U.S. Department of Energy

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Mass and Activity of Key Radionuclides Potentially Released from the Unsaturated Zone Over Time

Presented to:
Nuclear Waste Technical Review Board

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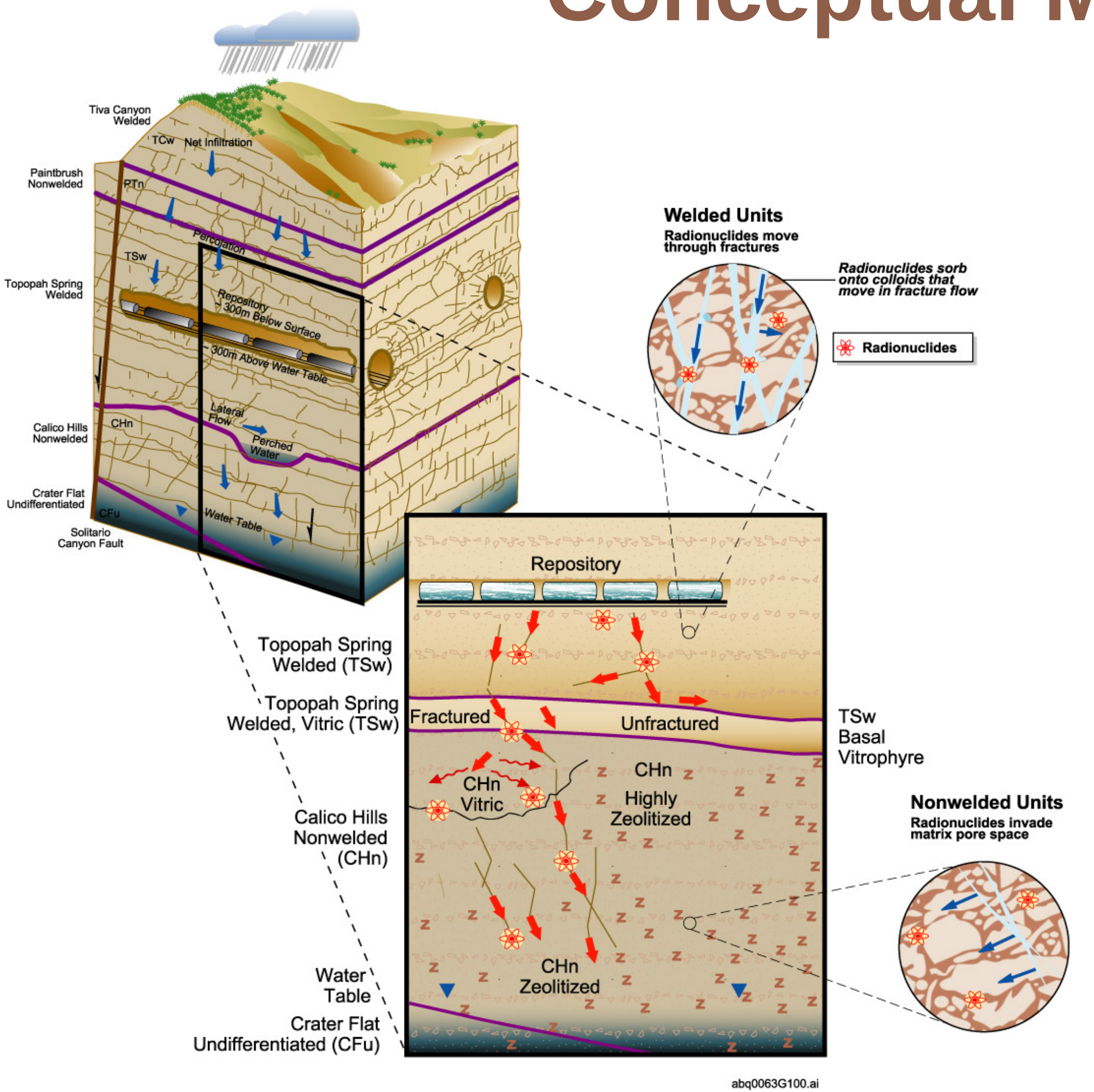
Outline

- Unsaturated Zone (UZ) Radionuclide Transport – Conceptual Models and Technical Basis
- Implementation of Unsaturated Zone Radionuclide Transport model for Total System Performance Assessment (TSPA)
- Results
  - Representative case
  - Sensitivity to flow model parameters
  - Diffusion processes and parameters
  - Fracture versus matrix releases
  - Spatial variability
- Conclusions

Unsaturated Zone Transport Conceptual Model



- **Combined fracture and matrix flow: dual permeability model formulation**
- **Radionuclide transport through fractures and matrix: advection, diffusion, sorption, colloid-facilitated transport**
- **Radionuclide transport is simulated using ambient flow fields**
- **Releases to either the fractures or matrix**

Scientific Basis

- **Fracture vs. matrix flow**
  - **Busted Butte experiment results confirm matrix flow in vitric Calico Hills units**
  - **Alcove 8, Niche 3 results confirm the process of fracture flow and matrix diffusion in the TSw units**
  - **Cl-36 results suggest the possibility of fracture-dominated transport of conservative species through the unsaturated zone**
  - **Model of combined fracture and matrix flow and transport is consistent with many observations of solute transport in vadose zones (beyond Yucca Mountain)**
- **Flow and Transport Parameters**
  - **Process flow and transport models are informed by data sets either by direct calibration (e.g. water content, matric potential) or by consistency checks (Cl-36, C-14)**

Implementation of UZ Radionuclide Transport in TSPA Model

- **Dual permeability particle tracking model, with probabilistic travel time delays to account for sorption and diffusion**
- **Full decay-chain capability**
- **Particle release locations and mass per particle are determined dynamically from engineered barrier system radionuclide mobilization and transport calculations**
- **Particles are released into the fracture or matrix continuum**
- **Radionuclide mass versus time at various locations at the water table is computed and input to the saturated zone model**
- **Validation achieved by comparison to 1, 2, and 3D models, including the UZ transport process model**

