-k Particle Tracking Model

- **Cell-based particle tracking model routes particles from one grid cell to the next in proportion to the water flux**
- **The residence time in a cell is determined probabilistically based on a simplified submodel for transport in a dual-k medium**
- **Particle arrivals at the water table are converted to radionuclide mass arrival**

Model Formulation
Matrix Diffusion and Sorption

- **Transport at the sub-grid scale is conceptualized as a system of parallel flow in the fractures and matrix**
- **Particles travel between the fractures and matrix due to water movement (advection) and molecular diffusion (matrix diffusion)**
- **Equilibrium, reversible, linear sorption model (K_d model) is used for sorption**



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Relationship to other Total System Performance Assessment Submodels
Unsaturated Zone Flow and Climate

- **Calibrated, steady-state flow fields are used in transport abstraction model**
  - **Dual-permeability formulation**
  - **Three infiltration scenarios are used to capture uncertainty in flux through the mountain**
- **Climate change is simulated**
  - **TSPA model shifts to a new flow field when climate changes in the model**
  - **Water table is assumed to be higher under future, wetter climates**

Net Infiltration in 3D Flow Model

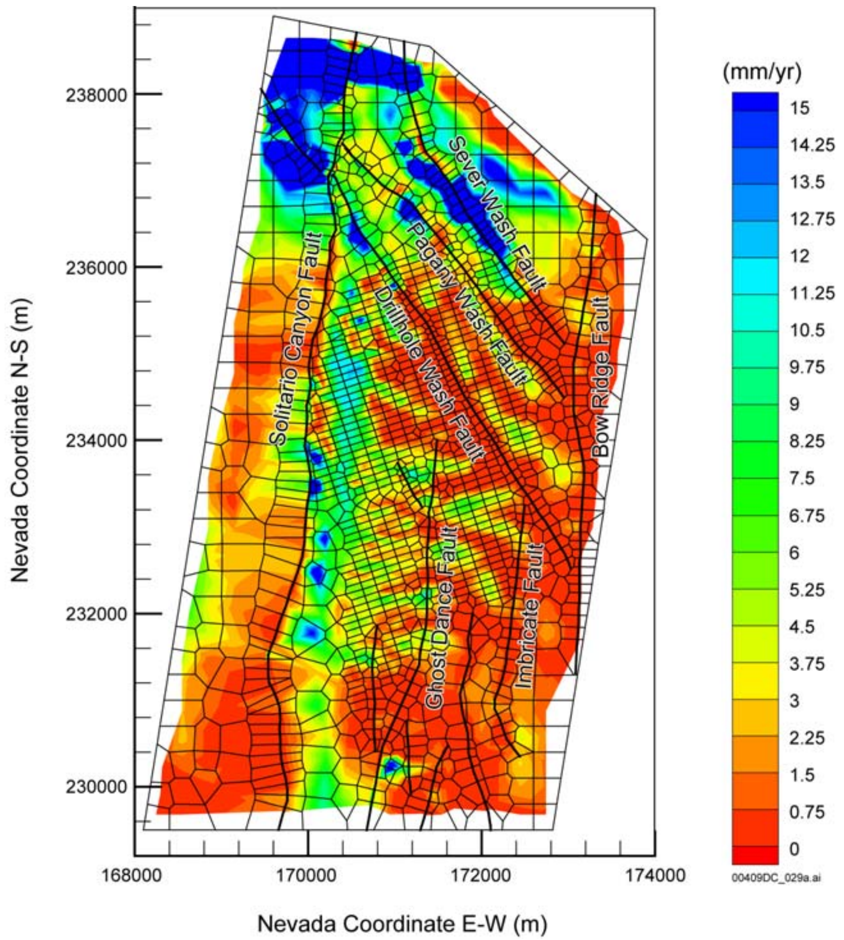

Figure 3-1 of TBD 10: Unsaturated Zone Transport

Relationship to other Total System Performance Assessment Submodels

Radionuclide Releases from Engineered Barrier Systems

- **Radionuclide releases occur at single grid points to simulate individual waste package failures**
- **Release rates are correlated to percolation flux at the repository horizon**
- **Radionuclide mass is added to the UZ transport abstraction model as particles with specified mass**

