



U.S. Department of Energy
Office of Civilian Radioactive Waste Management



Sorption, Matrix Diffusion, and Colloid-facilitated Transport in the Unsaturated Zone Radionuclide Transport Model

Presented to:

**U.S. Nuclear Waste Technical Review Board Panel
on the Natural System**

Presented by:

**George J. Moridis
Yongkoo Seol
Lawrence Berkeley National Laboratory**

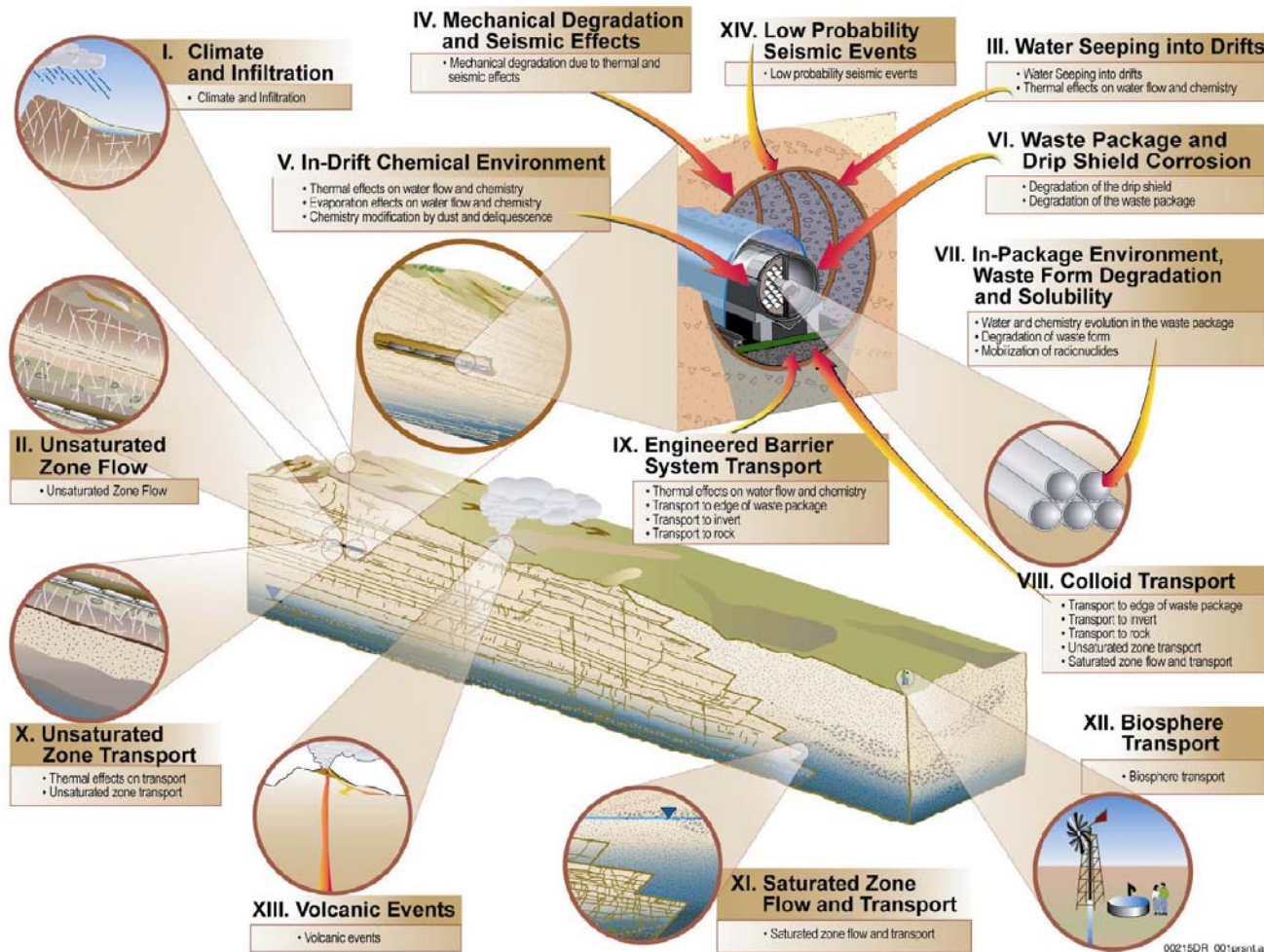
**March 9-10, 2004
Las Vegas, Nevada**

Outline

- **Relation of transport to other post-closure processes**
- **Discussion of radioactive species and transport processes**
- **Model validation/confidence building**
 - Field tests of various scales
- **Mountain-scale solute transport studies**
 - 3 radionuclides covering the spectrum of sorption (strong, weak, no sorption)
 - 3 climatic regimes, 3 levels within each regime
 - Instantaneous and continuous release
- **Mountain-scale colloid transport studies**
 - 4 colloid sizes
 - Different filtration behavior (weak vs. strong)
- **Uncertainties**
- **Conclusions and Comments**



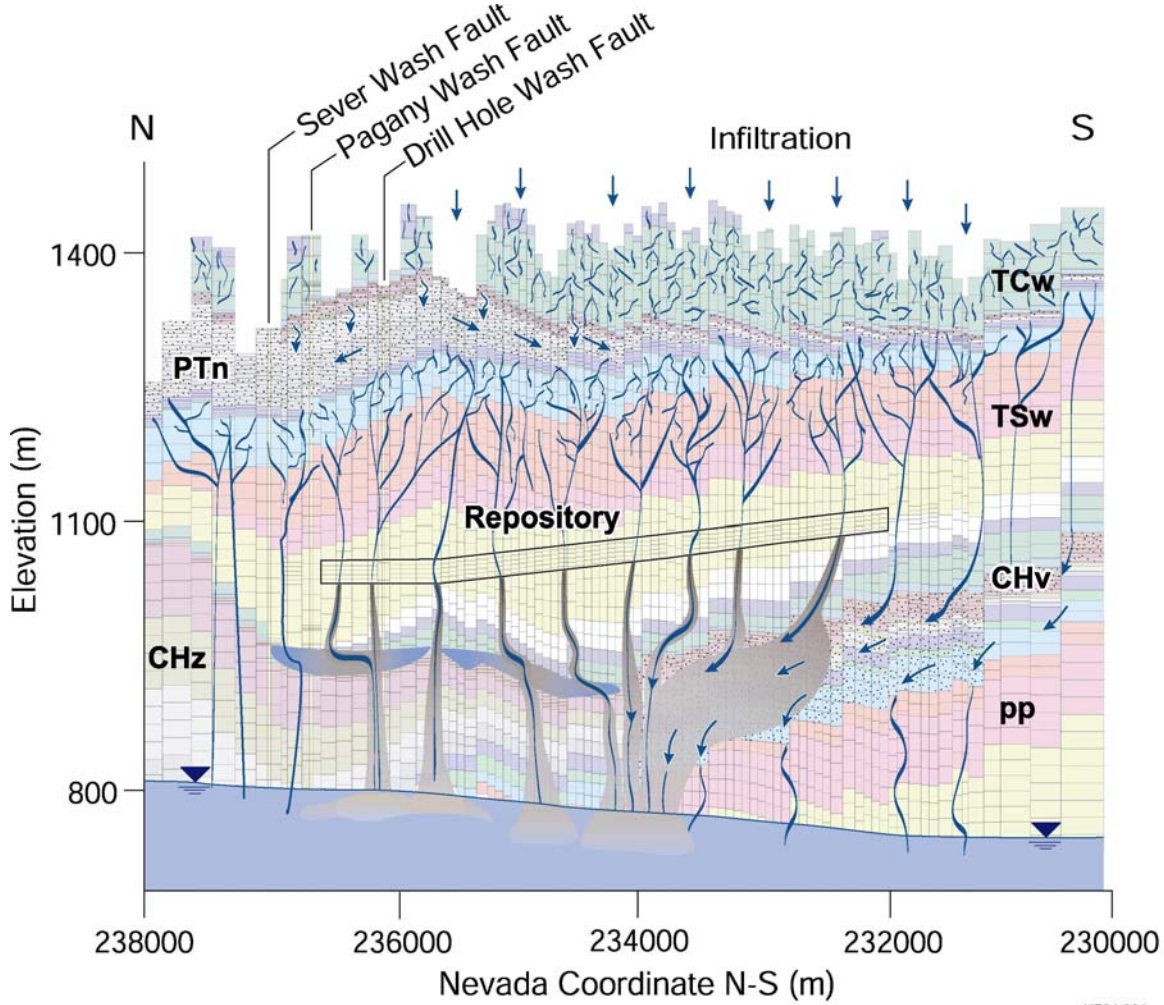
Relationship to the Other Components of Postclosure Technical Basis



Transport strongly linked to other processes: End of chain



Hydrogeology: Dominant Factor Affecting Transport



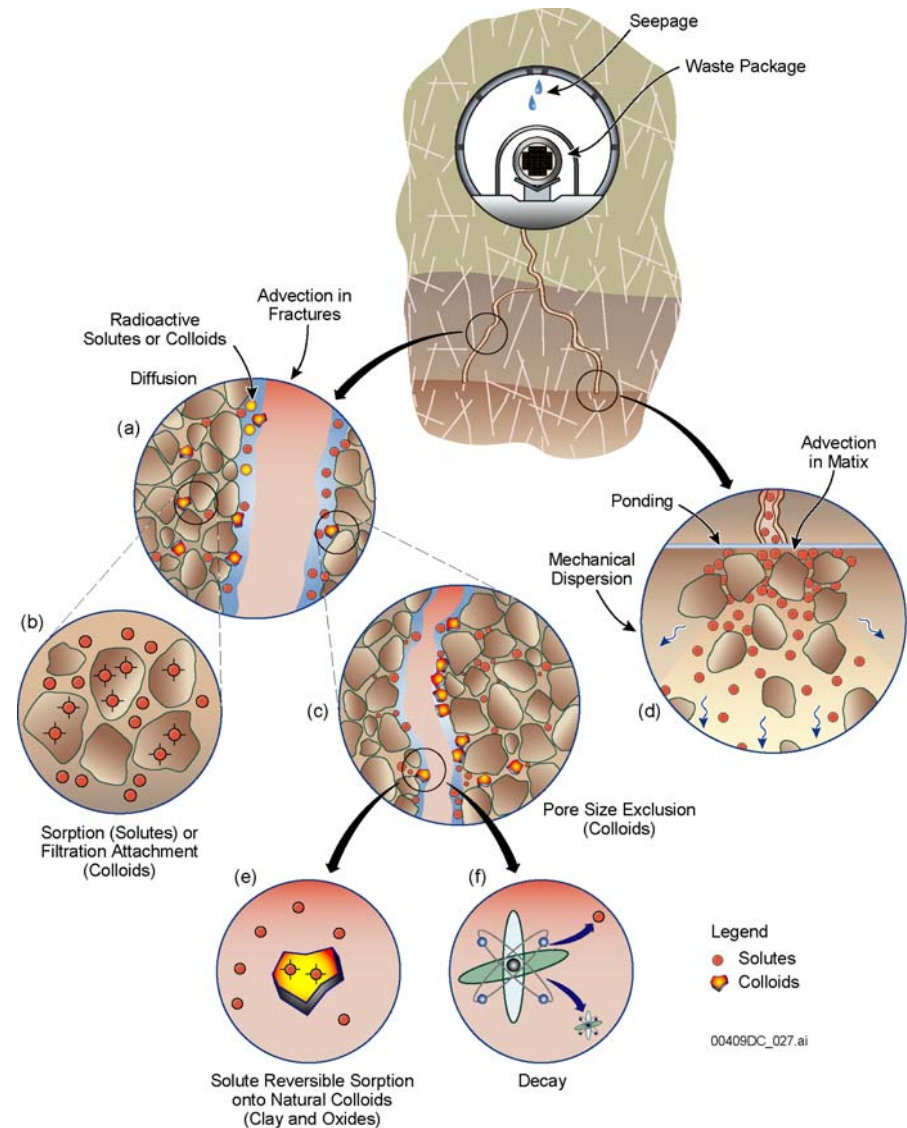
- Hydrogeology: Dominant factor affecting transport

Unsaturated Zone Flow Features. The major hydrogeologic units are the Tiva Canyon welded (TCw), the Paintbrush nonwelded (PTn), and the Topopah Spring welded (TSw) units. CHz (zeolitic), CHv (vitric), and PP (Prow Pass) refer to hydrogeologic units within the major Calico Hills hydrogeologic unit. Arrows in the PTn layer indicate local lateral component of flow.



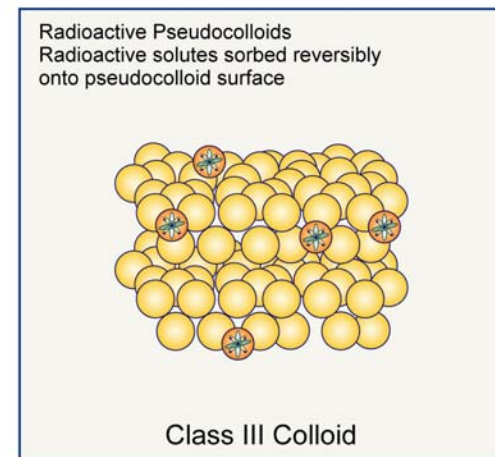
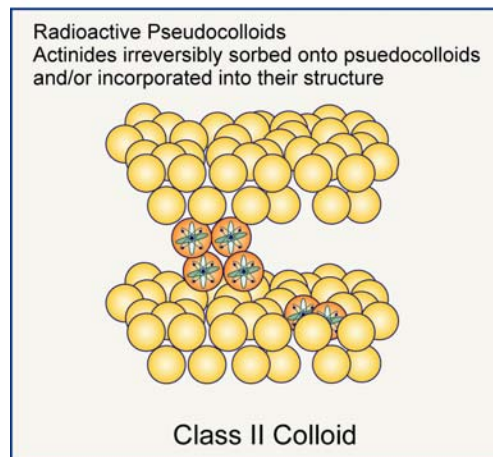
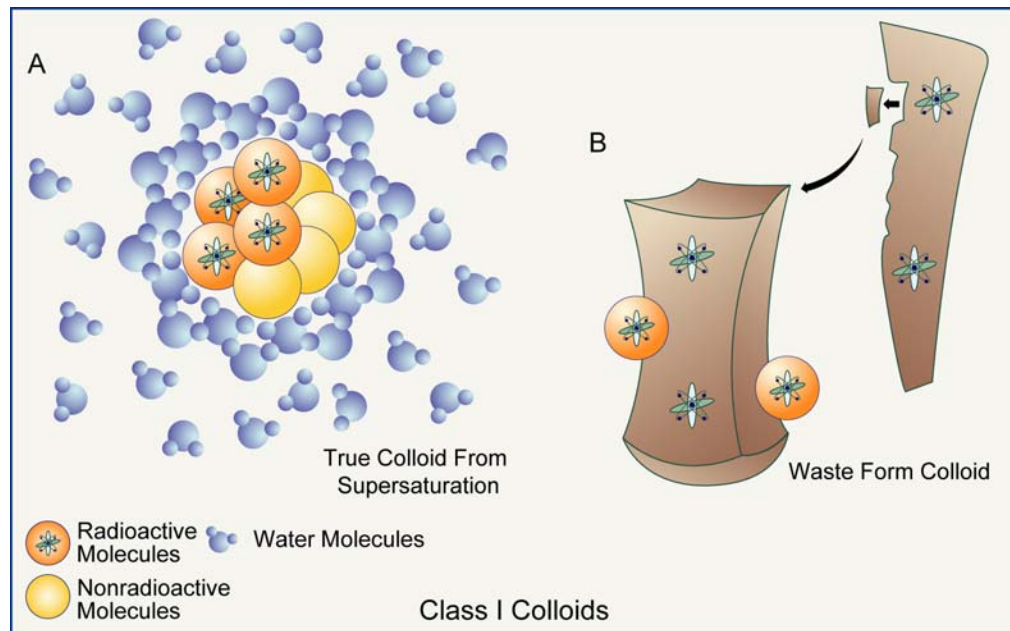
Processes in Transport