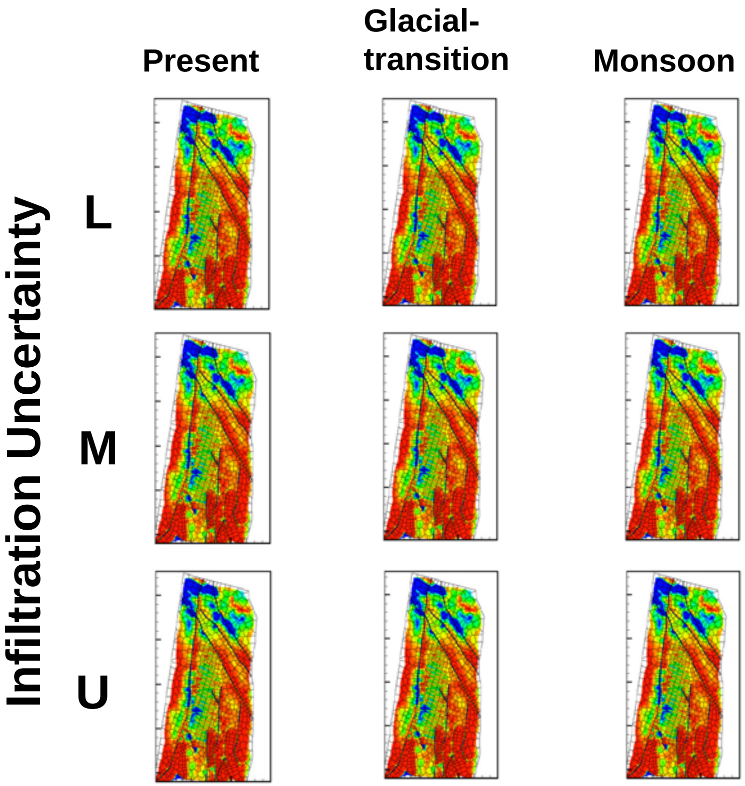
Radionuclides Considered

- **Conservative: C-14, I-129, Tc-99**
- **Weakly Sorbing: Np-237, U-232, U-234, U-235, U-236, U-238**
- **Strongly Sorbing: Am-241, Am-243, Cs-135, Cs-137, Pa-231, Pu-236, Pu-239, Pu-240, Pu-242, Ra-226, Sr-90, Th-229, Th-230, Th-232**
- **Colloid-Facilitated Transport: most strongly sorbing radionuclides**

Advective Transport

- 3D, steady state, dual-permeability flow fields from UZ flow model
- Instantaneous transition of flow field from one climate state to another
- Water table rise for future, wetter climates
- Uncertainty from infiltration model is propagated through the UZ transport model
- Sensitivity to flow-model parameters is explored through sensitivity analyses