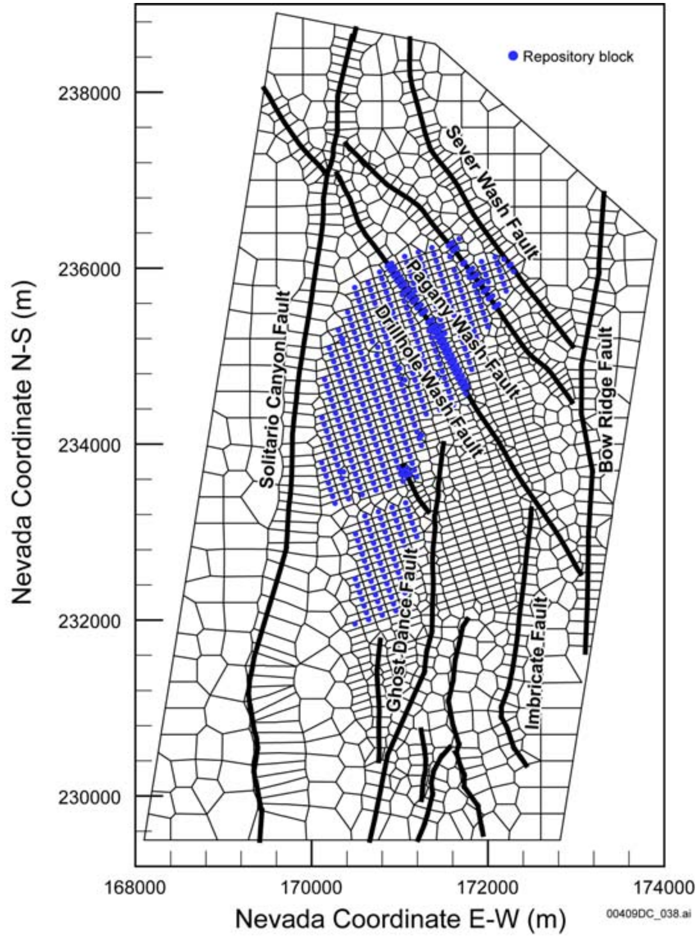

Figure 5-1 of TBD 10: Unsaturated Zone Transport

Relationship to other Total System Performance Assessment Submodels
Saturated Zone Flow and Transport

- **Location of radionuclide mass reaching the Saturated Zone (SZ) is identified**
- **Mass flux versus time arriving at each of four quadrants is recorded**
- **Subsequent SZ transport simulations assume a point source within one of the four regions**