- **Advection**
- **Matrix diffusion**
- **Dispersion**
- **Solutes: sorption**
- **Colloidal transport**
 - Pore size exclusion
 - Filtration/attachment
- **Radioactive decay**

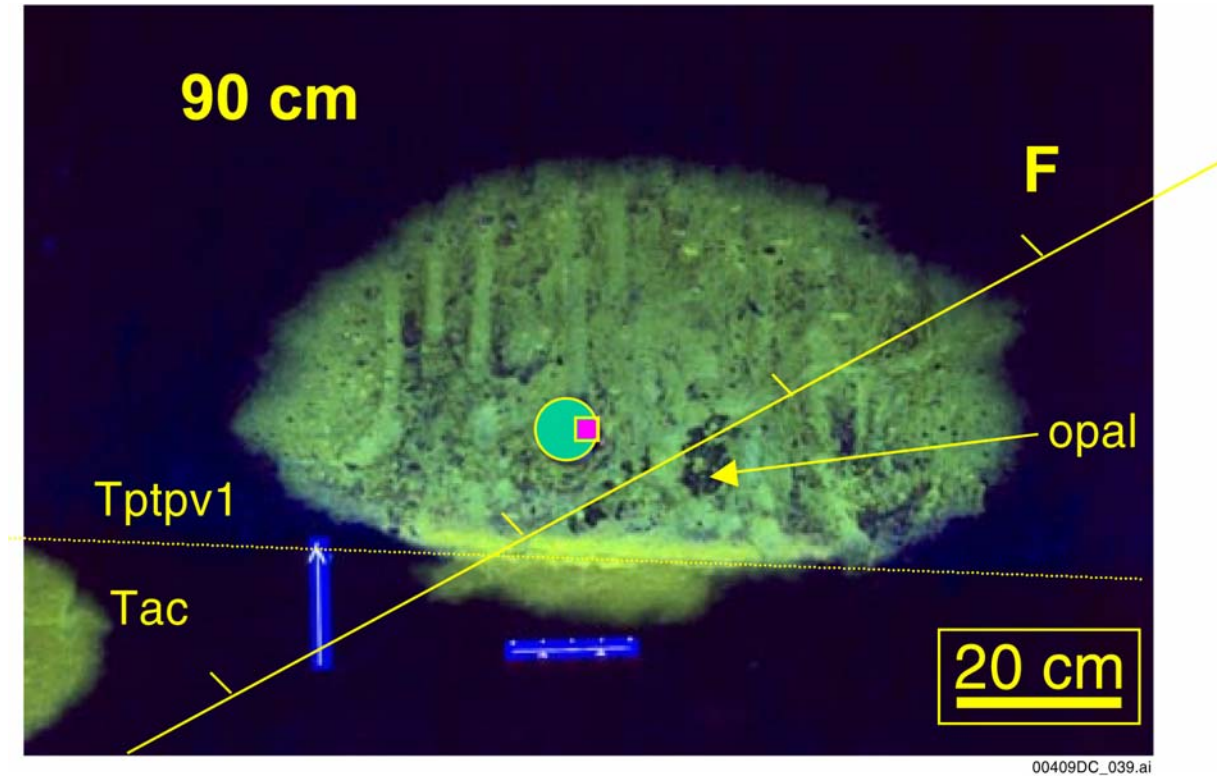


Radioactive Species

- **Solutes**
 - Various K_d
- **Colloids: 3 classes**



Confidence Building: The Busted Butte Test 1A (sub-meter scale)

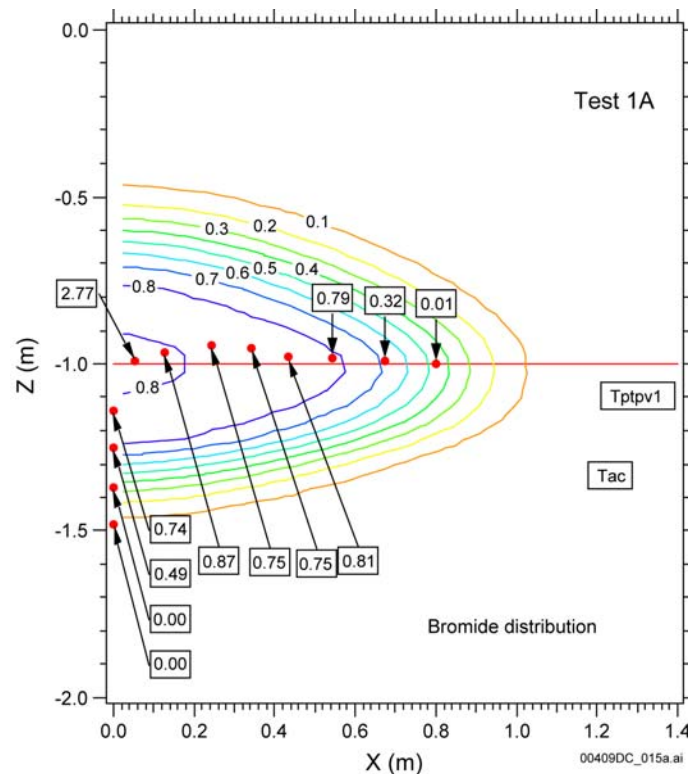
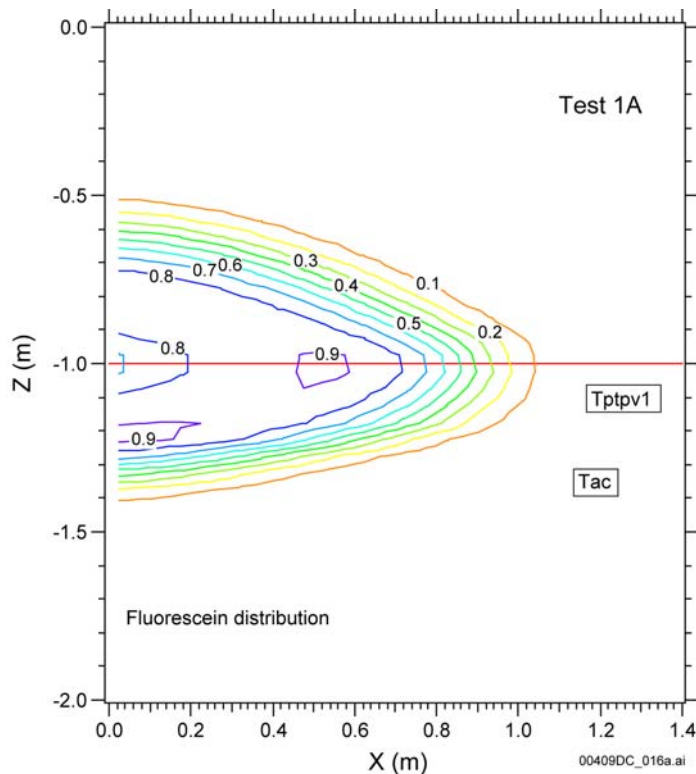


Fluorescein Plume at the Mineback Face ($y = 0.9$ m) at Borehole 3



Confidence Building: The Busted Butte Test 1A (sub-meter scale)

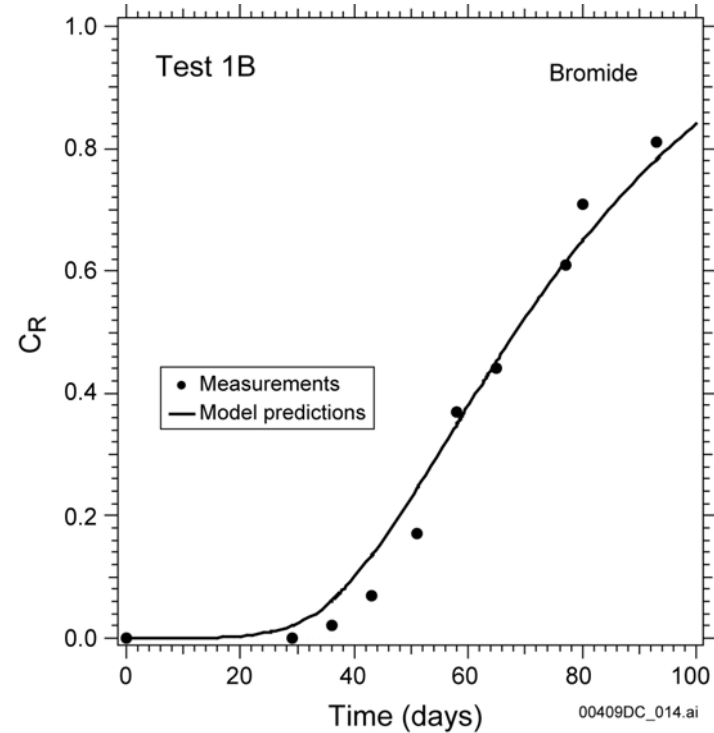
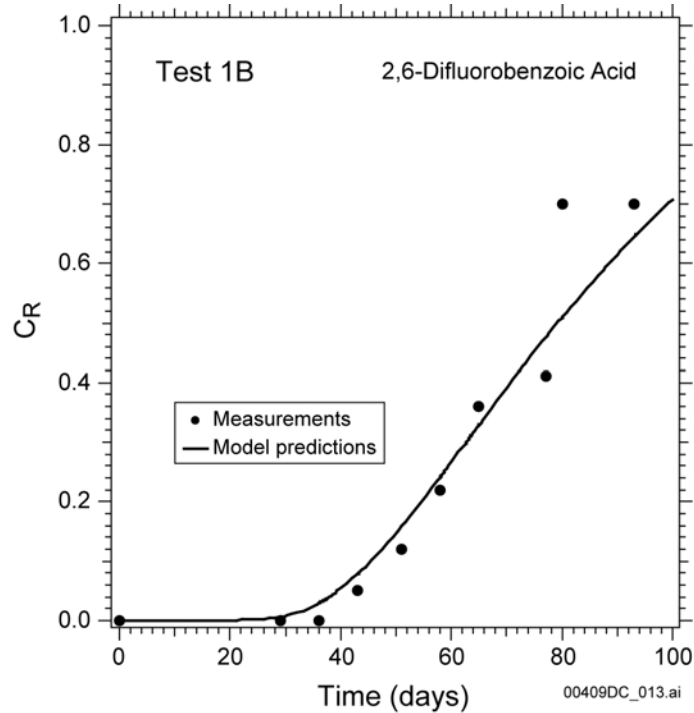
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Numerical Prediction of the Fluorescein Plume Using Calibrated Parameters (Busted Butte Test Phase 1A, Left) and Field Measurements and Numerical Prediction of the Bromide Distribution in Busted Butte Test Phase 1A (Right)



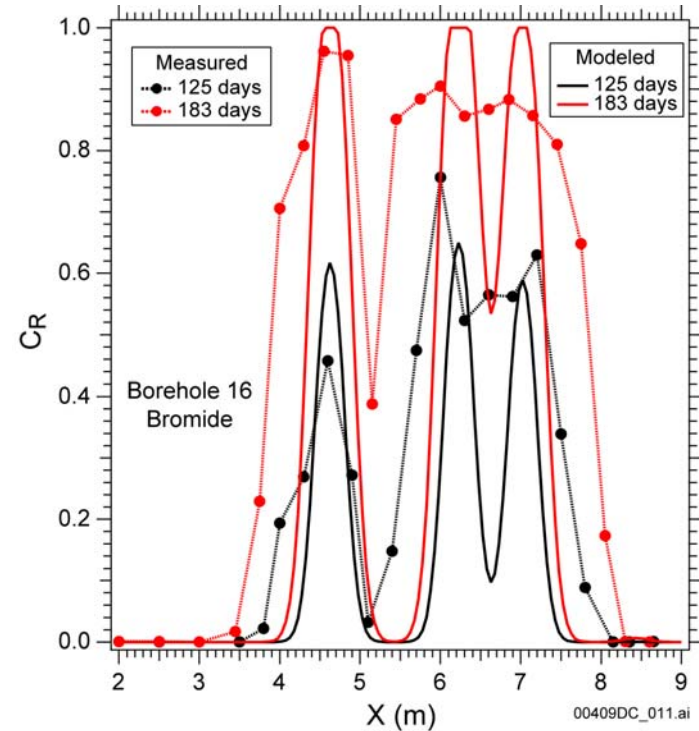
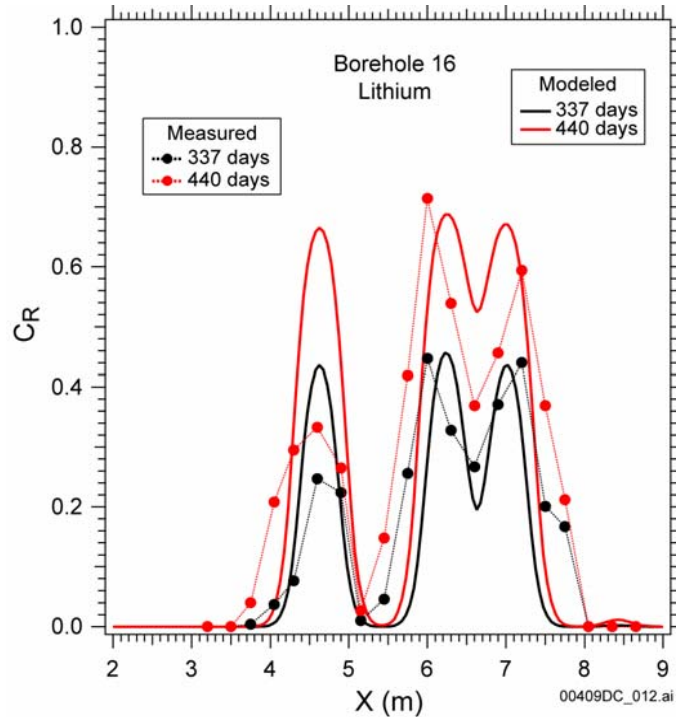
Confidence Building: The Busted Butte Test 1B (meter scale)



Observed and Numerically Predicted (Calibrated) Breakthrough Curves of 2,6-DFBA for the Busted Butte Phase 1B Test (Left), and Observed and Numerically Predicted (at Verification) Breakthrough Curves of Bromide in the Busted Butte Phase 1B Test (Right)