Climate-related variability

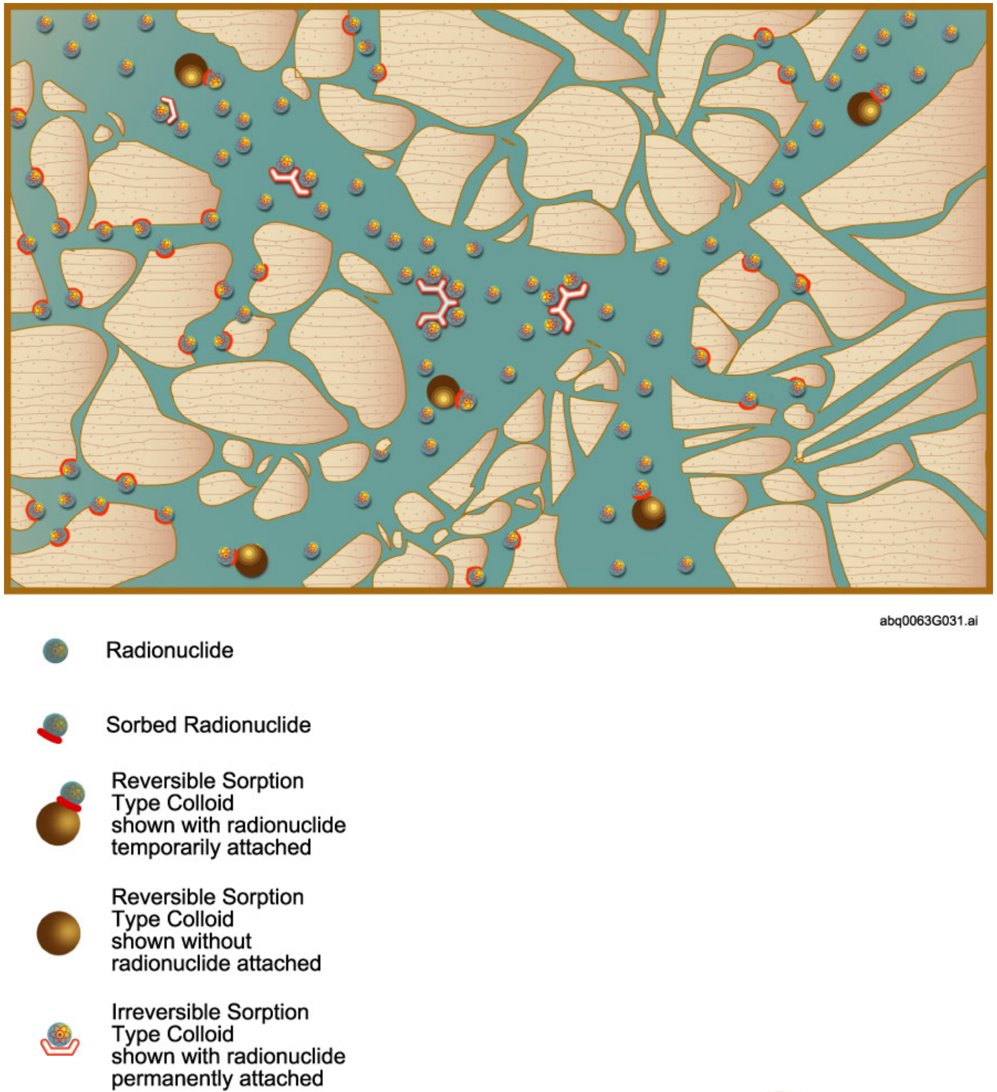


Transport Parameters and Uncertainties

- The unsaturated zone transport model incorporates probabilistically defined parameters to propagate uncertainty through the UZ model
- Sorption – reversible, equilibrium sorption model
  - Distributions developed for each radionuclide
  - Sorption to colloids is included
- Diffusion
  - Diffusion coefficient distribution from laboratory measurements
  - Uncertainty distributions for geometric parameters (aperture, fracture spacing)
  - Conceptual-model uncertainty for fracture-matrix interactions
- Colloid Transport Properties

Mathematical Implementation Using Particle Tracking – Colloid Transport Model

- **Reversible Sorption Type Colloid**
  - Colloid partitioning coefficient (K_c) describes the relative amount of radionuclide on colloids versus that in the aqueous phase
  - Only aqueous phase radionuclides can sorb or diffuse into the rock matrix
- **Irreversible Sorption Type Colloid**
  - Advective transport without diffusion into the rock matrix
  - Size exclusion model to prevent transport from fractures into some matrix units
  - Retardation via reversible filtration within the fracture continuum
  - A small fraction of the colloid inventory transports without retardation due to filtration (the "fast fraction")



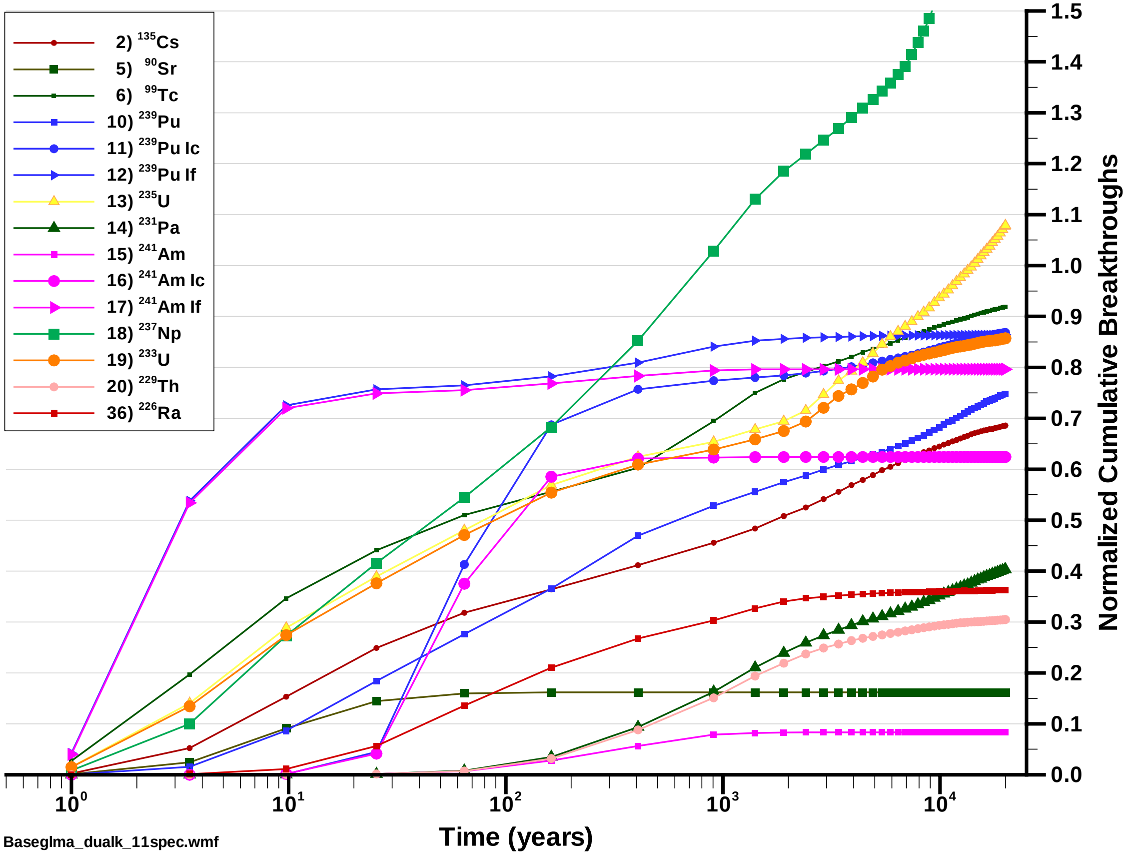
Results – Normalized Breakthrough Curves

- **This breakthrough curve (BTC) method measures the model-predicted distribution of arrival times at the water table**
  - **Representative case and other sensitivity analyses assume a release over the entire repository footprint**
  - **Method – particles are introduced at time 0, BTC is the cumulative number that arrive at the water table at various times**
  - **Curves are normalized to the number of particles introduced, so should approach 1 at long times in the absence of radioactive decay**
  - **Radionuclides participating in decay chains are introduced both as the radionuclide itself and as a parent which decays to the radionuclide – because all species are introduced in the simulation in this way, a few radionuclide BTCs go above 1**