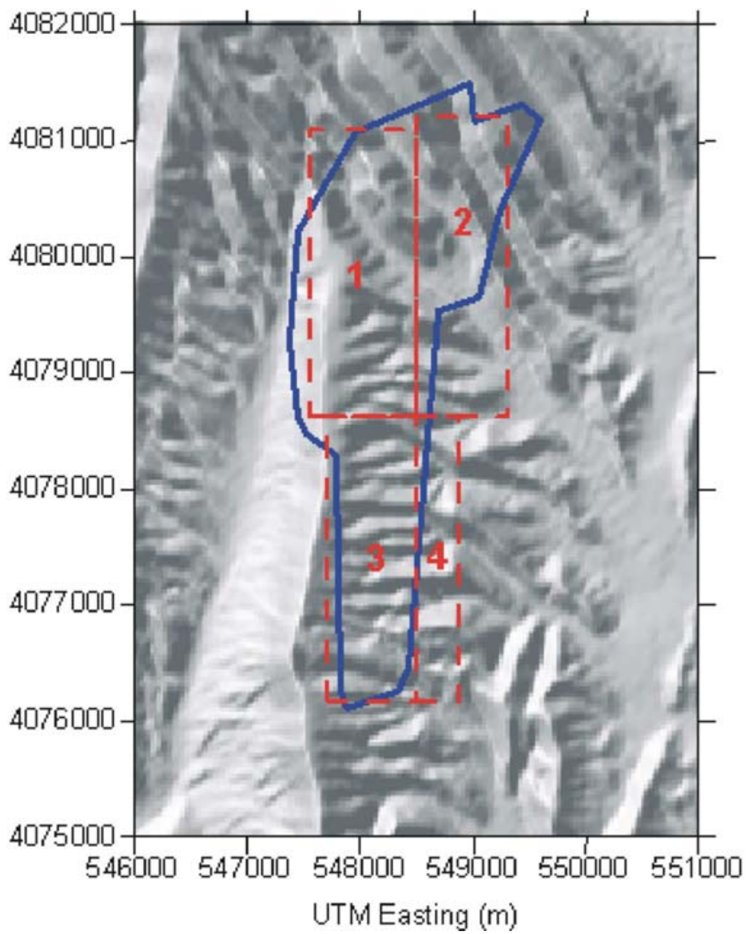

Figure 6-26 of SZ Flow and Transport Model Abstraction

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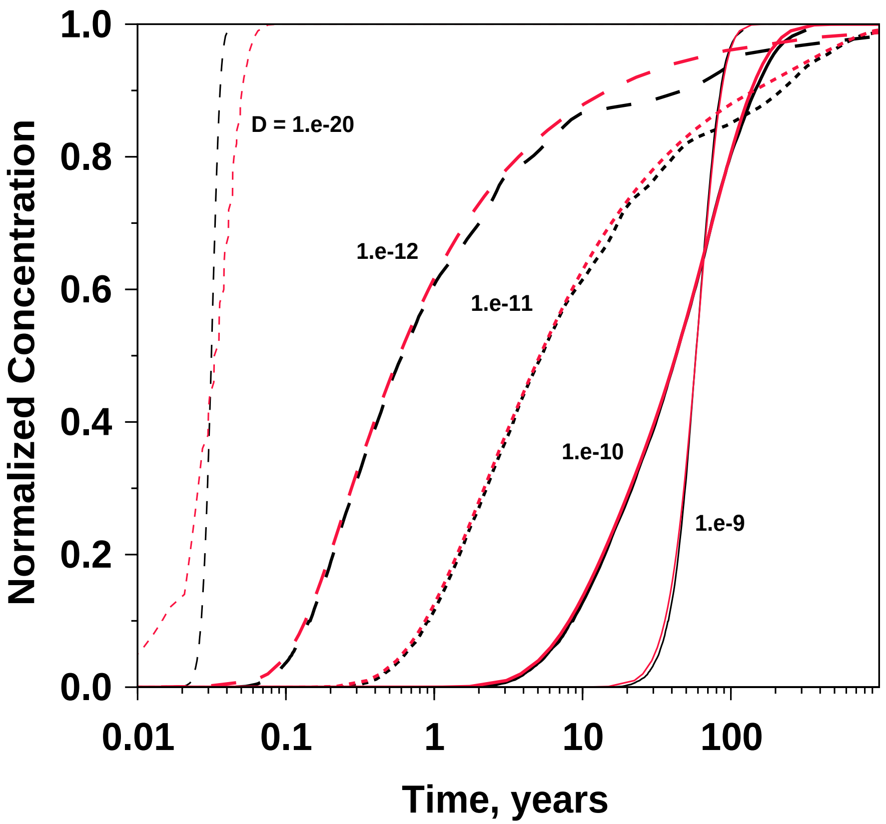
Validation
1-D Transport, diffusion