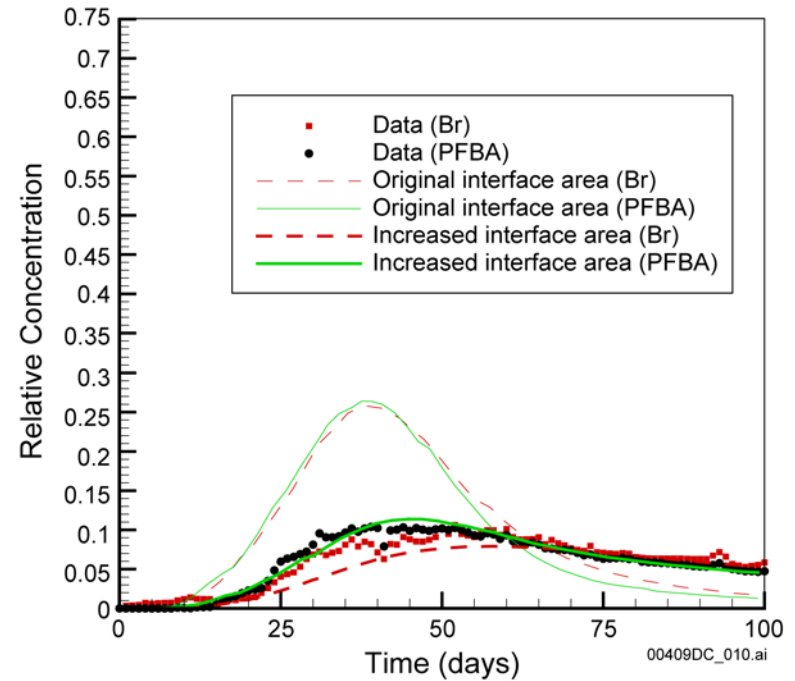
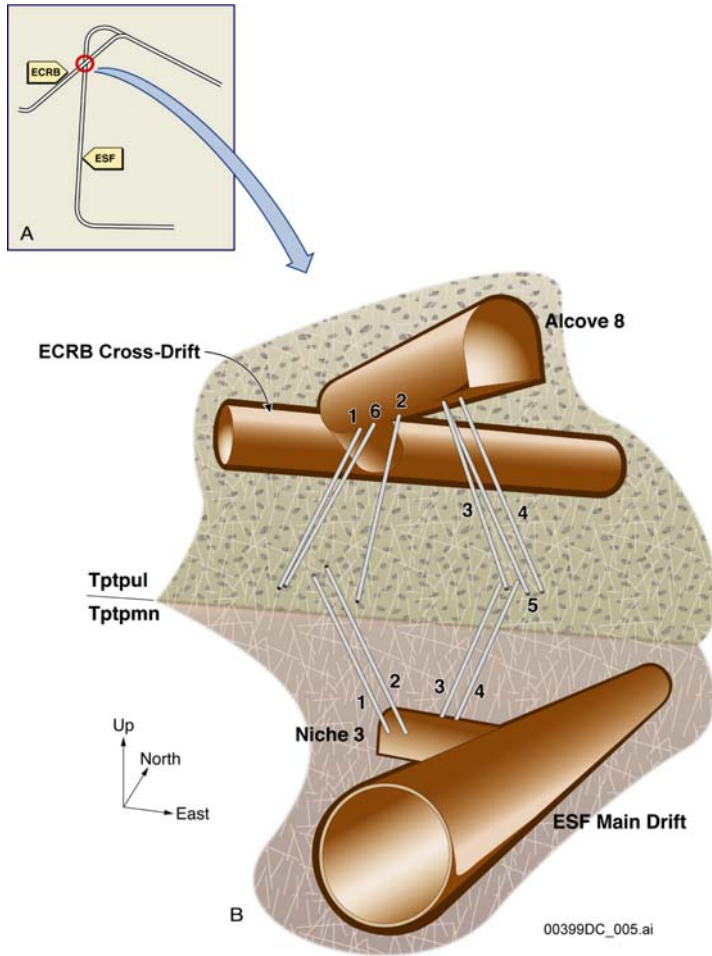
Confidence Building: The Busted Butte Test 2C (2-3 meter scale)



Observed and Numerically Predicted (Calibrated) Breakthrough Curves of Li^+ in the Busted Butte Phase 2C Test (Left), and Observed and Numerically Predicted Breakthrough Curves of Br^- in the Busted Butte Phase 2C Test (at Verification) (Right)



Confidence Building: The Alcove 8-Niche 3 Test (20-30 meter scale)



Comparisons between Simulated Breakthrough Curves at the Niche for Two Different Fault-Matrix Interface Areas and the Observed Data

Test Bed for the Alcove 8-Niche 3 Tests



3-D Mountain-Scale Transport Studies

- **Objectives**
 - **By stressing the system under impossibly aggressive (conservative) conditions, to**
 - ◆ **Determine the main pathways of potential radionuclide transport to the water table**
 - ◆ **Identify the dominant processes affecting transport and retardation**
 - ◆ **Evaluate the relative importance of processes and phenomena**
 - ◆ **Determine the relative transport behavior of general types of radioactive species (solutes vs. colloids, nonsorbing vs. sorbing)**
- **Not an attempt to predict travel times to the water table under any possible/plausible scenario**



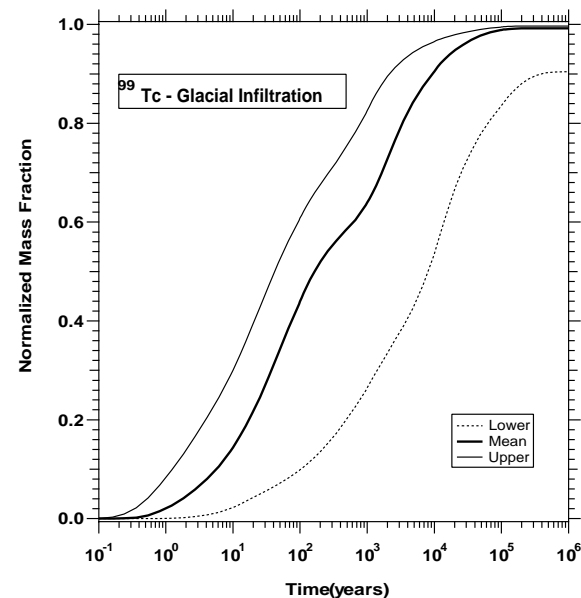
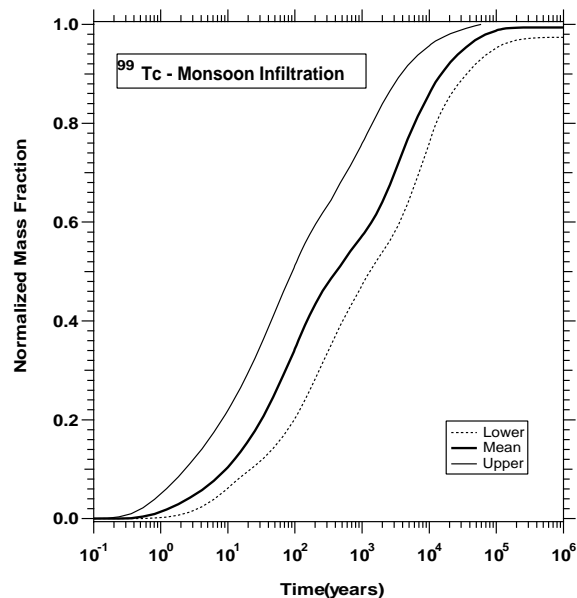
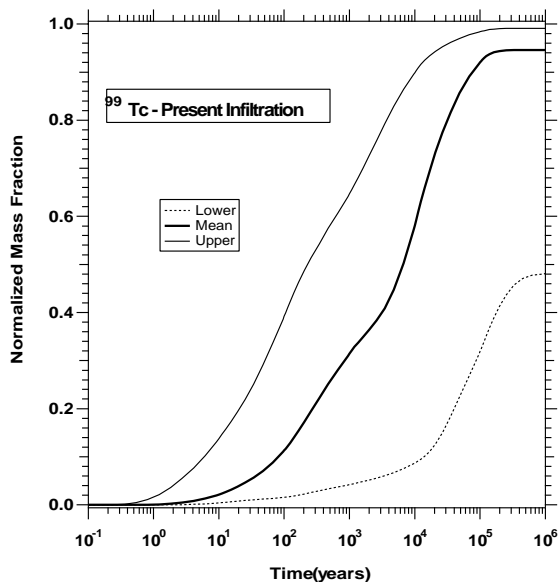
In This Study: Conservative Approach

- **No drip shields are considered, and flow through the canisters is assumed**
- **All the radioactive packages in the entire repository rupture simultaneously**
- **The radionuclides are released directly into the fractures (no retardation effects of the invert with porous media properties)**
- **The effects of the shadow zone are ignored**
- **The vertical fractures are open and continuous throughout the UZ (no retardation through solute sorption and/or colloid attachment onto the fracture walls and the fracture minerals)**
- **The horizontal fractures are modeled as interconnected, and are also connected (directly or indirectly) to the vertical fractures**
- **The distribution coefficients were estimated over longer concentration intervals using an approach that results in milder slopes and lower K_d values**
- **Potential chemical stabilization (e.g., through precipitation) of solids is ignored**
- **Colloid stability is assumed**

NOTE: Significant Uncertainties in UZ hydrology.



3-D Mountain-Scale Transport Studies



Transport of ⁹⁹Tc (nonsorbing) Instantaneous Release, Various Climatic Regimes

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.

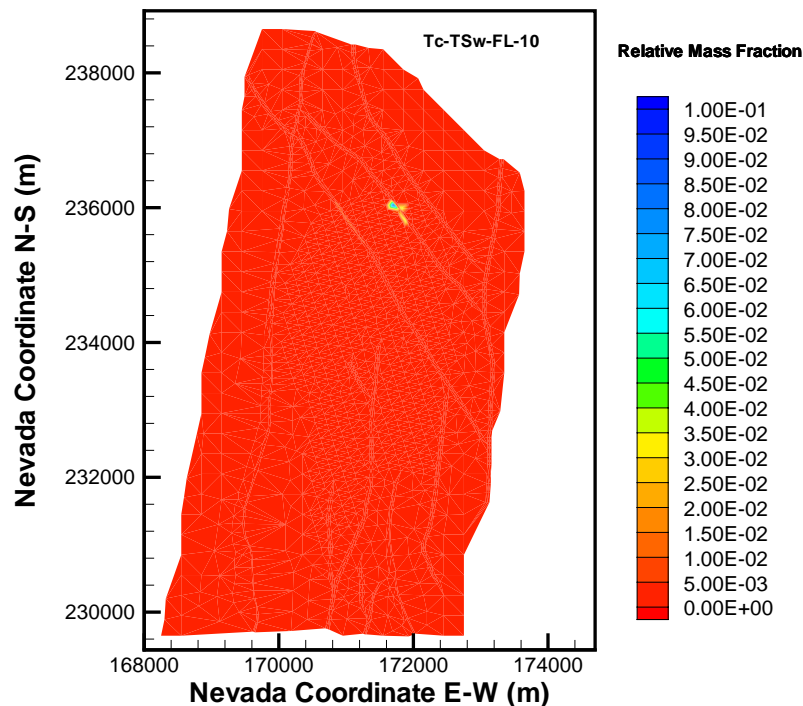


3-D Mountain Scale Transport Studies

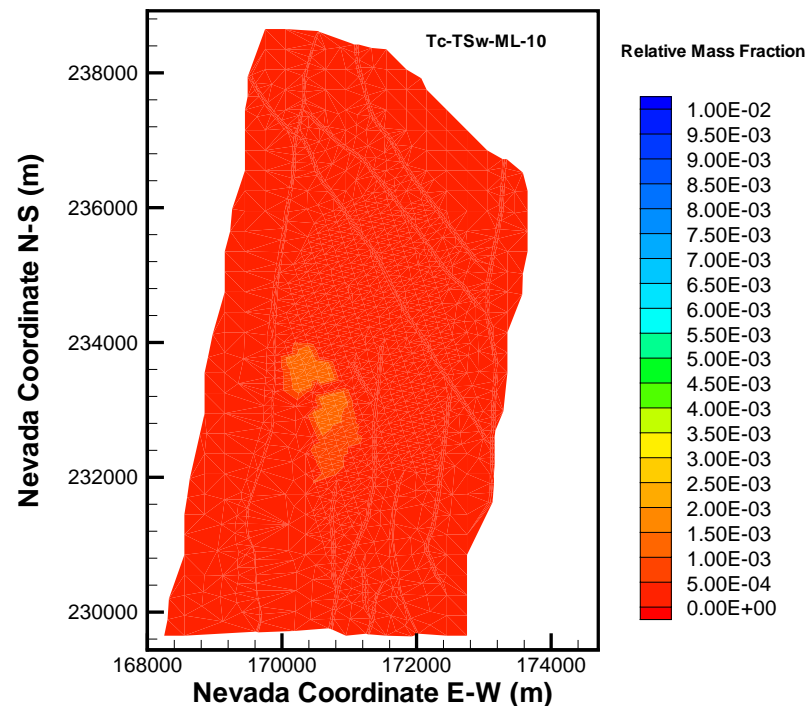
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Instantaneous Release

T = 10 yrs, Fracture Relative Concentration



T = 10 yrs, Matrix Relative Concentration



Transport Patterns of ^{99}Tc (nonsorbing)
Bottom of the TSw

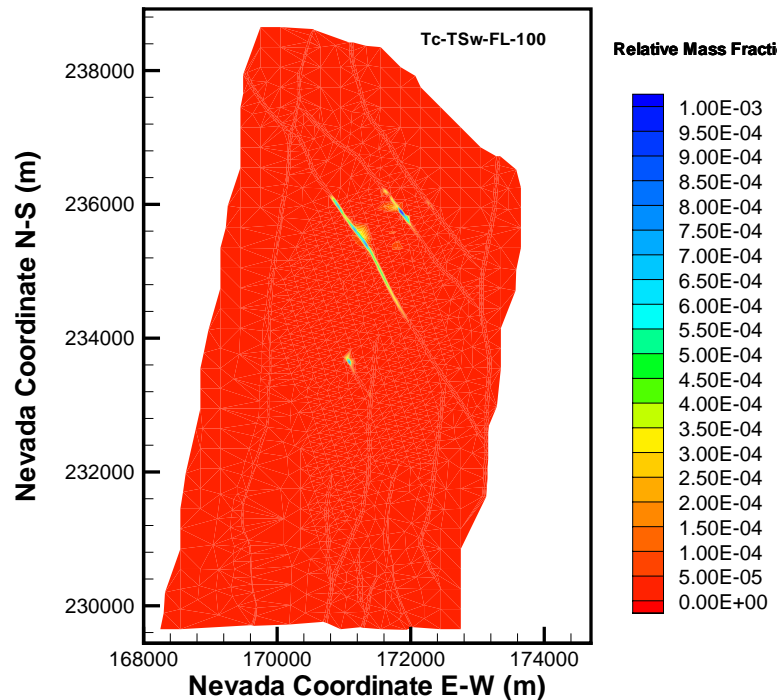


3-D Mountain Scale Transport Studies

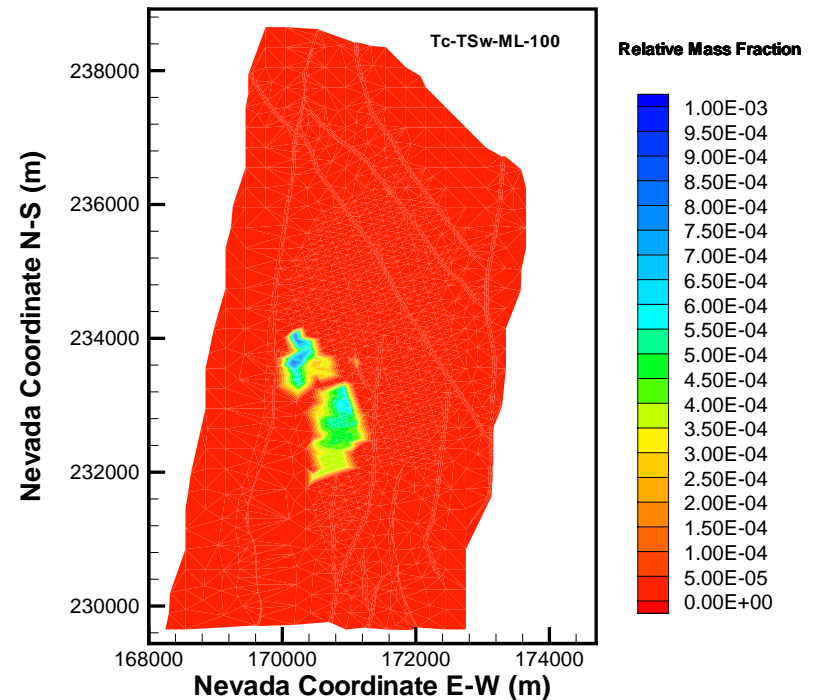
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Instantaneous Release