Results – Representative Case, Various Radionuclides

Glacial-transition climate, mean infiltration scenario

- **Colloidal species travel most rapidly through the UZ, and have the narrowest distribution of arrival times**
- **Conservative and sorbing species migrate more slowly**
- **Distribution of arrival times are much broader due to matrix diffusion**
- **Radioactive decay reduces the activity of many radionuclides in the UZ**



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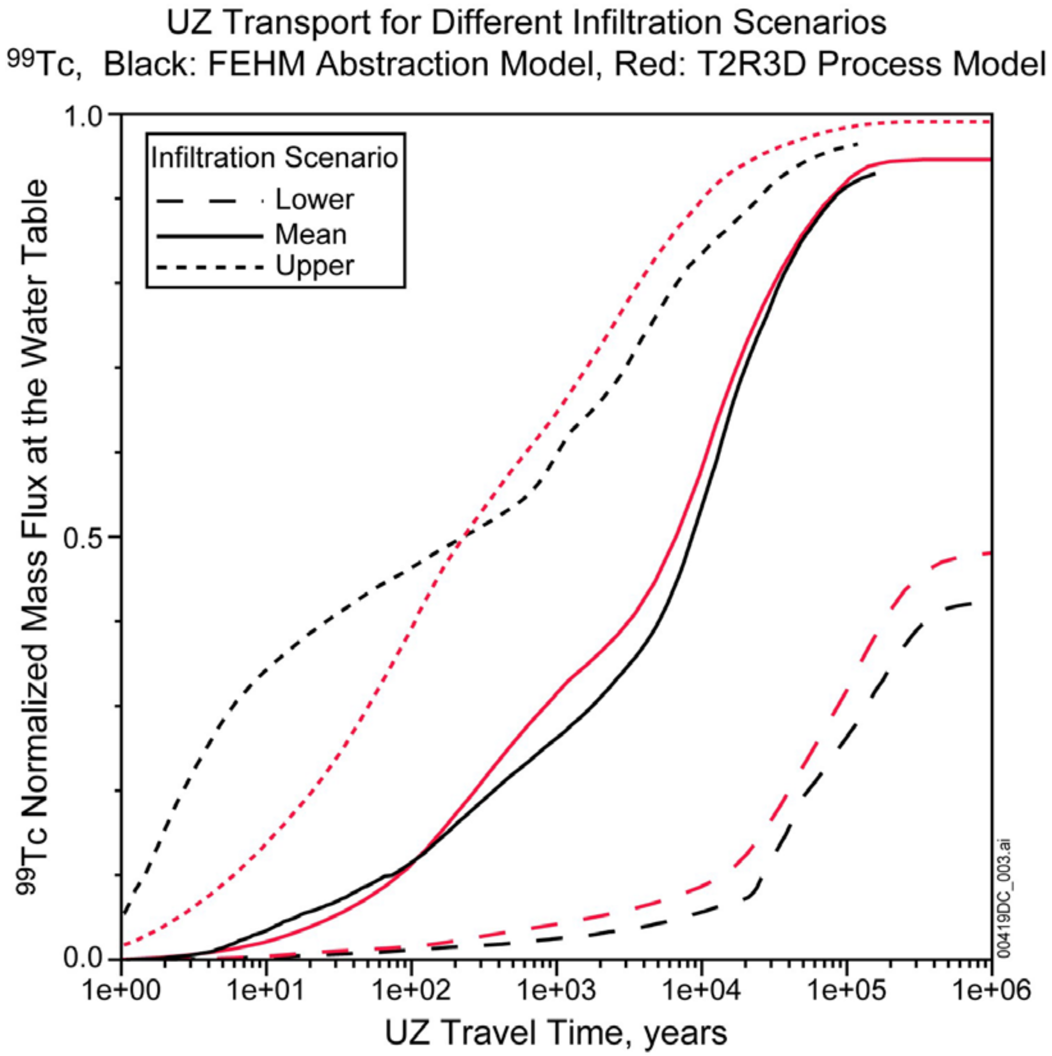
Results – Sensitivity to Infiltration Scenario

Present-day climate

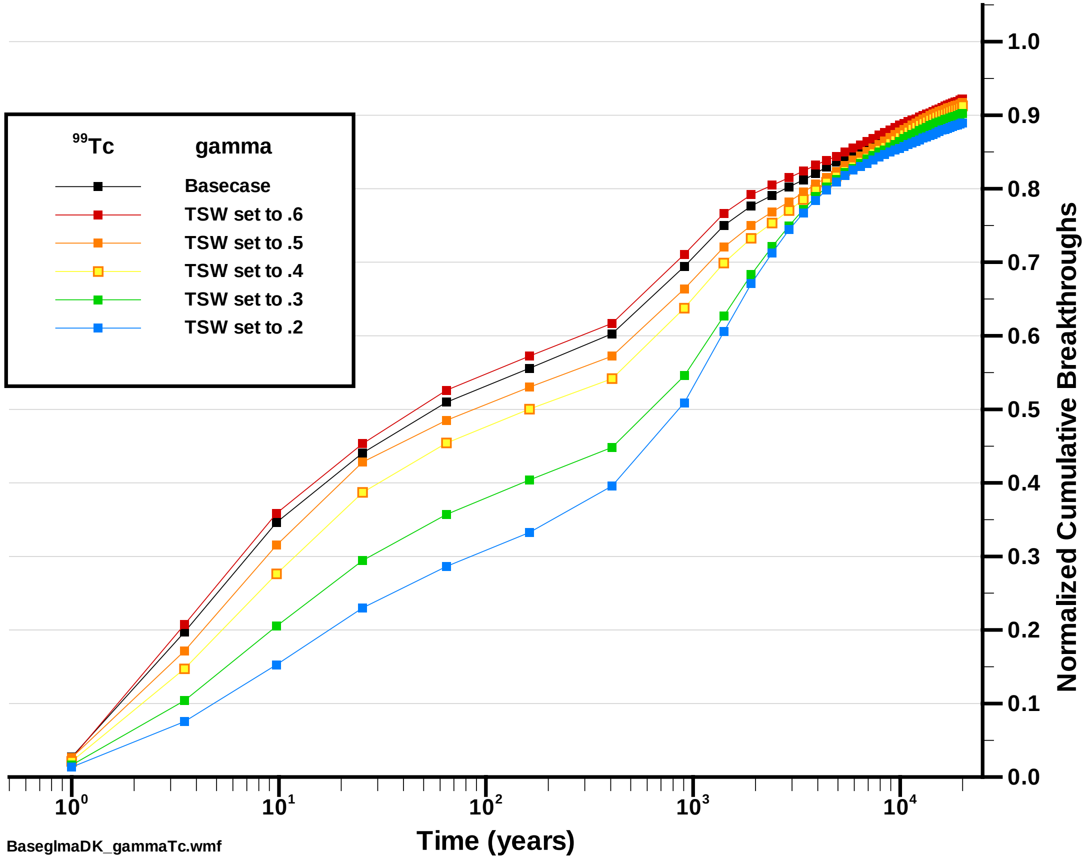
- **Comparisons illustrate the TSPA abstraction model reproduces the process model results**
- **Infiltration uncertainty has a dramatic impact on transport model results**