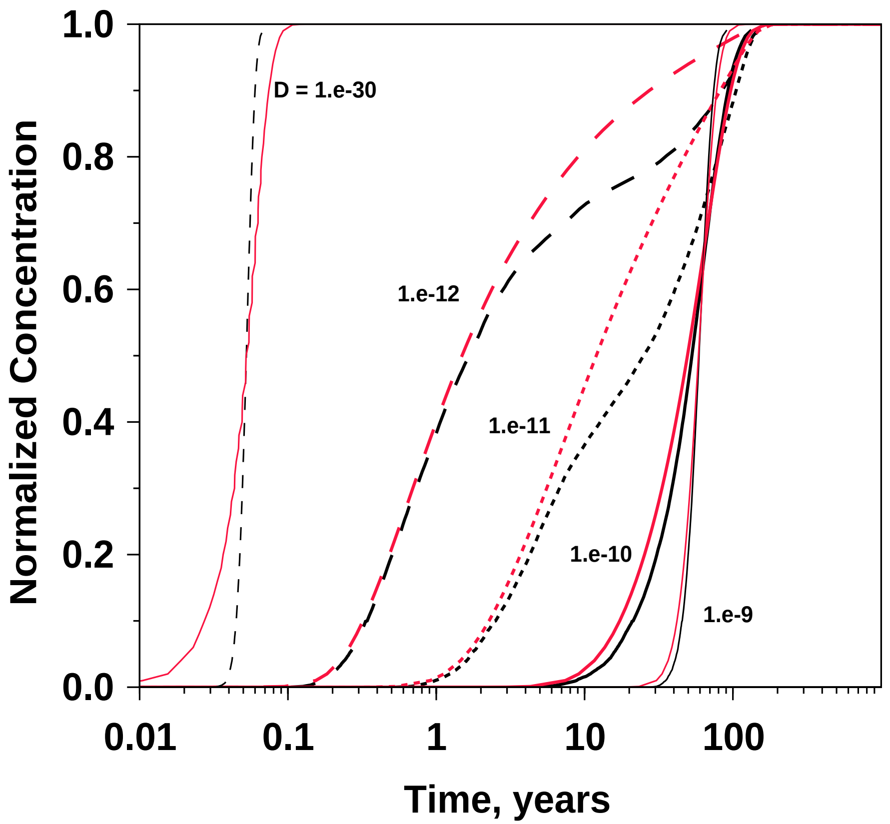
99% Fracture Flow

Black - Particle Tracking; Red - Discrete Fracture Model



60% Fracture Flow

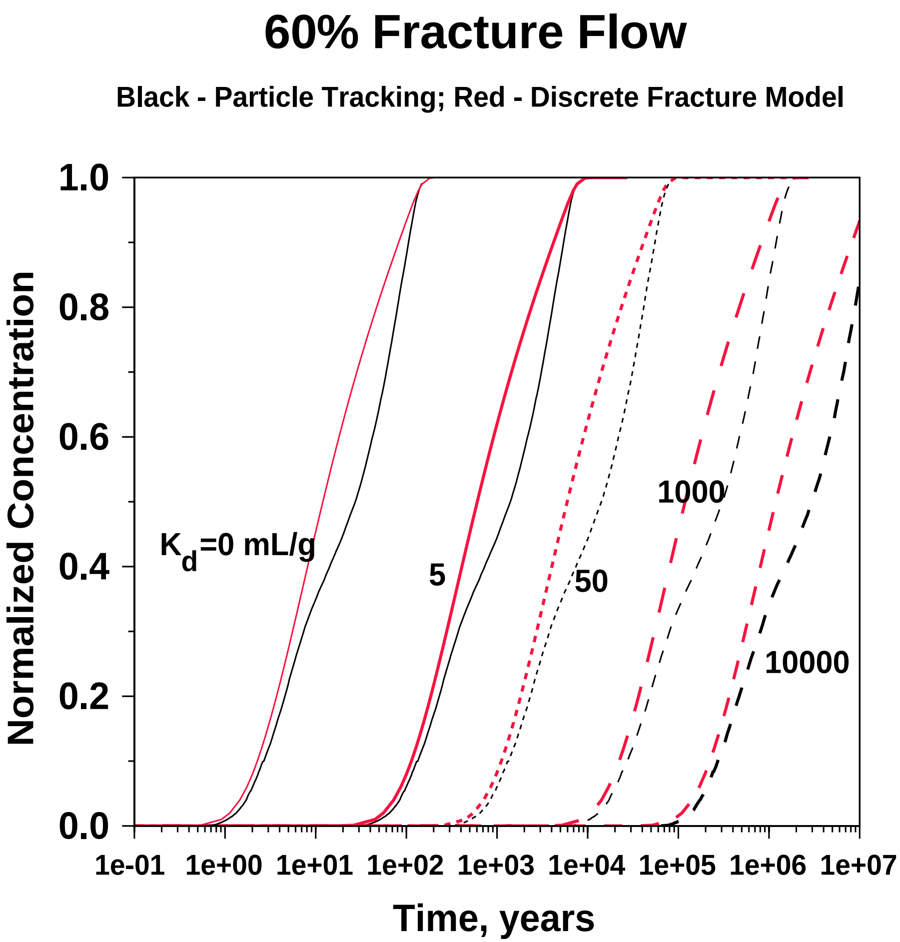
Black - Particle Tracking; Red - Discrete Fracture Model



For model validation purposes only: travel times are not necessarily representative of Yucca Mountain UZ transport

Validation
1-D Transport, Diffusion and Sorption

- **Testing over a wide range of sorption and diffusion parameters compares favorably to a discrete fracture model**
- **This confirms that the basic building blocks of the particle tracking model perform well over the range of parameters required by the TSPA model**



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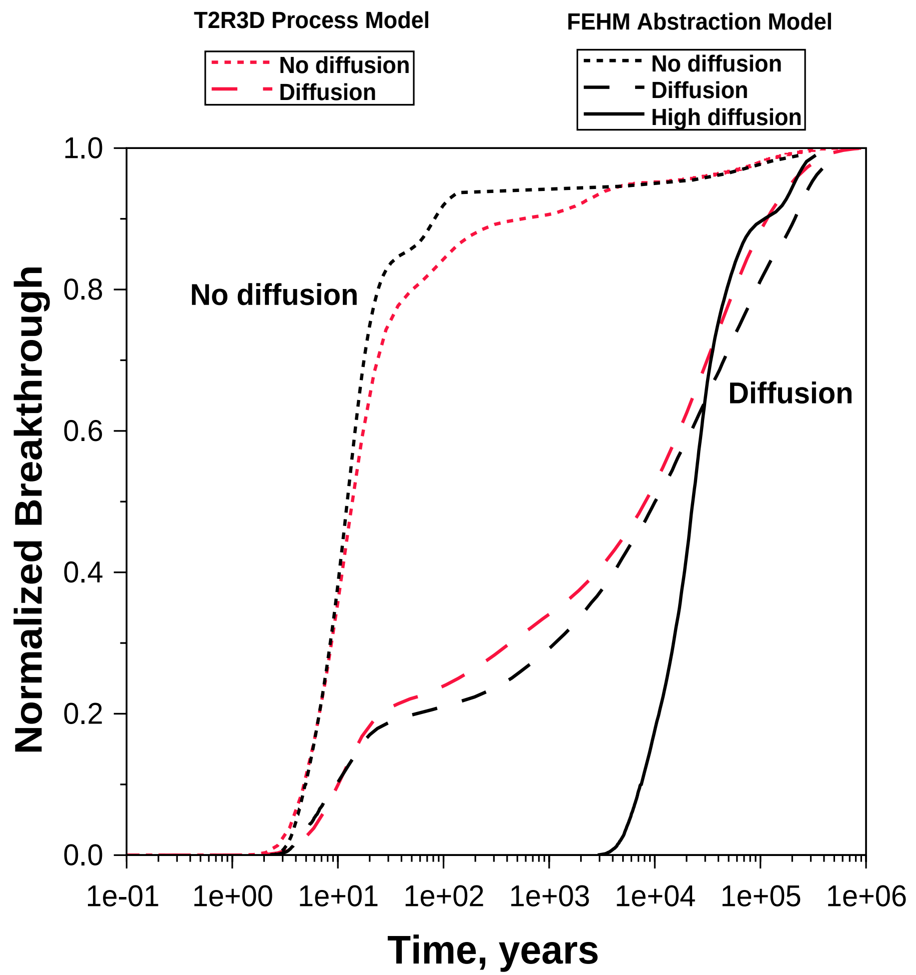
Validation