T = 100 yrs, Fracture Relative Concentration



T = 100 yrs, Matrix Relative Concentration



⁹⁹Tc at the Bottom of the TSw: Different Transport Patterns in North and South

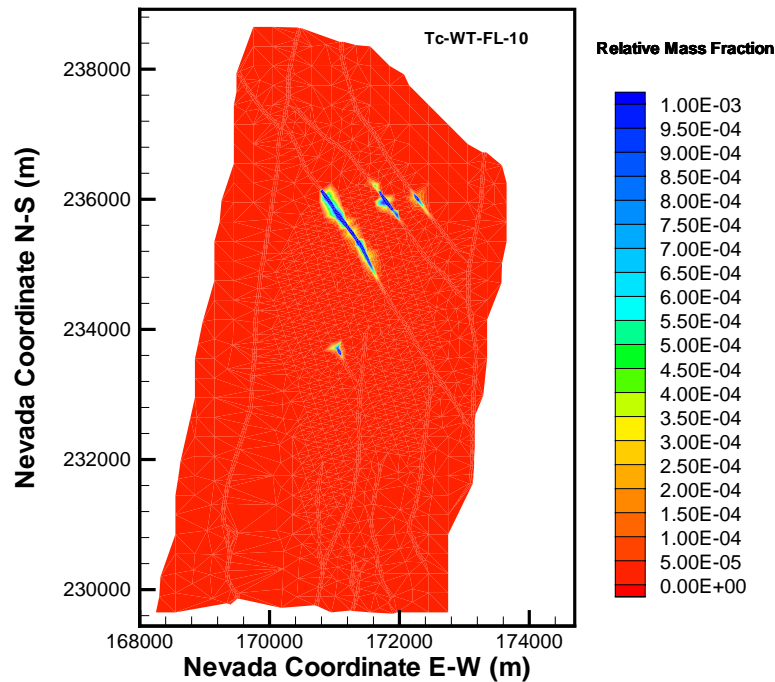


3-D Mountain Scale Transport Studies

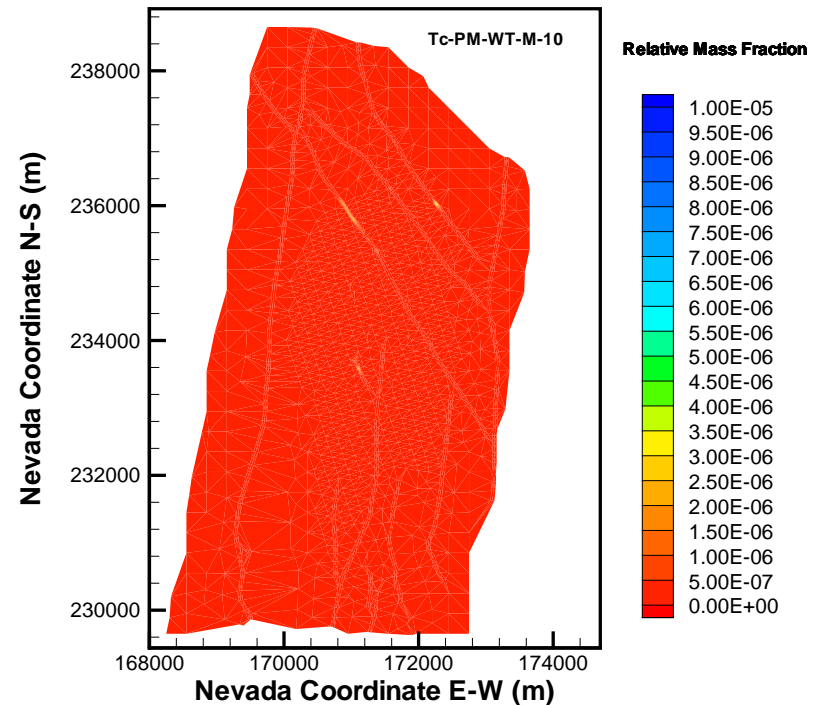
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Instantaneous Release

T = 10 yrs, Fracture Relative Concentration



T = 10 yrs, Matrix Relative Concentration



^{99}Tc at the Water Table: Different Transport Patterns, Dominance of Faults

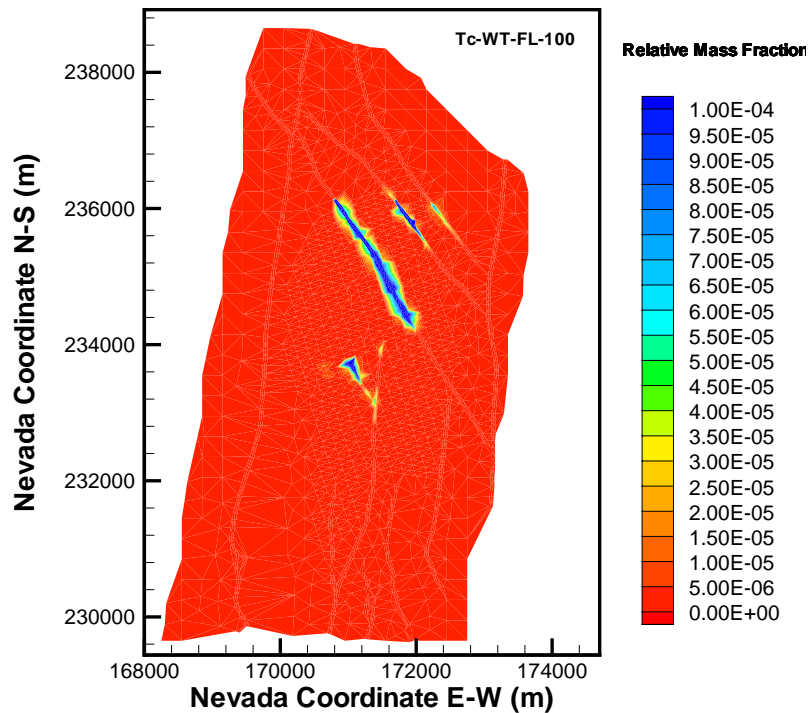


3-D Mountain Scale Transport Studies

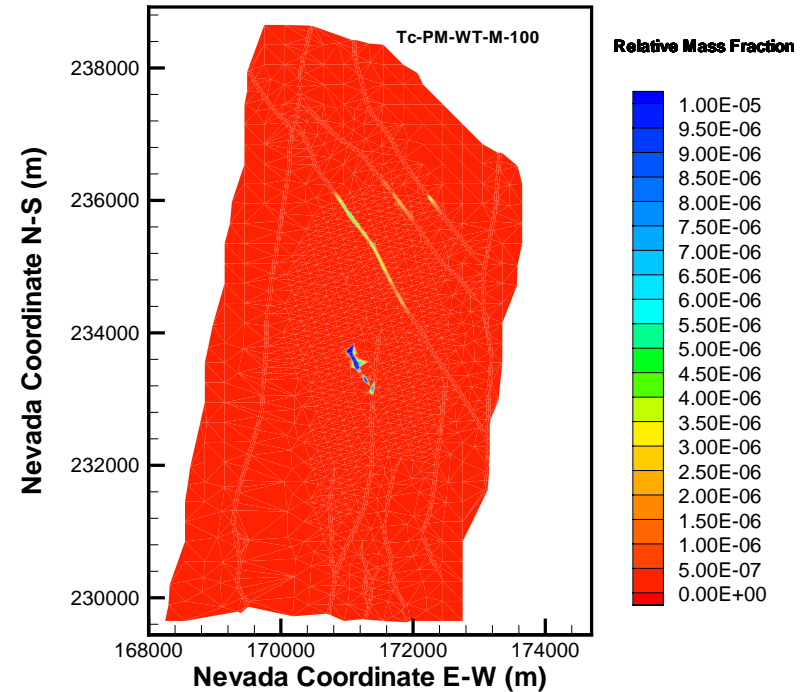
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Instantaneous Release

T = 100 yrs, Fracture Relative Concentration



T = 100 yrs, Matrix Relative Concentration

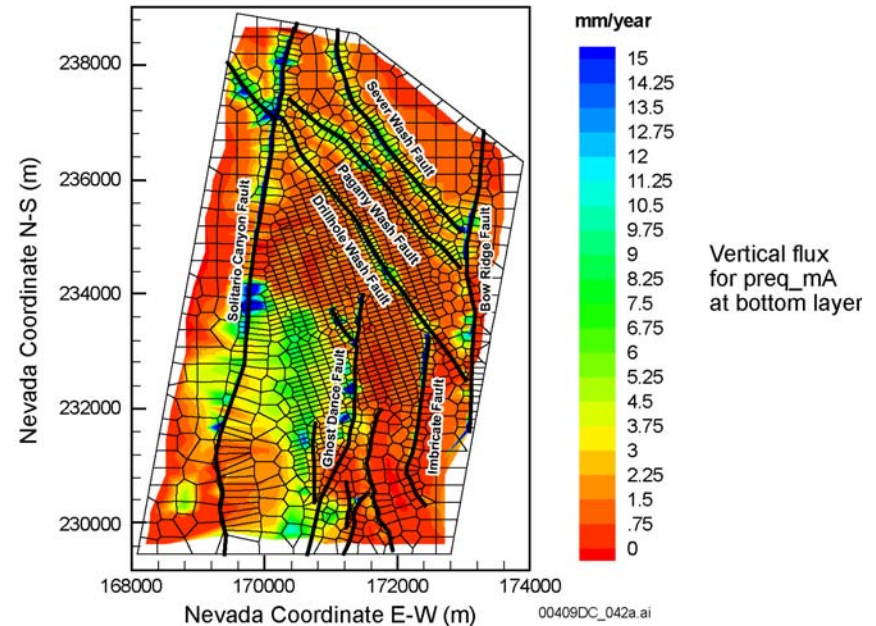
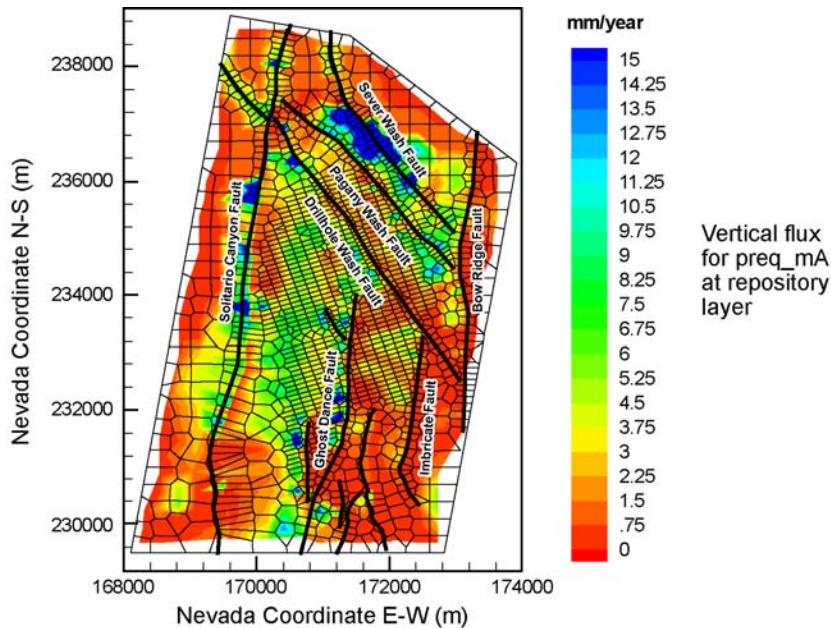


**^{99}Tc at the Water Table: Dominance of Faults
Difference from Pattern at the Bottom of the TSw**



3-D Mountain Scale Transport Studies

(Continued)

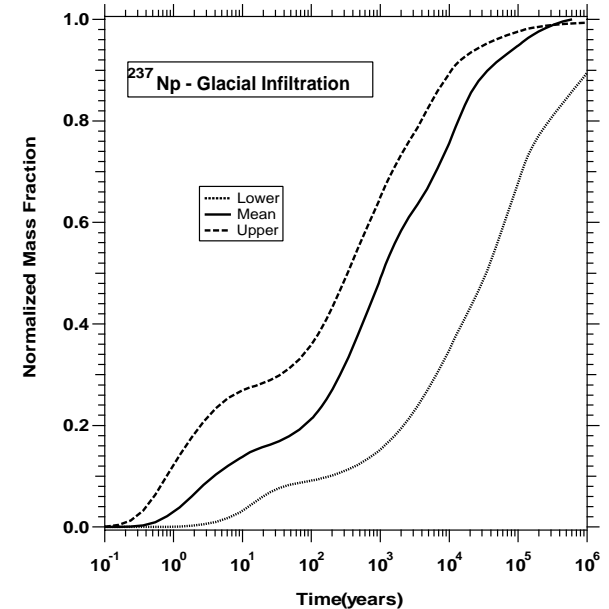
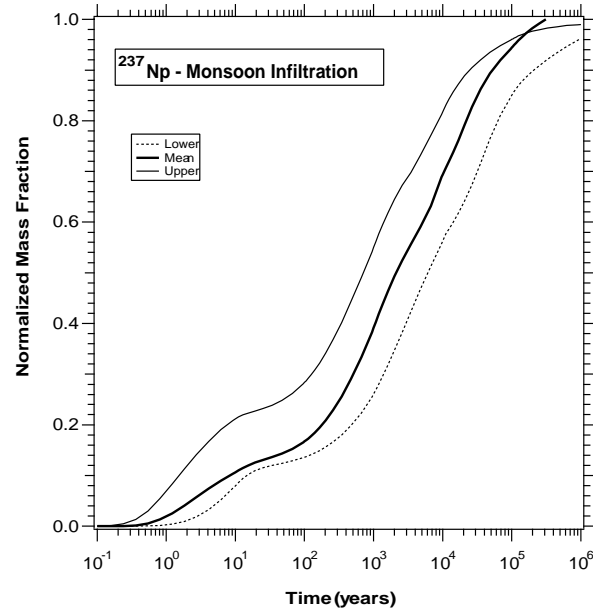
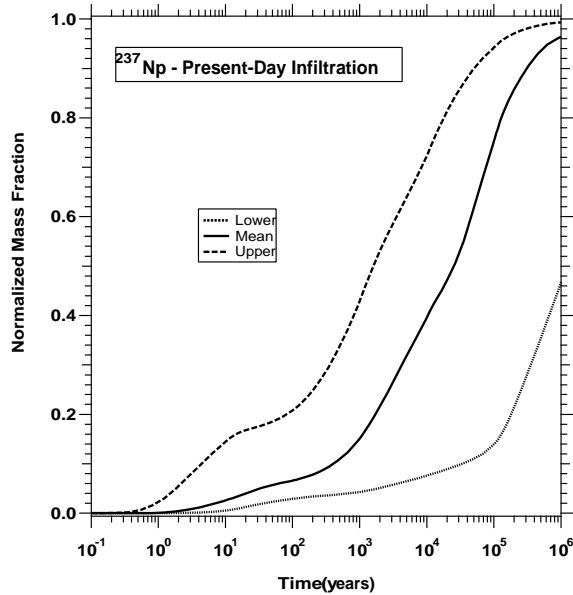


Percolation Fluxes at the Repository Level and at the Water Table Level

Direct Correlation of Water Flow and Transport Patterns



3-D Mountain Scale Transport Studies (Continued)



Transport of ²³⁷Np (mildly sorbing) Instantaneous Release, Various Climatic Regimes

The data shown in these figures 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.