Sensitivity to Active Fracture Model Parameter Gamma – Tc-99

Glacial-transition climate, mean infiltration scenario

- **Flow model calibrations are relatively insensitive to several model parameters**
- **Sensitivity analyses are used to explore these uncertainties**
- **Active fracture model gamma parameter has a moderate impact on the breakthrough curve**
- **TSPA models use flow parameters at the conservative but reasonable end of the range**



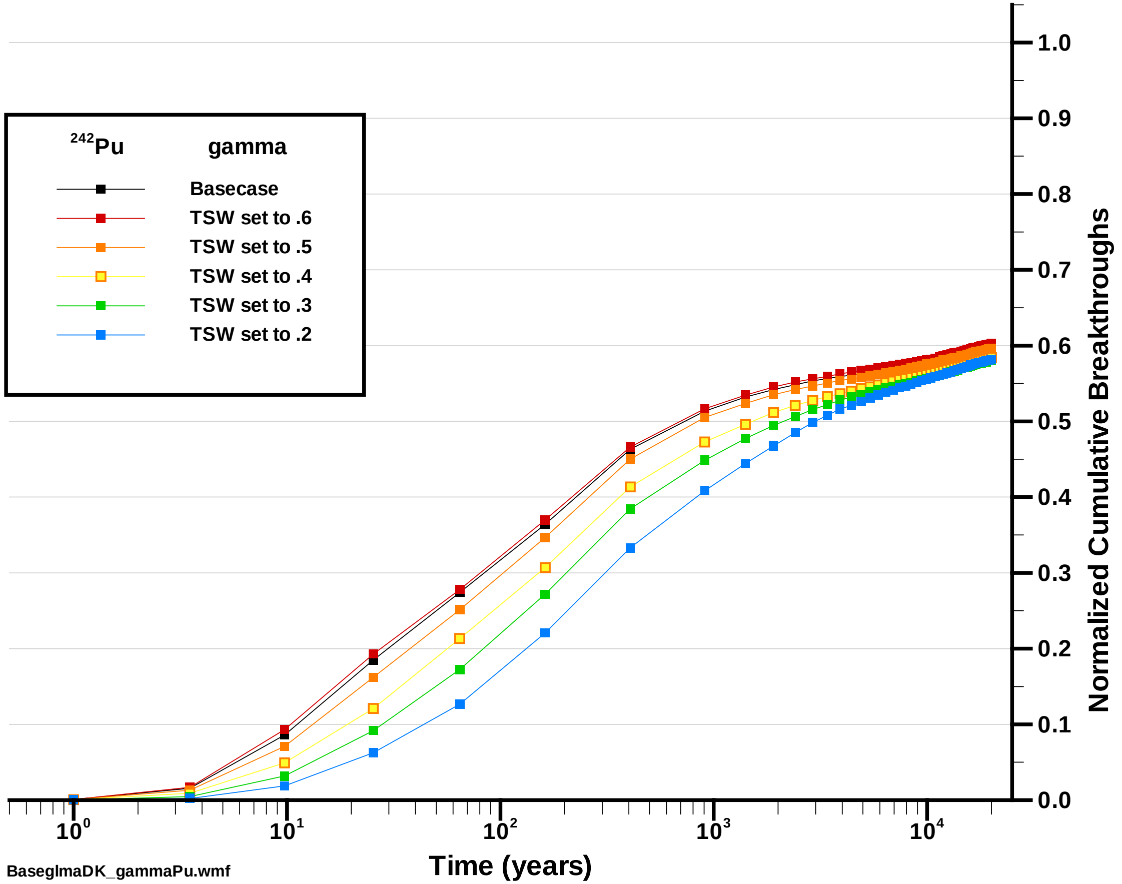
Sensitivity to Active Fracture Model Parameter Gamma – Pu-242

Glacial-transition climate, mean infiltration scenario

- Active fracture model gamma parameter also has a moderate impact on the breakthrough curve of sorbing radionulcides

Other flow model parameter results (not shown here)