2-D Mountain-Scale Transport, Comparison to Process Model

- **Release over the entire repository domain**
- **No-diffusion case confirms that the particle routing and residence time calculations are properly implemented**
- **Diffusion case confirms that the dual-k matrix diffusion model is properly implemented**



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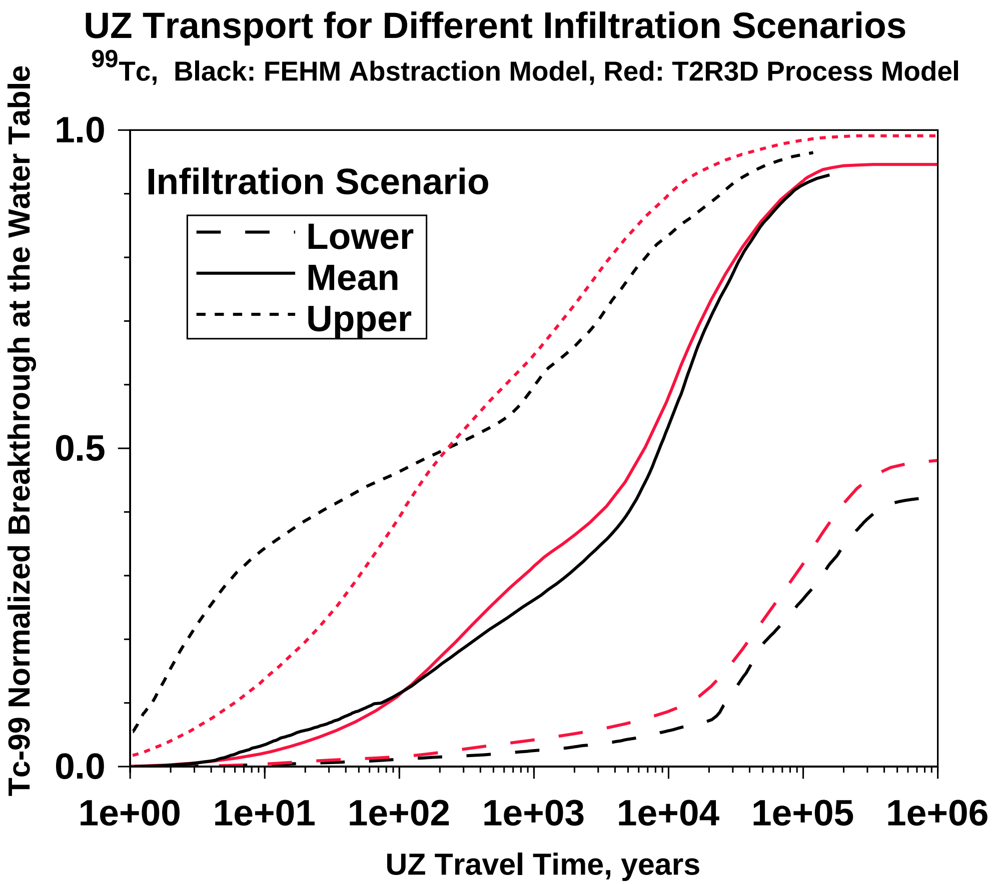
Validation

3-D Mountain-Scale Transport, Comparison to Process Model

- **Release over the entire repository domain**
- **Good agreement with 3-D process model over a wide range of infiltration scenarios**
- **Plot shows the large impact of infiltration uncertainty on UZ transport model performance**



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 unsaturated zone portion of the Yucca Mountain flow system.