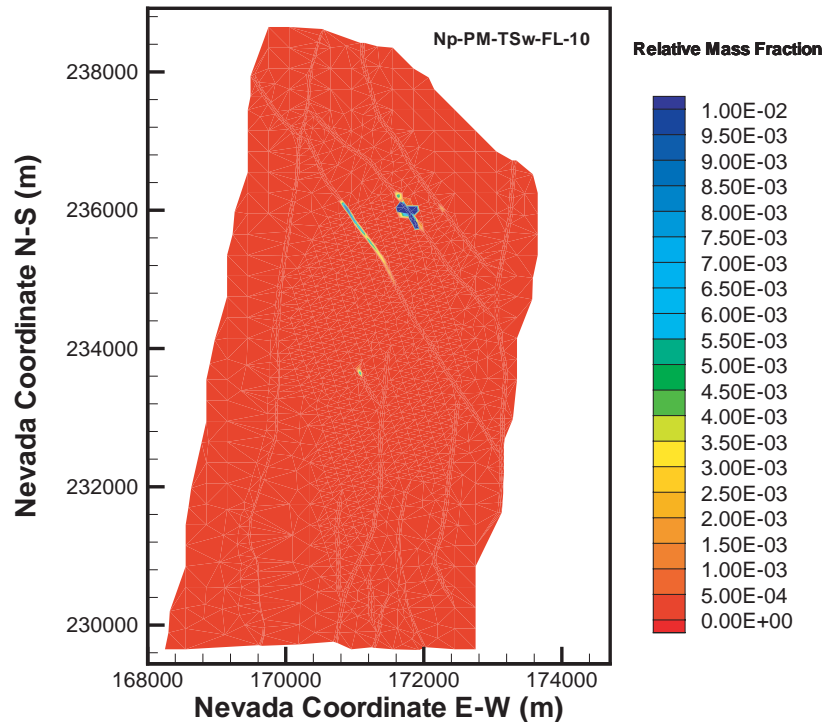


3-D Mountain Scale Transport Studies

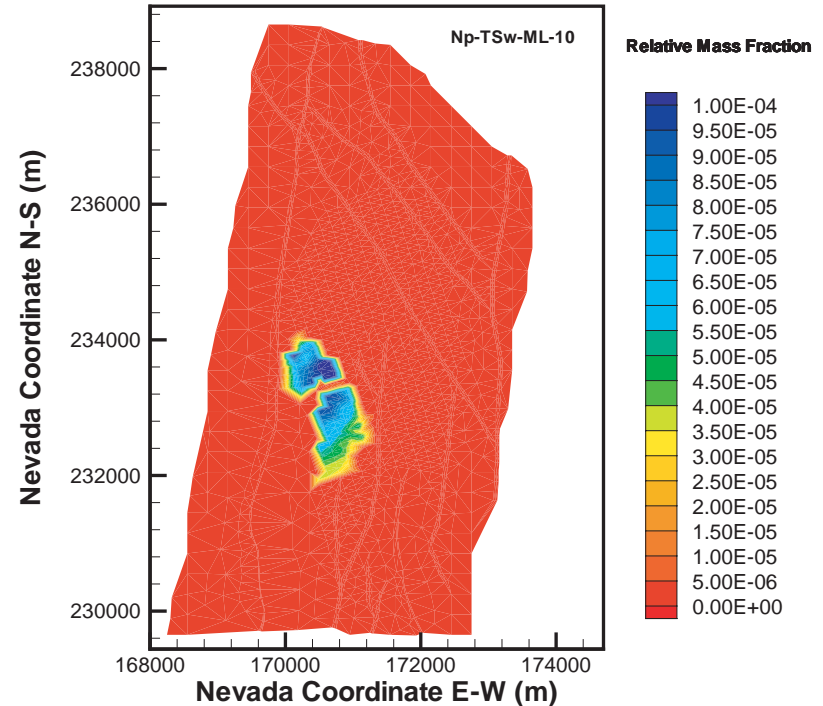
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Instantaneous Release

T = 10 yrs, Fracture Relative Concentration



T = 10 yrs, Matrix Relative Concentration



Transport Patterns of ^{237}Np (mildly sorbing)
Bottom of the TSw: Transport Similar to that of ^{99}Tc

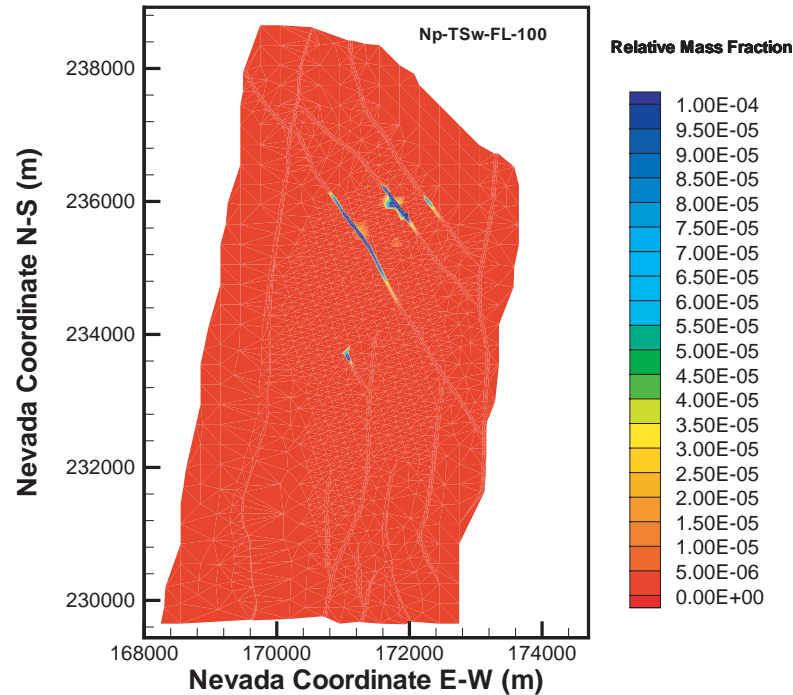


3-D Mountain Scale Transport Studies

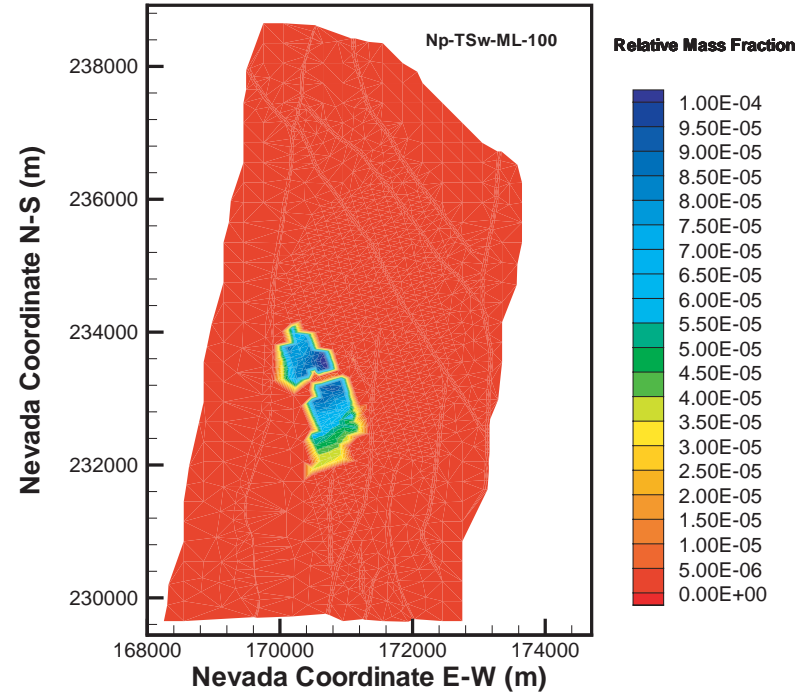
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Instantaneous Release

T = 100 yrs, Fracture Relative Concentration



T = 100 yrs, Matrix Relative Concentration



Transport Patterns of ^{237}Np (mildly sorbing)
Bottom of the TSw: Transport Pattern Similar to that of ^{99}Tc

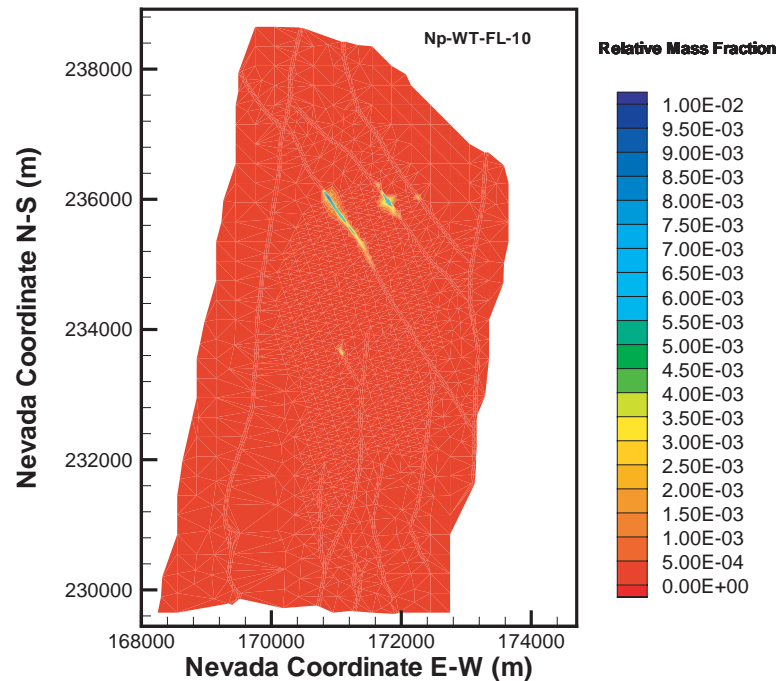


3-D Mountain Scale Transport Studies

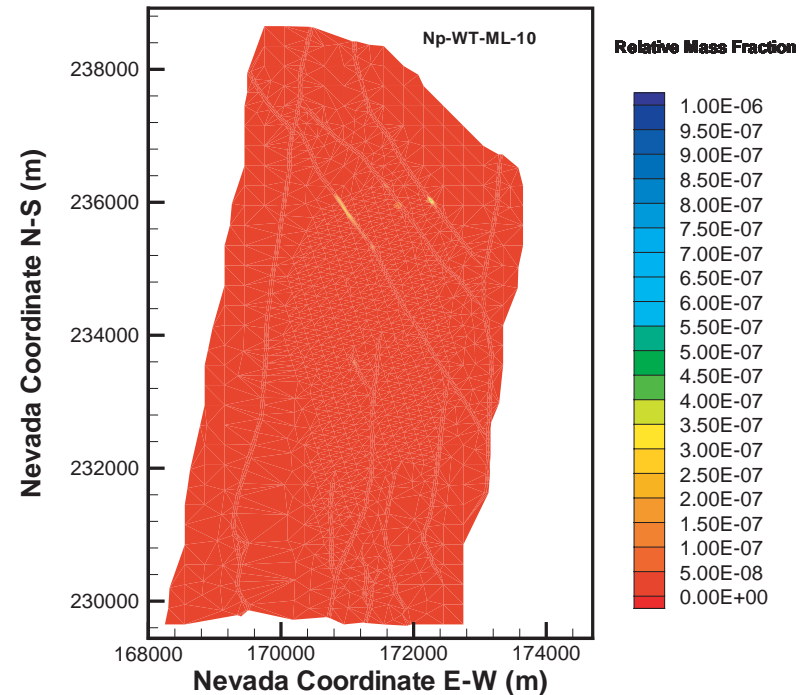
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Instantaneous Release