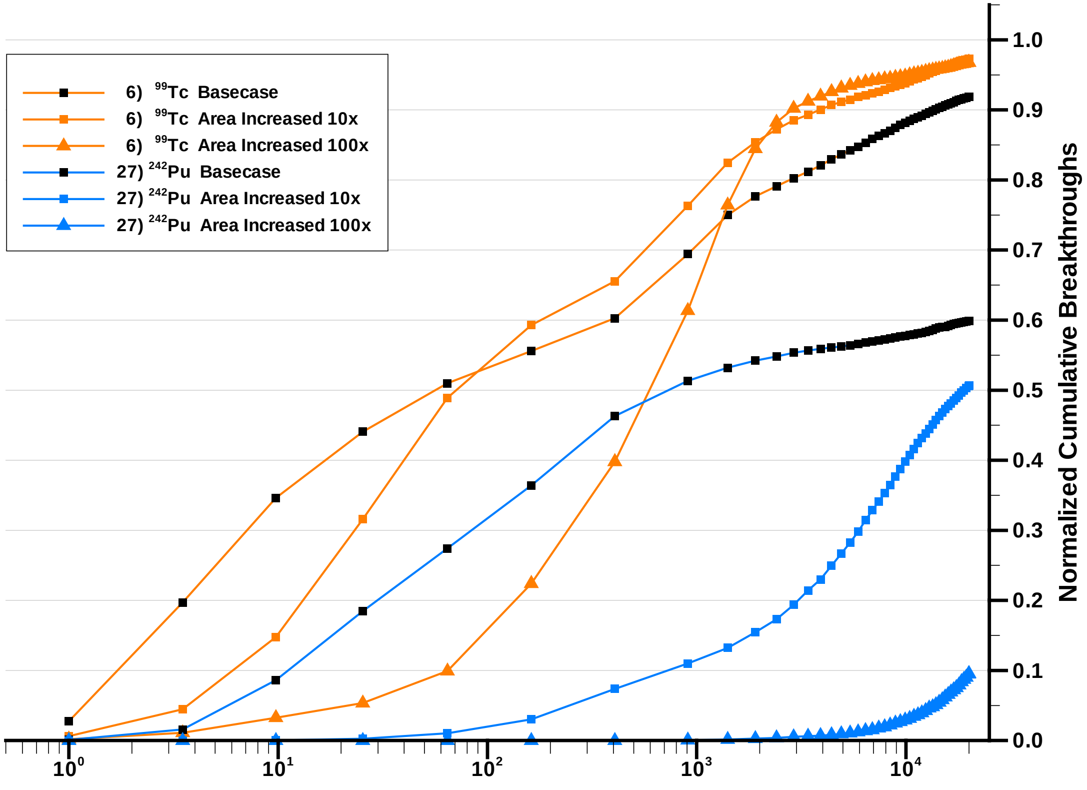
- Other sensitivity analyses show low to moderate impact of flow model parameter uncertainties on the breakthrough curves



Sensitivity to Diffusion Coefficient – Tc-99 and Pu-242

Present-day climate, mean infiltration scenario

- **Diffusion coefficient has a large impact on the breakthrough curve**
- **For fracture transport, diffusion subdues the transport velocities of radionuclides traveling in the fractures by enabling migration into the slow-moving fluid in the rock matrix**
- **The impact of diffusion is most prevalent for sorbing radionuclides**
- **Uncertainty in diffusion coefficient is captured in TSPA model**



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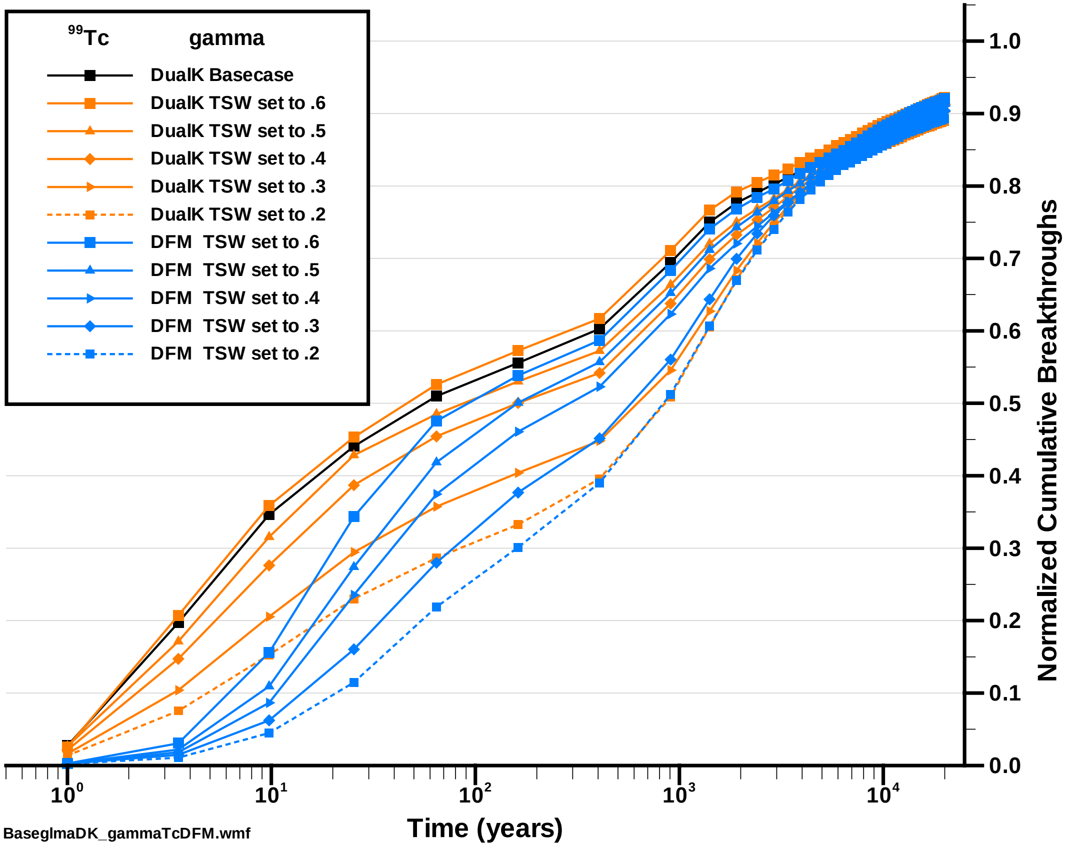
Sensitivity to Fracture-Matrix Interaction Model – Tc-99