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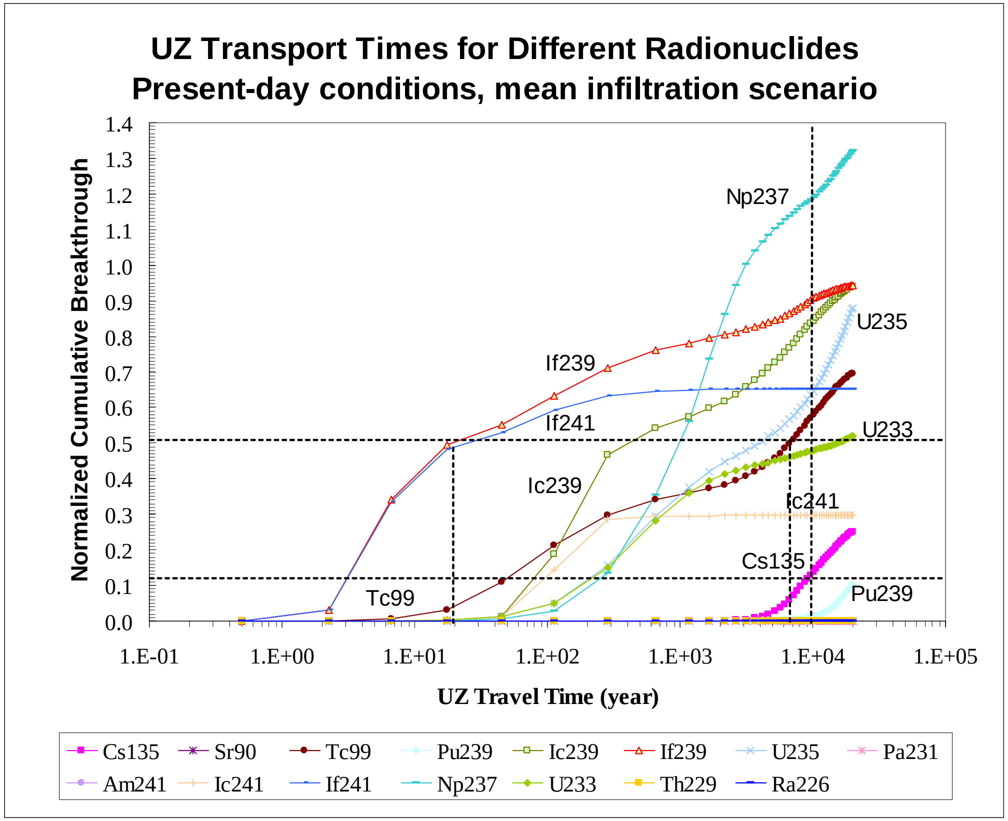
Transport Processes and Parameters
Colloids

- **Colloid-facilitated radionuclides are modeled as species with low diffusion**
- **Rapid travel times through fractures**
- **Size exclusion and filtration options are available**
- **NOTE: Impact of colloid-facilitated transport on dose will be controlled by the release rates of radionuclides irreversibly bound to colloids**



If239 – Pu239 on unretarded colloids
Ic239 – Pu239 on retarded colloids
If241 – Am241 on unretarded colloids
Ic241 – Am241 on retarded colloids

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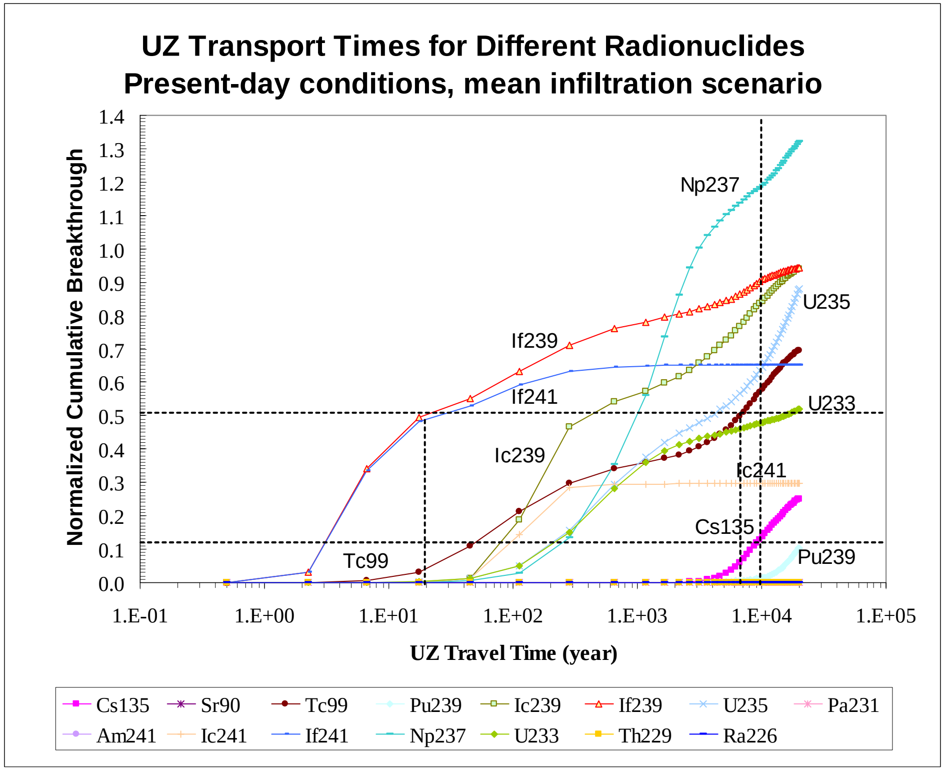
Transport Processes and Parameters
Sorption, Dispersion

- **Rock properties influencing transport: Obtained from process model for UZ flow**
- **Sorption K_d: Probability distributions are developed for key radionuclides on three main rock types**
- **Longitudinal dispersivity set to constant value due to low sensitivity**
- **NOTE: Dose will also depend on radionuclide release rates, SZ transport, and biosphere models**