T = 10 yrs, Fracture Relative Concentration



T = 10 yrs, Matrix Relative Concentration



**^{237}Np at the Water Table: Dominance of Faults
Transport Pattern Similar to that of ^{99}Tc**

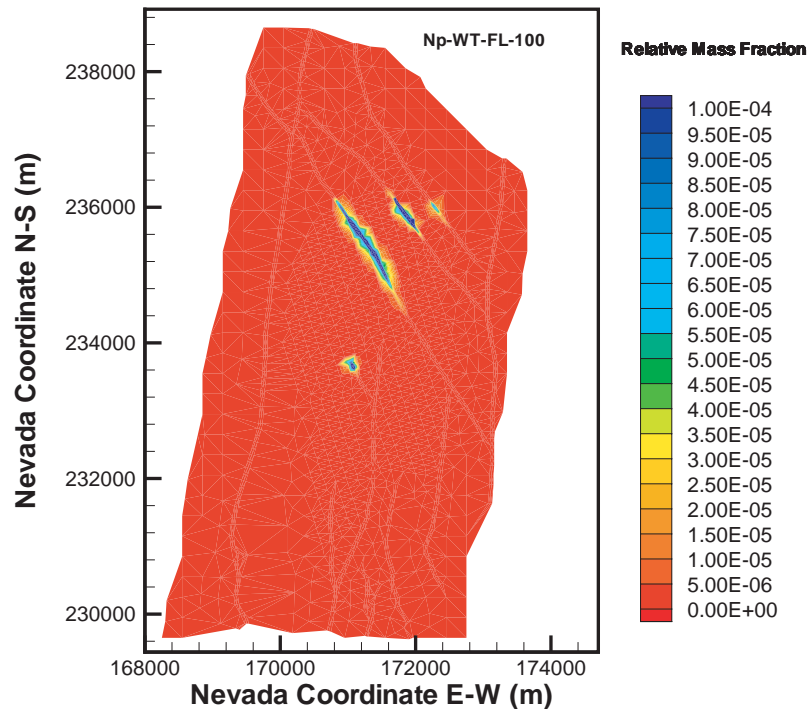


3-D Mountain Scale Transport Studies

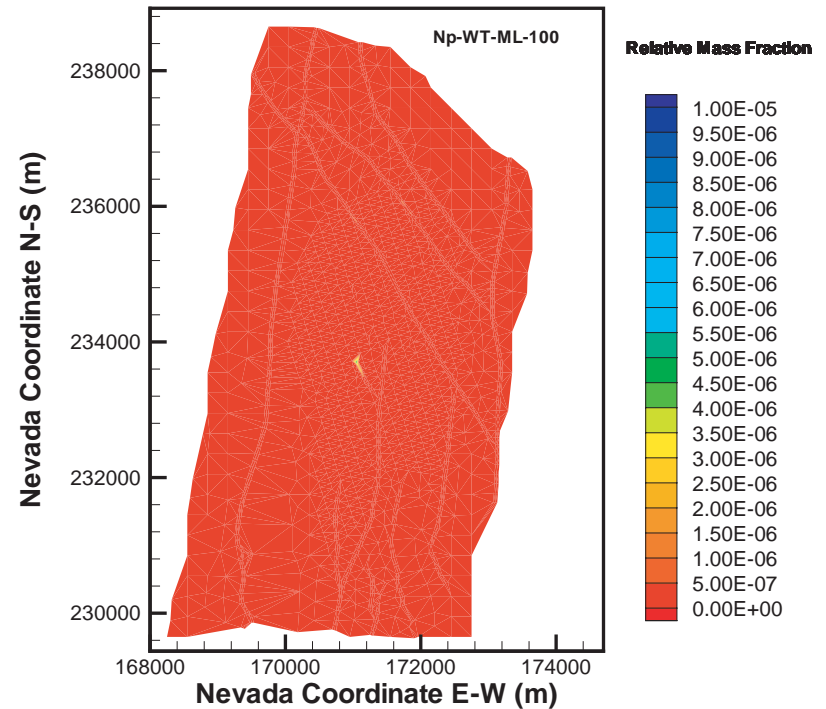
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Instantaneous Release

T = 100 yrs, Fracture Relative Concentration



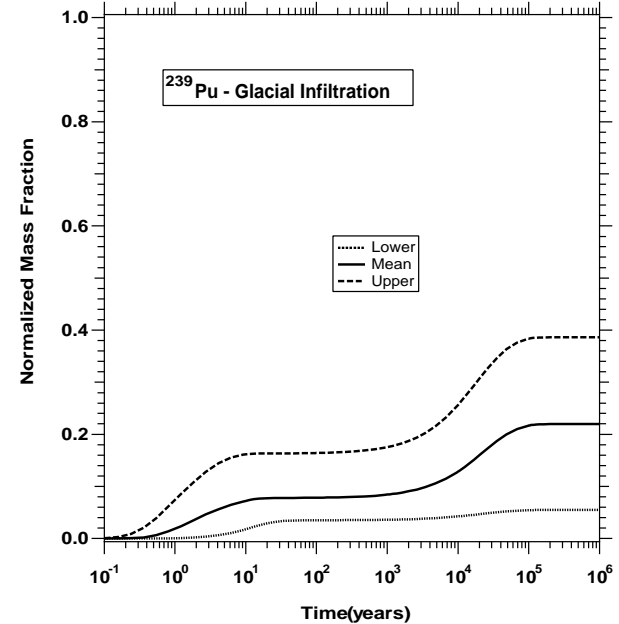
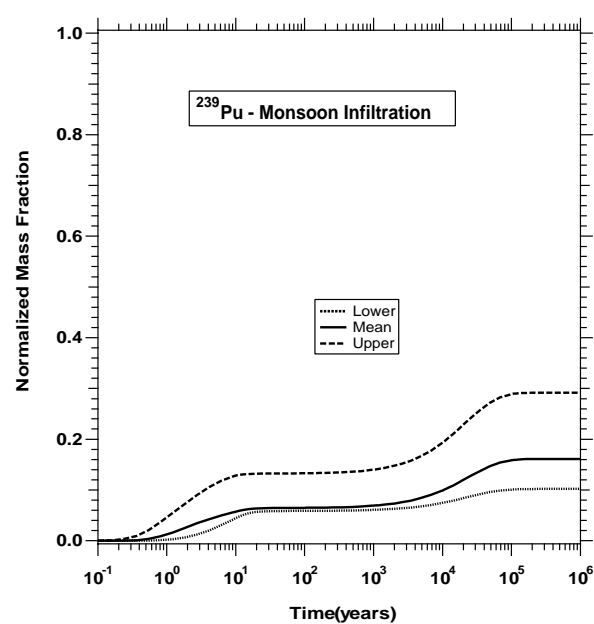
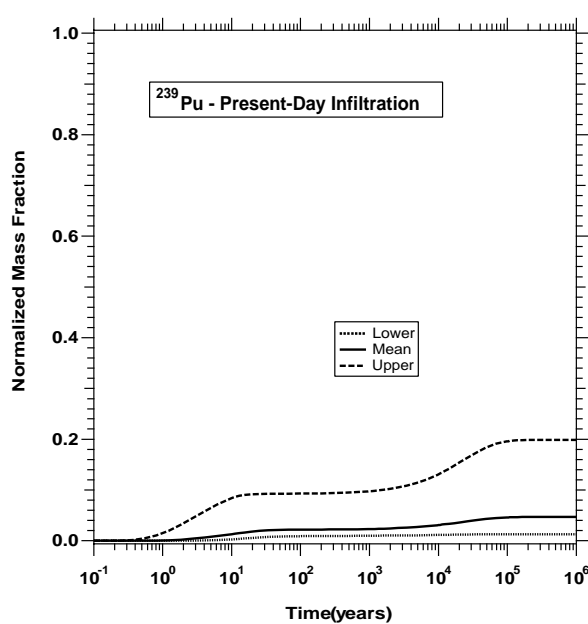
T = 100 yrs, Matrix Relative Concentration



**^{237}Np at the Water Table: Dominance of Faults
Transport Pattern Similar to that of ^{99}Tc**



3-D Mountain Scale Transport Studies (Continued)



Transport of ²³⁹Pu (strongly sorbing) Instantaneous Release, Various Climatic Regimes

The data shown in these figures 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.

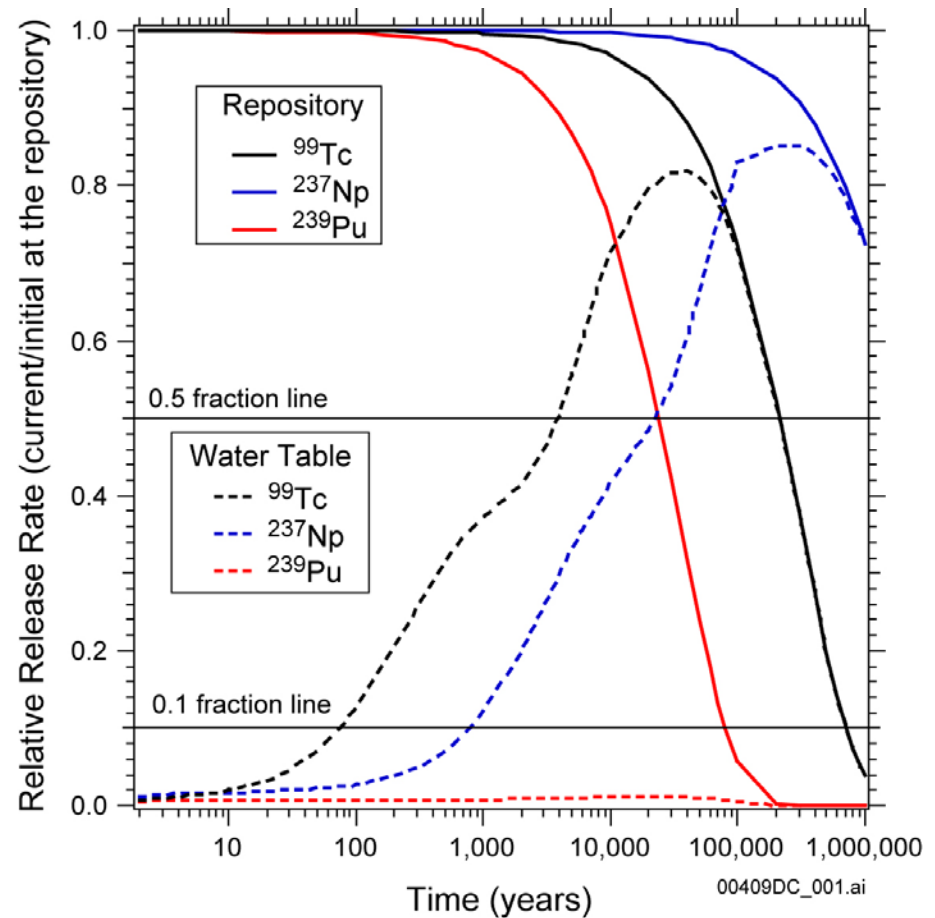


3-D Mountain Scale Transport Studies

(Continued)

Continuous Release

Normalized Relative Release R_F of ^{99}Tc , ^{237}Np , and ^{239}Pu at the Water Table Mean Present-Day Climate Scenarios



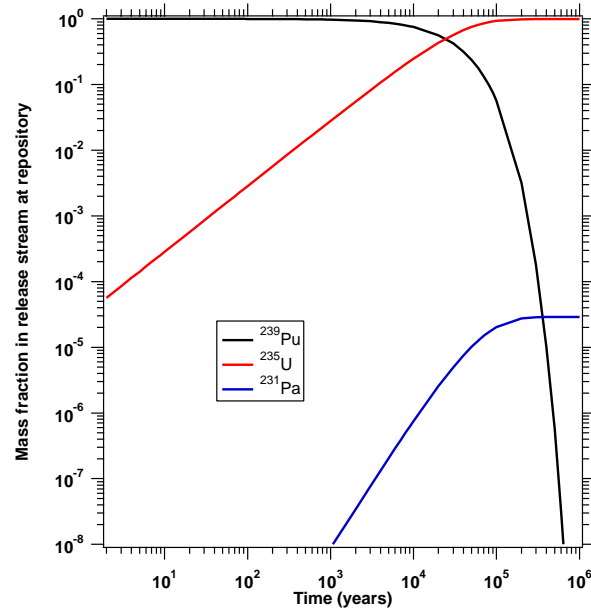
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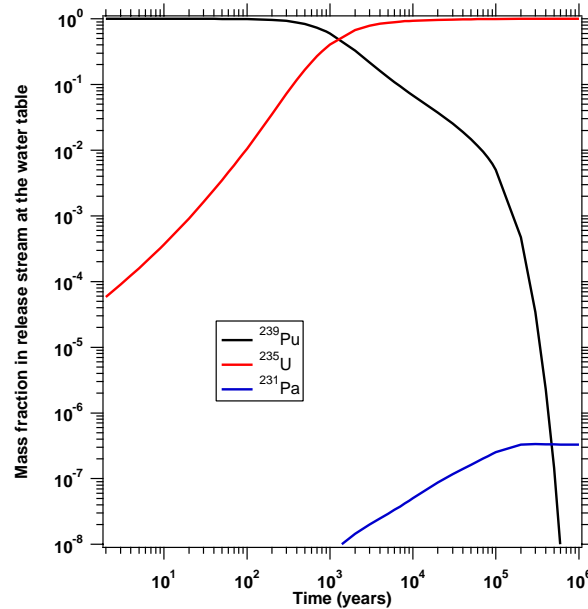
3-D Mountain Scale Transport Studies

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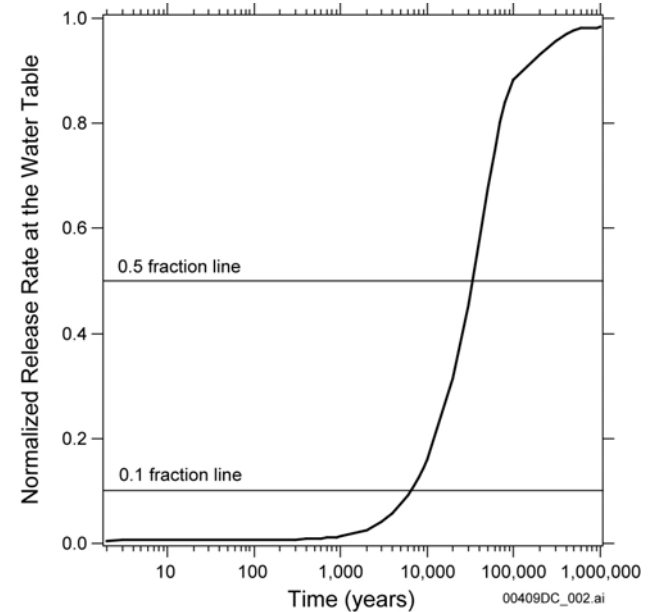
Continuous Release



Mass fractions in the repository release stream



Mass fractions in the water arriving at the water table



Normalized relative release R_F of the sum of all members of the ^{239}Pu chain

The Importance of Daughter Products

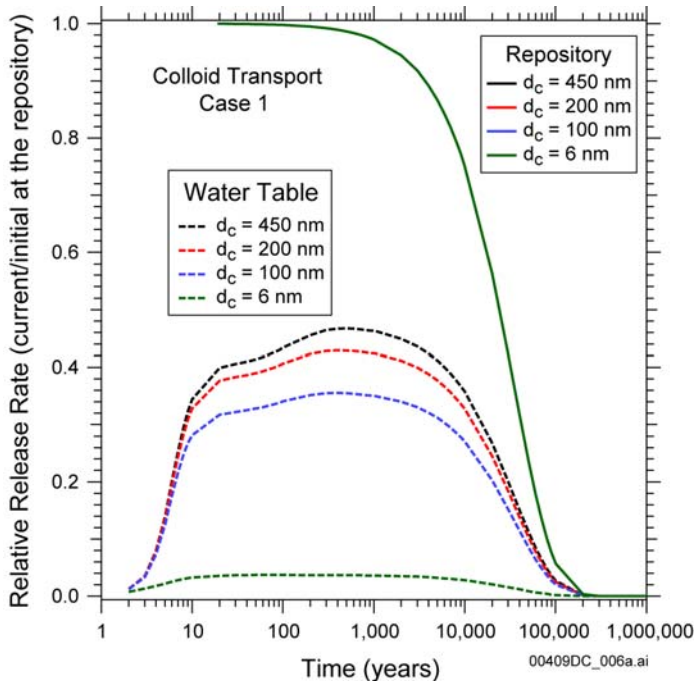
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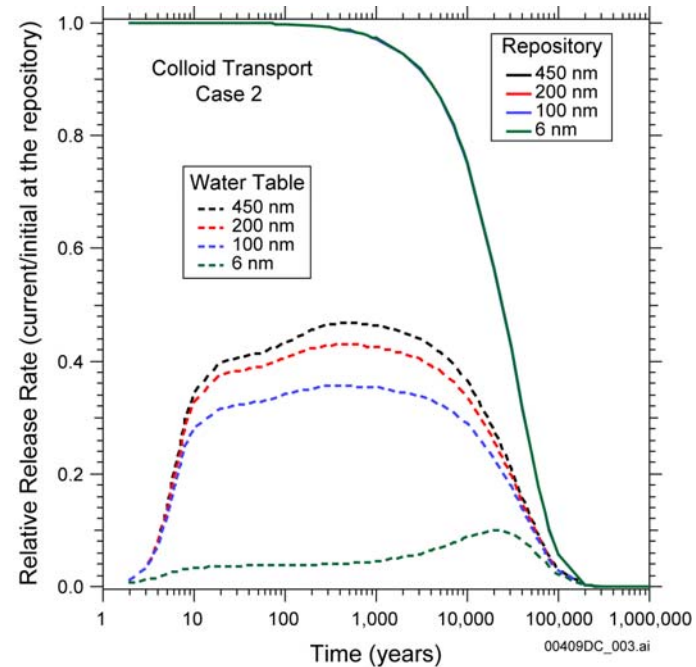
3-D Mountain Scale Studies of Colloid Transport