Glacial-transition climate, mean infiltration scenario

- **The conceptual model uncertainty associated with the diffusion to and from the fractures (fracture-matrix interaction model) has a significant impact on breakthrough curves**
- **Less early-time breakthrough is predicted with the (alternative) discrete fracture model because sharp gradients near the fracture are captured in this model**



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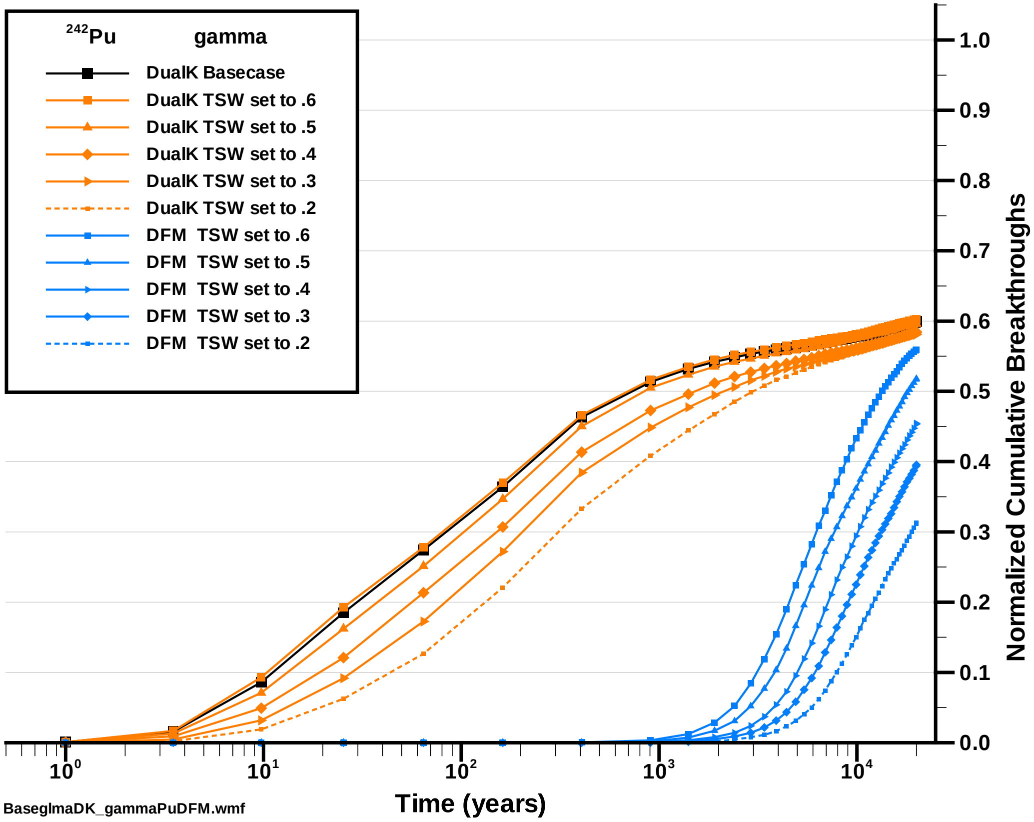
Sensitivity to Fracture-Matrix Interaction Model – Pu-242

Glacial-transition climate, mean infiltration scenario

- The impact is even more dramatic for sorbing radionuclides
- The TSPA model conservatively uses the dual-k model
- A discrete fracture model (or equivalent) could be used in the future if the model is validated against field data
- Alternatively, a dual-k model with enhanced diffusion coefficients could be used



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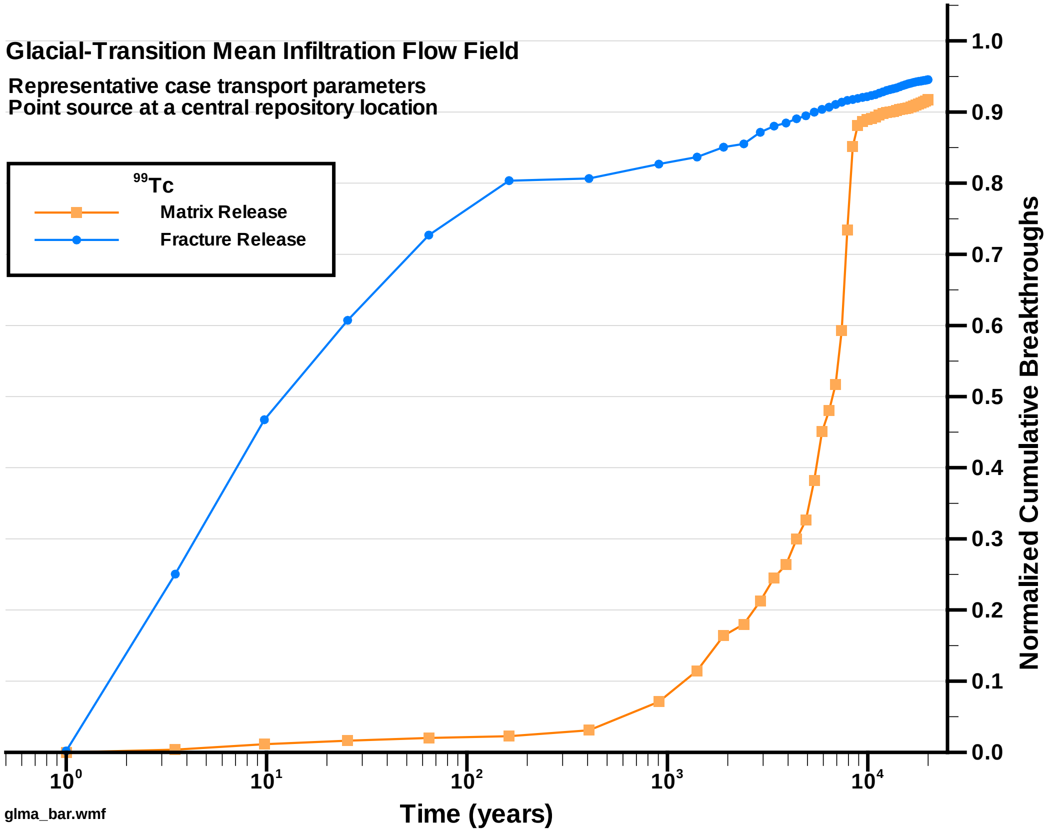
Fracture Versus Matrix Releases