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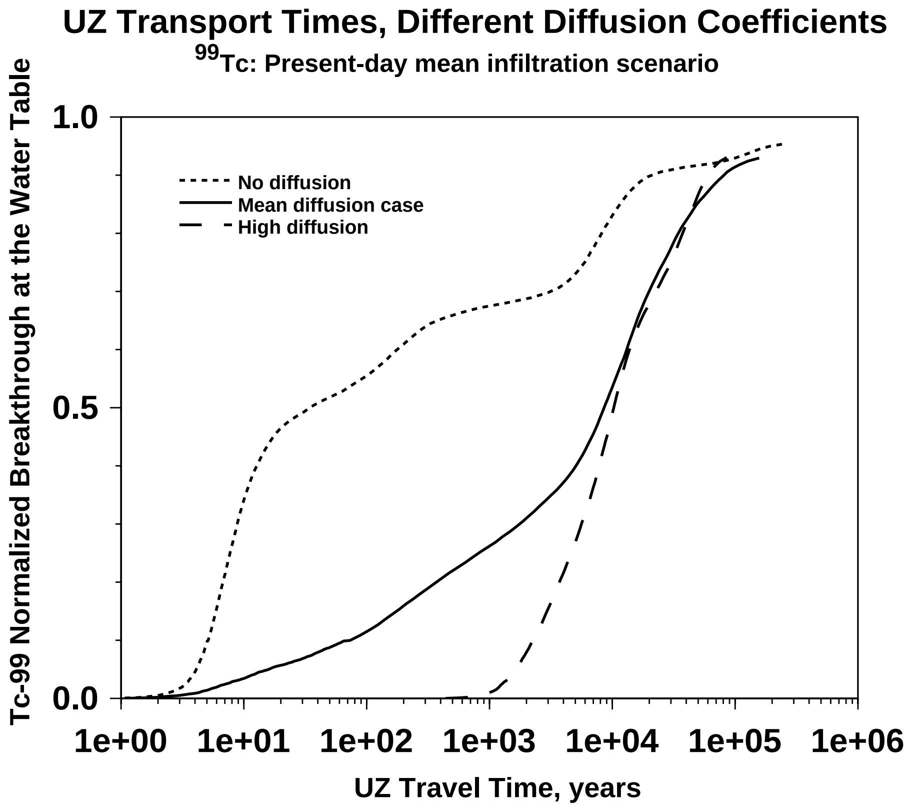
Transport Processes and Parameters
Matrix Diffusion

- **Early breakthrough without diffusion is dominated by rapid transport through fractures and faults**
- **Matrix diffusion allows radionuclides to sample slow-moving fluid in the matrix**
- **Parameters influencing diffusion are represented stochastically:**
  - **Diffusion coefficient: based on laboratory measurements**
  - **Fracture spacing and aperture: based on combination of field observations of fracture frequency and flow model results**
- **Active Fracture Model parameters: Uncertainty is represented stochastically**