Continuous Release (PuO_2 Colloids)

Mean Present-Day Climate



Straining and slow declogging



Straining and fast declogging

Significant Effect of Colloid Size on Transport

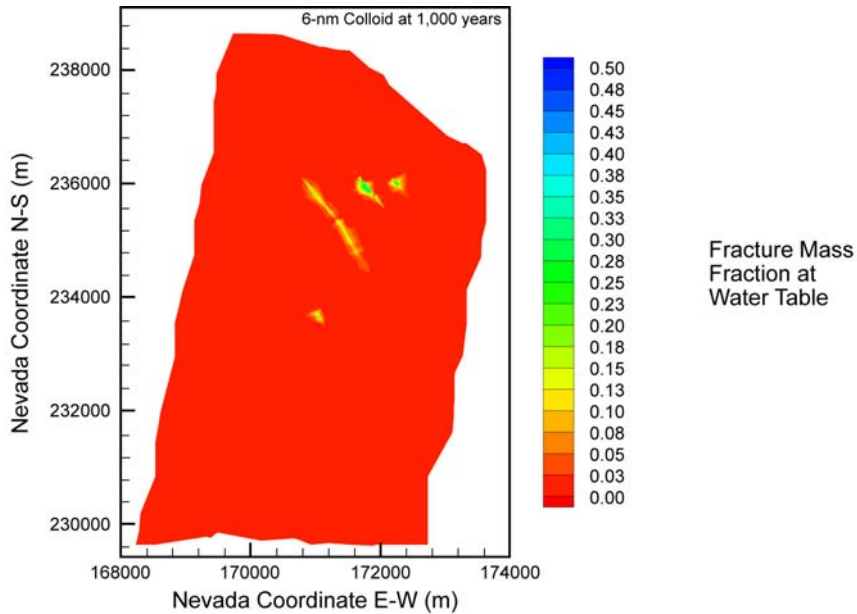
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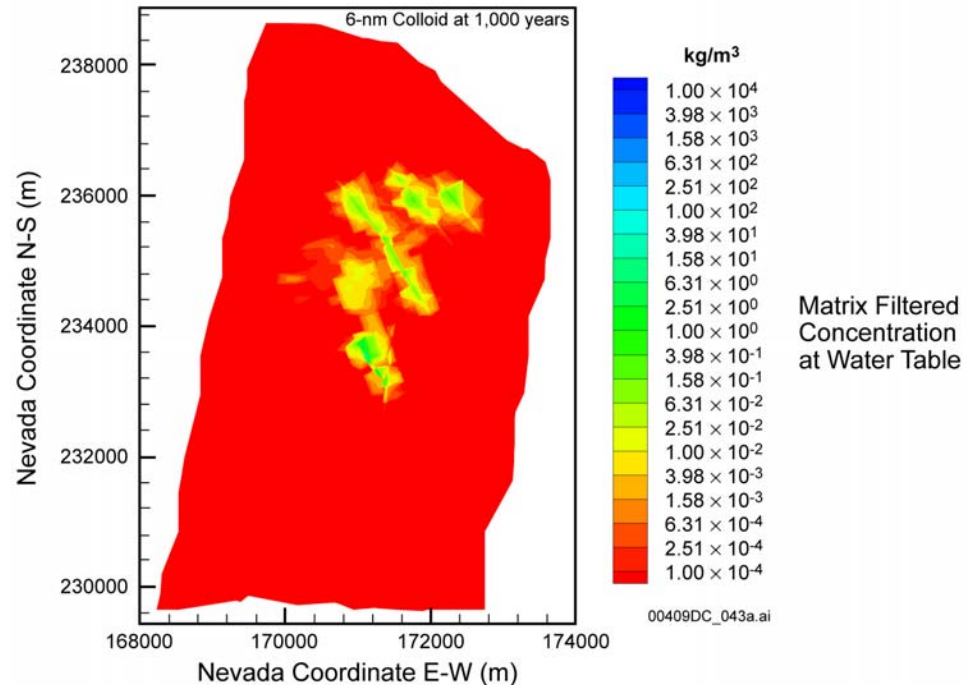
3-D Mountain Scale Transport Studies

Continuous Release, 6 nm Colloid

T = 1000 yrs, Fracture Relative Concentration



T = 1000 yrs, Matrix Filtered Relative Concentration



Dominance of Faults

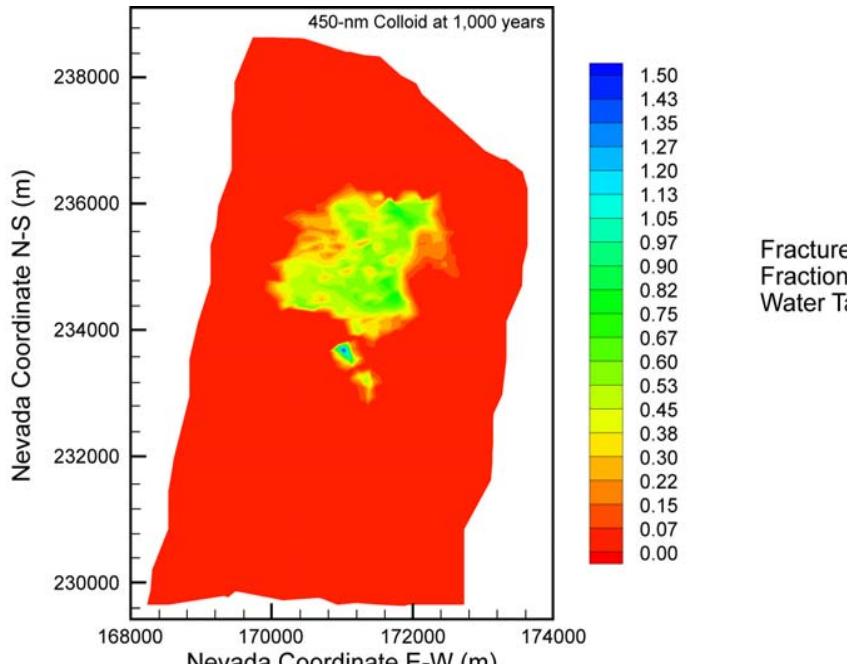


3-D Mountain Scale Transport Studies

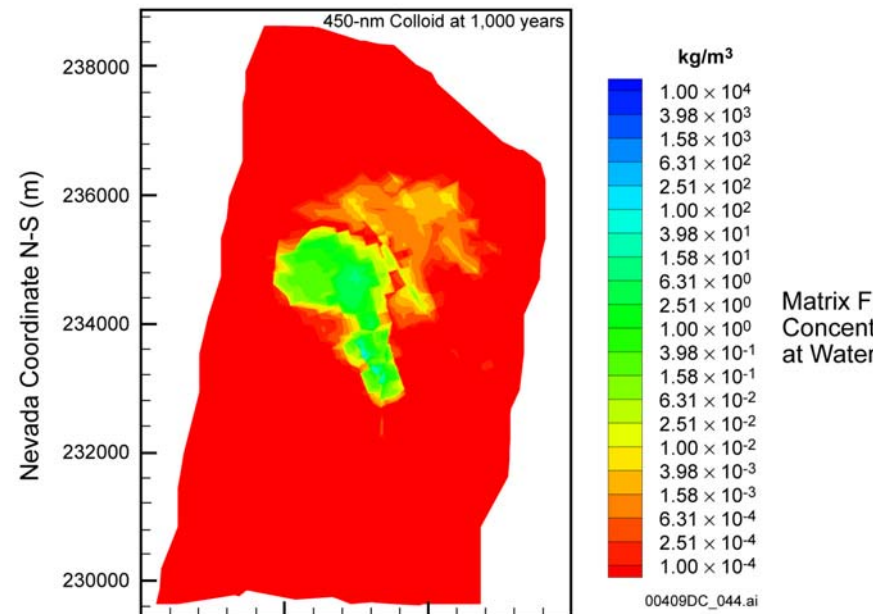
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Continuous Release, 450 nm Colloid

T = 1000 yrs, Fracture Relative Concentration



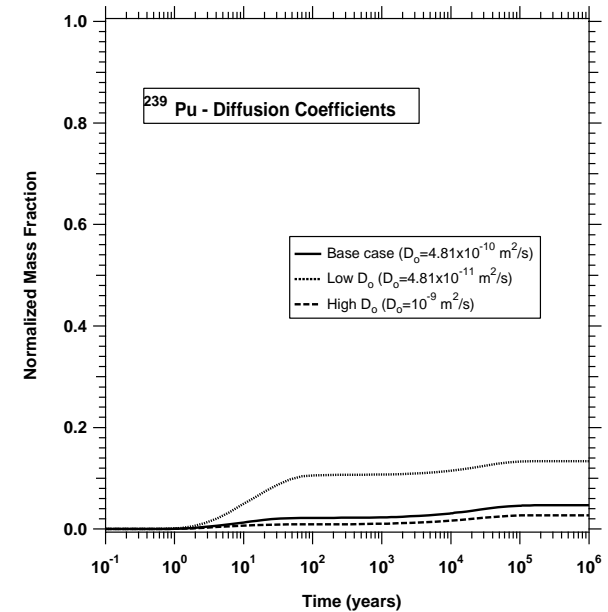
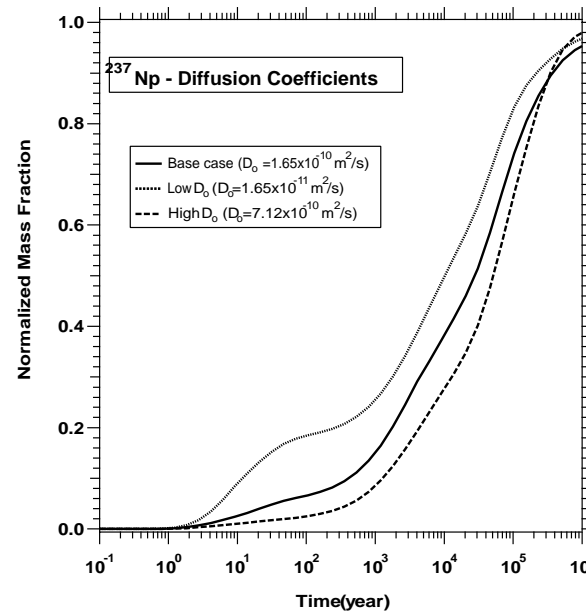
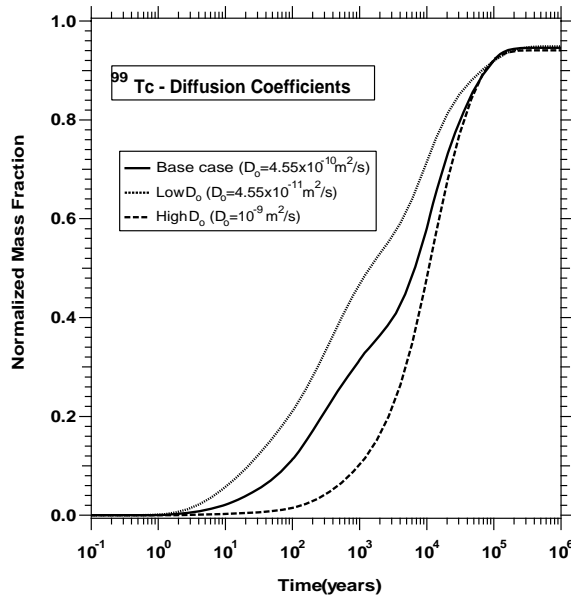
T = 1000 yrs, Matrix Filtered Relative Concentration



Colloid Size Leads to Differences in the Transport Pattern



3-D Mountain Scale Transport Studies (Continued)

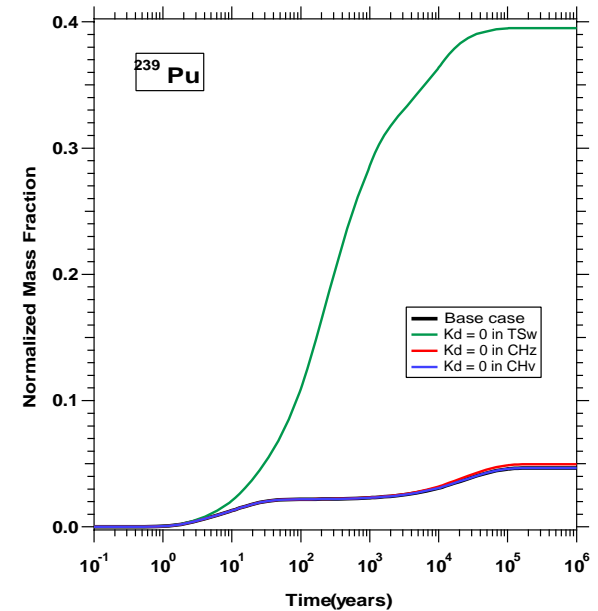
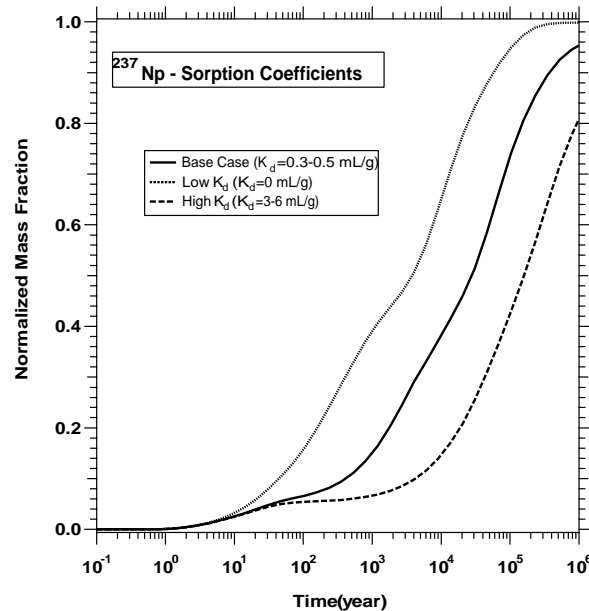
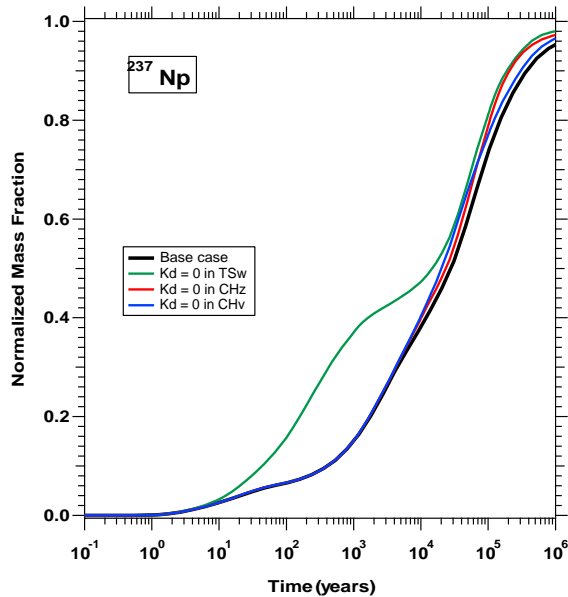


Impact of Uncertainties in the Value of the Diffusion Coefficients

The data shown in these figures 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.