Tc-99, glacial-transition climate, mean infiltration scenario, point release

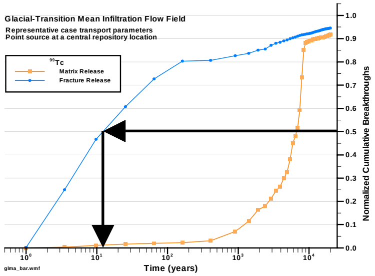
- Flow is fracture-dominated at the repository horizon
- Matrix releases have significantly longer travel times because radionuclide must diffuse to the flowing fractures to travel rapidly
- Smaller diffusion coefficients yield longer travel times (the opposite of the fracture release case)

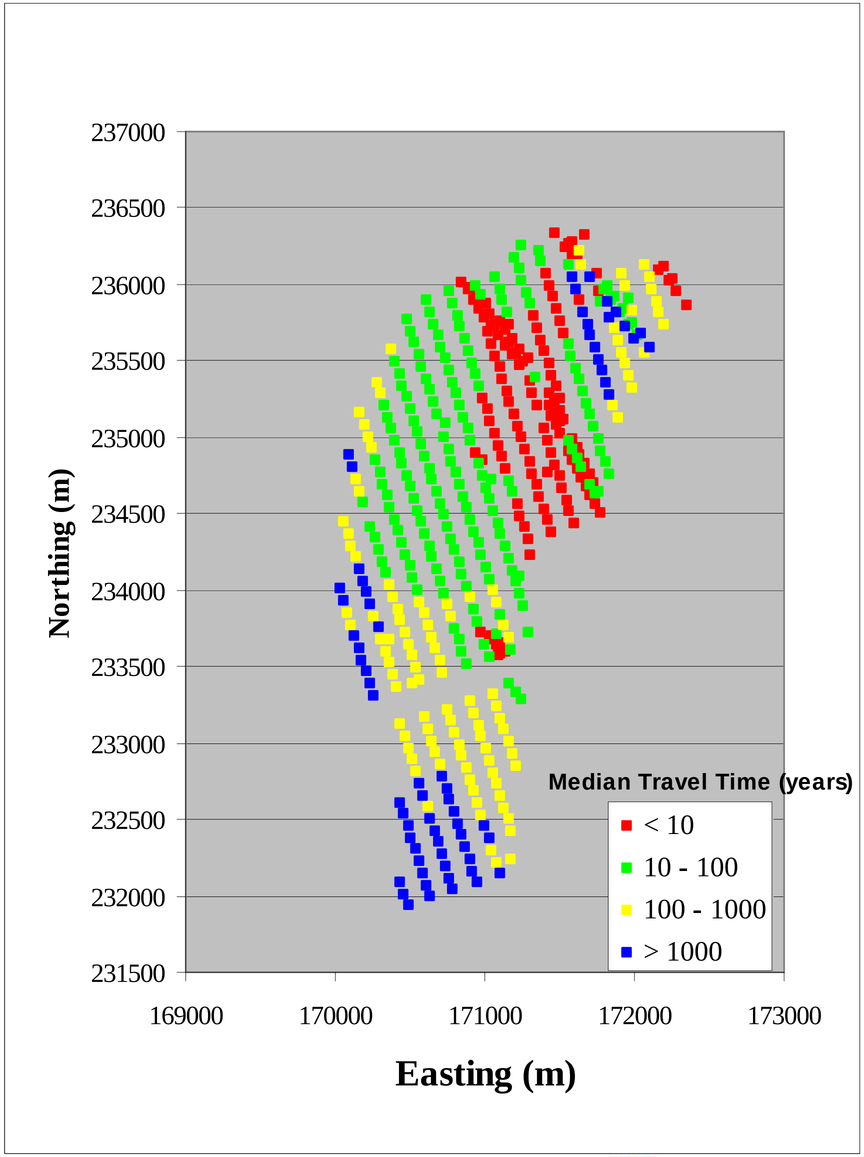


Spatial Variability – Median Travel Time of Tc-99

Glacial-transition climate, mean infiltration scenario

- **Large variability in breakthrough curve depending on where the releases occur**
  - **Hydrogeologic variability**
  - **Percolation flux variability**
- **If only a few waste packages fail, this results in an uncertainty in travel time**
- **If most packages fail, this effect results in a spread in the distribution of arrival times**
- **All distributed release simulations presented earlier include this variability in the breakthrough curves**





Conclusions

- Radionuclide transport in the Unsaturated Zone for TSPA is simulated considering all relevant transport processes
- Uncertainties that are most important to the travel times through the UZ are:
  - Infiltration rate
  - Diffusion model parameters
  - Diffusion conceptual model
- Uncertainties in flow model parameters have low to moderate impact on the travel times
- TSPA model takes a reasonably conservative approach for uncertainties not directly represented via parameter uncertainty distributions
- Matrix releases yield much longer travel times
  - Fracture releases – lower D yields shorter travel times
  - Matrix releases – lower D yields longer travel times
- Spatial variability of travel times results from different percolation fluxes and hydrogeology across the repository