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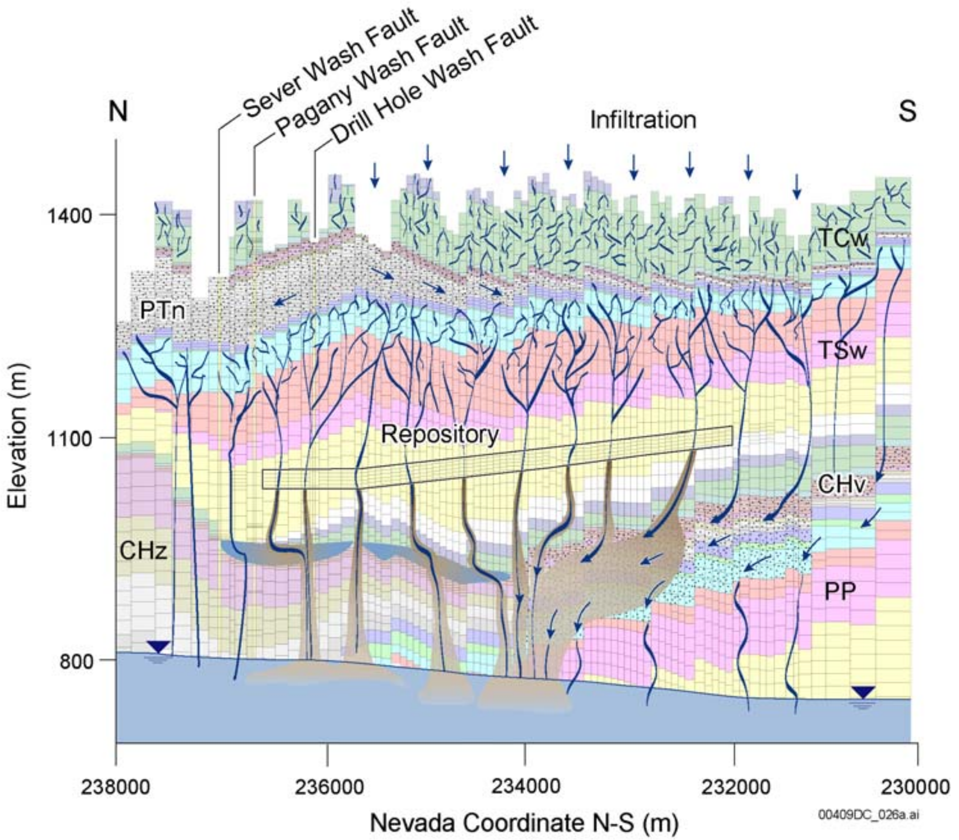
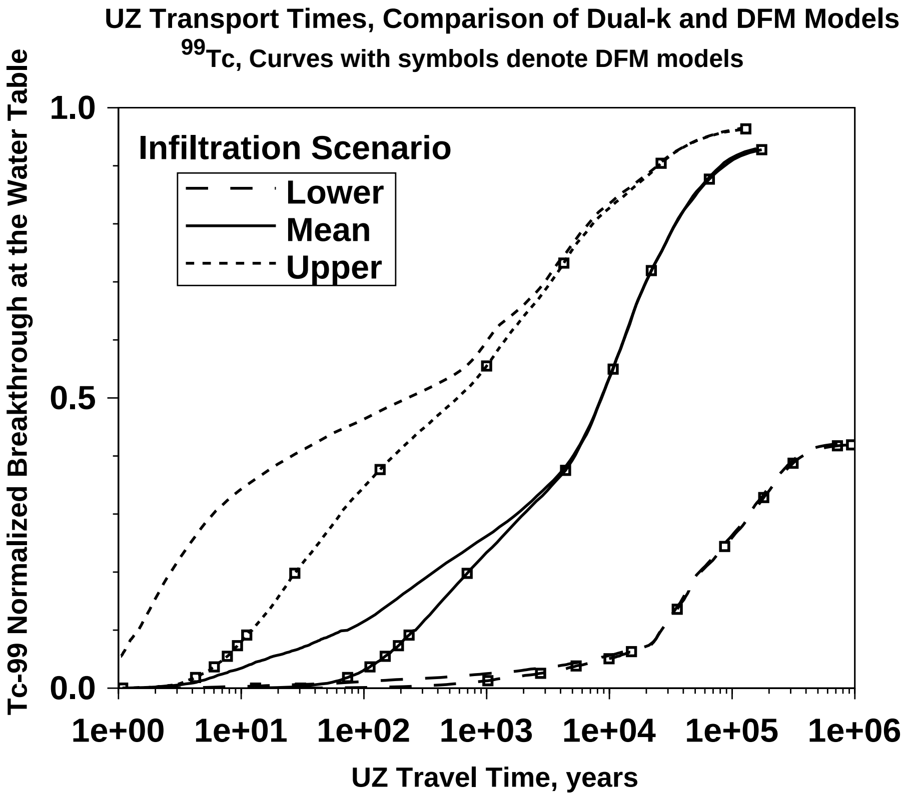
Transport Processes and Parameters
Matrix Diffusion: Active Fracture Model

- **Active Fracture Model (AFM) accounts for the fact that only some fractures flow**
- **Spacing between *flowing* fractures is larger than spacing observed in the tunnels**
- **AFM for transport is implemented in the abstraction model**
- **Result: Shorter first arrival times for the fastest moving radionuclides**



Transport Processes and Parameters
Matrix Diffusion: Conceptual Model Uncertainty

- Dual-k fracture/matrix interaction model: Concentration gradient represented with a single matrix grid block
- Discrete Fracture Model (DFM): Concentration gradient close to the fracture is modeled explicitly
- Particle-tracking model allows either conceptual model to be tested
- Dual-k predicts shorter first arrival times for the fastest moving radionuclides.
  Long-time behavior is the same for both models
- TSPA model uses the dual-k formulation



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Conclusions

- **Abstraction model is a computationally efficient version of the process model**
  - **UZ Flow: flow fields based on the UZ flow model, with climate change included**
  - **Transport - dual-permeability model with sorption and matrix diffusion**
- **Validation runs in 1-D, 2-D, and 3-D confirm the acceptability of the abstraction model**
- **Abstraction model is coupled to other TSPA submodels in a way that retains the spatial variability of radionuclide transport**

Conclusions
(Continued)

- Predicted UZ radionuclide travel times from the abstraction model span a large range
- Representative median UZ travel times, present-day conditions, mean infiltration scenario:
  - Colloid-facilitated radionuclides: ~20 yr
  - Nonsorbing ^{99}Tc: ~6000 yr
  - Strongly sorbing radionuclides: >10,000 yr
- Future, wetter climate conditions will yield shorter UZ travel times
- Parameter uncertainties have been quantified and will be propagated through the TSPA model
- Conceptual model uncertainty for fracture/matrix interactions and matrix diffusion can also be examined