3-D Mountain Scale Transport Studies (Continued)

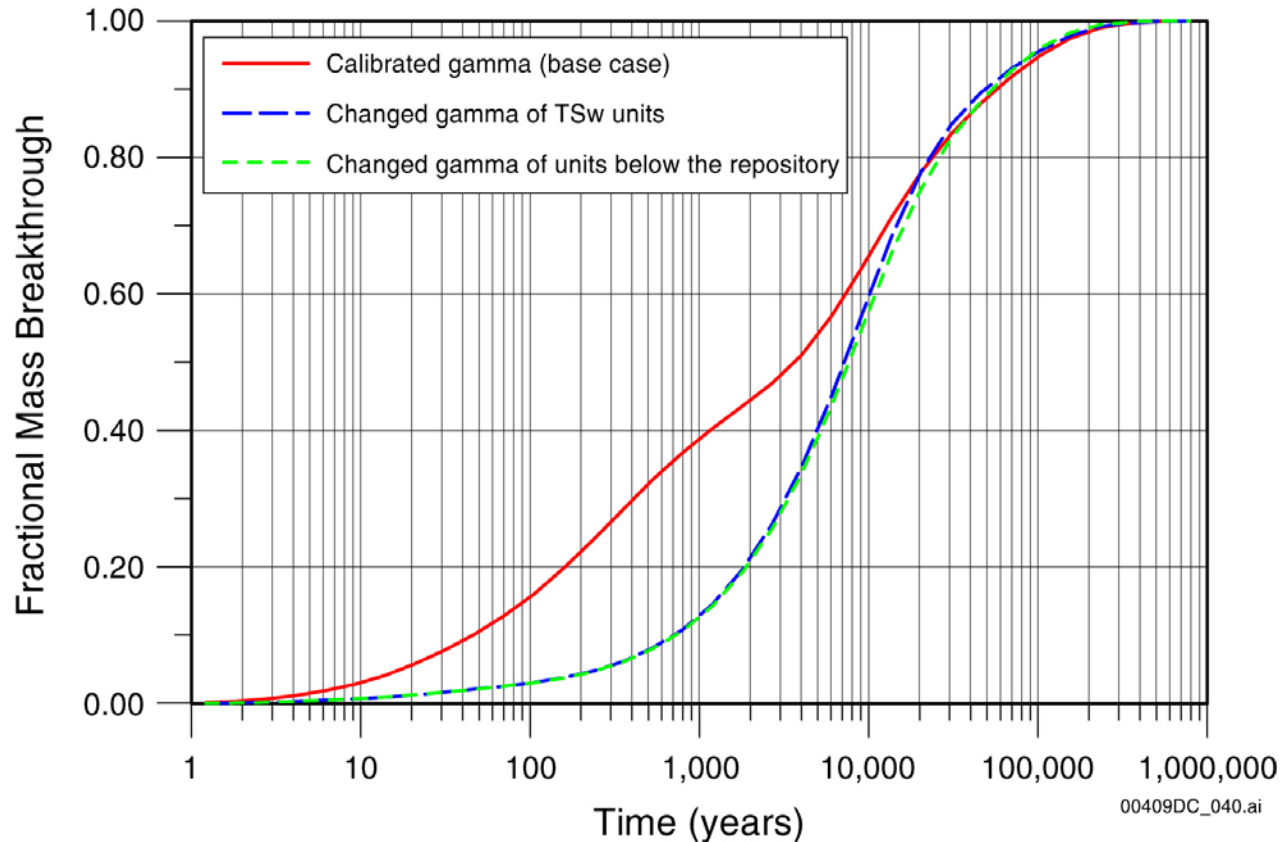


Impact of Uncertainties in the Value of the Sorption Coefficients Relative Importance of the Main Hydrogeologic Units

The data shown in these figures 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.



Impact of Uncertainties in the Value of the Parameter γ of the Active Fracture Matrix Model with Matrix Diffusion



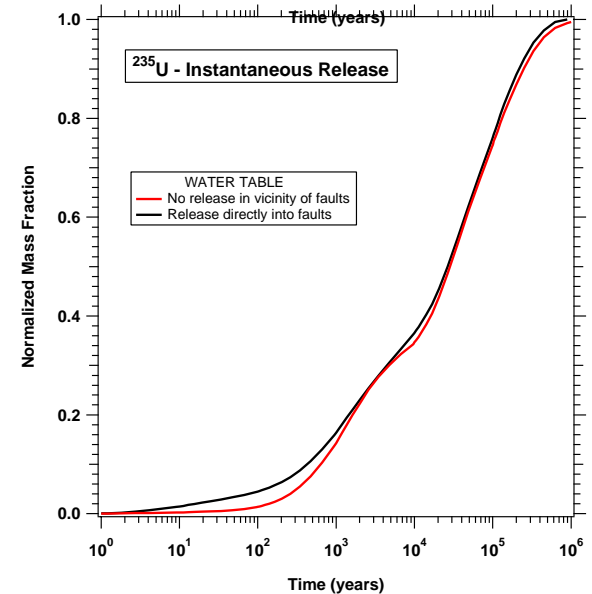
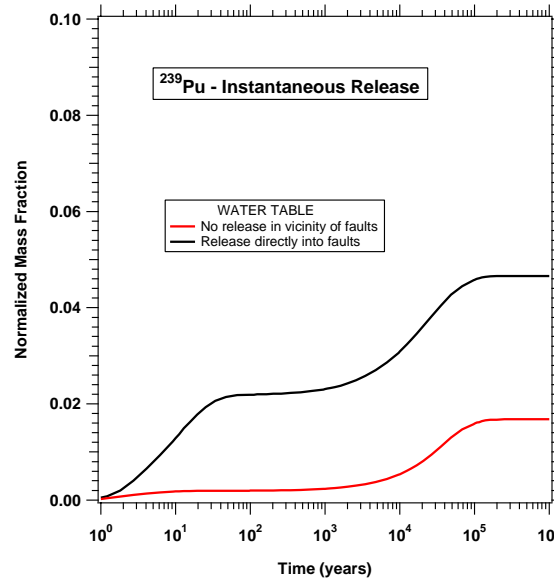
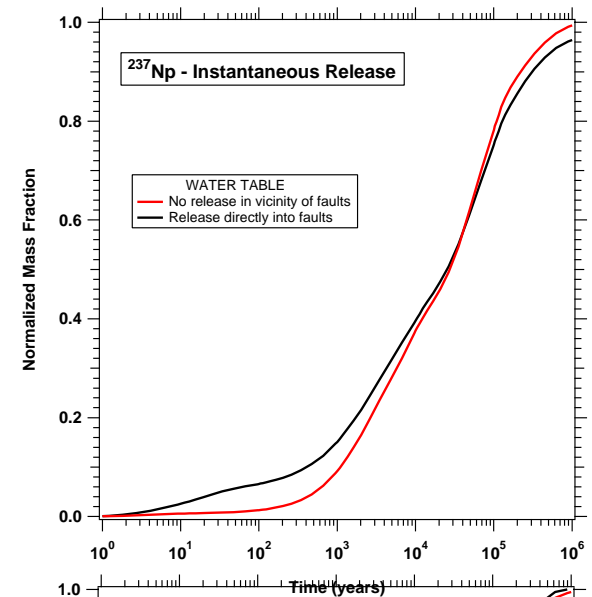
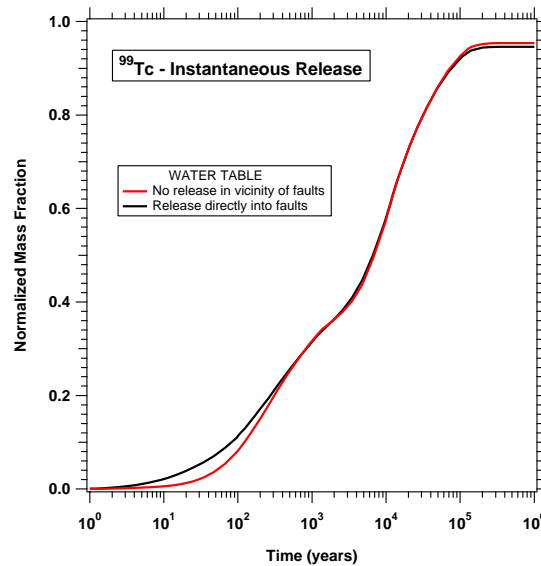
00409DC_040.ai

The data shown in these figures 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.



**No Direct
Releases into
the Faults:
NO EFFECT!**

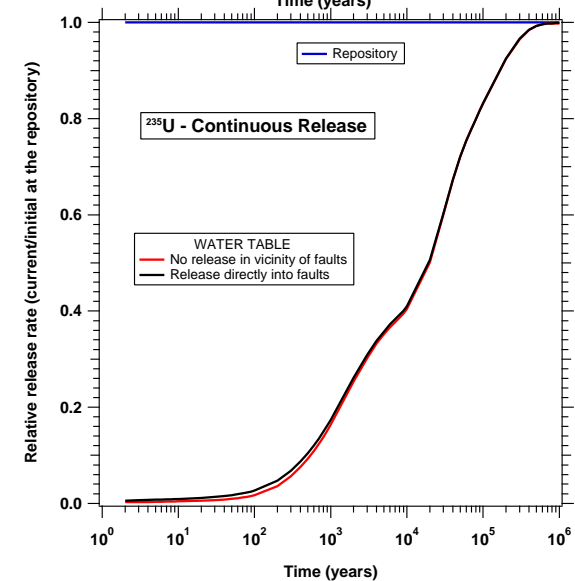
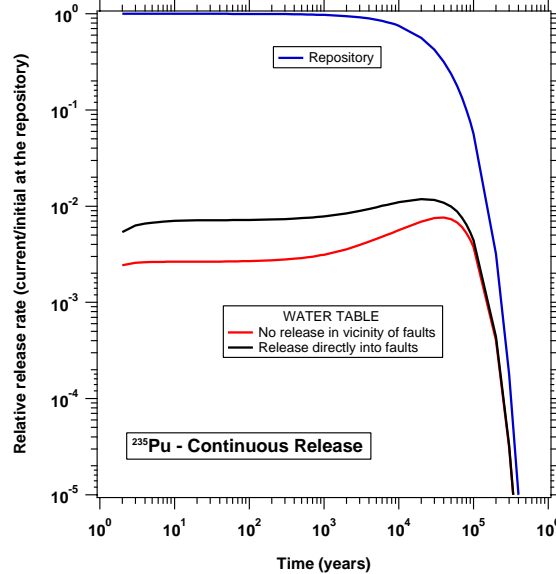
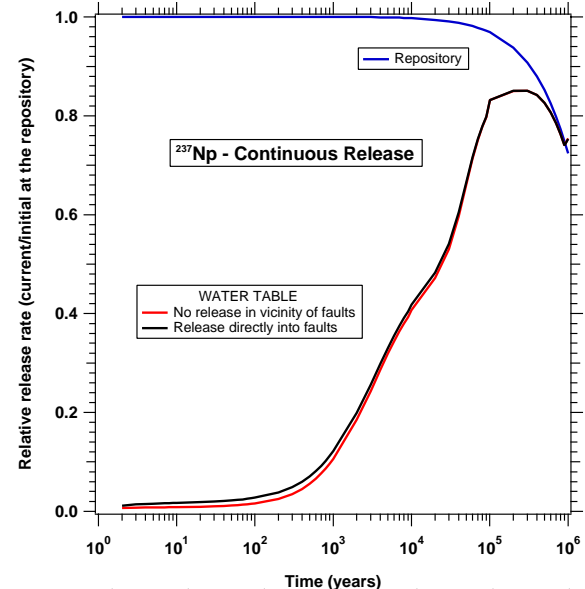
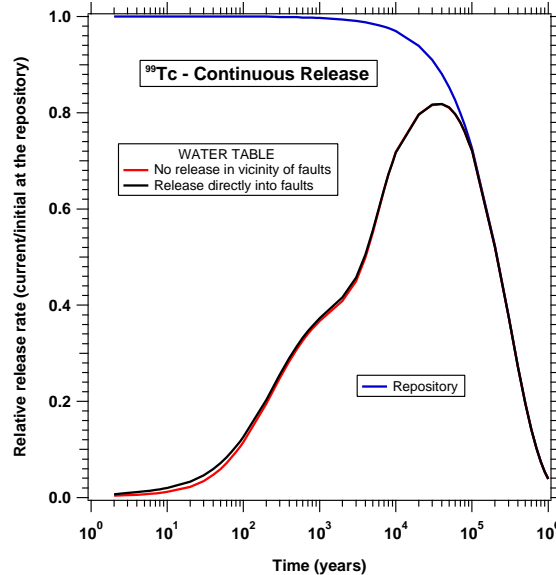
**Instantaneous
Releases**



The data shown in these figures 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.



**No Direct
Releases into
the Faults:
NO EFFECT!**



**Continuous
Releases**

The data shown in these figures 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.



In This Study: Conservative Approach

- **No drip shields are considered, and flow through the canisters is assumed**
- **All the radioactive packages in the entire repository rupture simultaneously**
- **The radionuclides are released directly into the fractures (no retardation effects of the invert with porous media properties)**
- **The effects of the shadow zone are ignored**
- **The vertical fractures are open and continuous throughout the UZ (no retardation through solute sorption and/or colloid attachment onto the fracture walls)**
- **The horizontal fractures are modeled as interconnected, and are also connected (directly or indirectly) to the vertical fractures**
- **The distribution coefficients were estimated over longer concentration intervals using an approach that results in milder slopes and lower K_d values**
- **Potential chemical stabilization (e.g., through precipitation) of solids is ignored**
- **Colloid stability is assumed**

NOTE: Significant Uncertainties in UZ hydrology.



Conclusions

- **Radionuclide transport is dominated and controlled by faults, which provide fast pathways for downward migration to the water table**
- **The transport patterns follow the infiltration and percolation distributions**
- **There is a direct relationship between increasing infiltration (wetter climatic regime) and shorter arrival times at the repository**
- **Radionuclides move faster and reach the water table earlier in the northern part of the repository, which is characterized by the presence of highly fractured zeolitic CHz layers**



Conclusions

(Continued)

- **The highly conductive Drill Hole Wash and Pagany Wash faults are the main pathways of transport in the northern part of the repository**
- **Diffusion into the rock matrix is the only mechanism for nonsorbing solutes. Mechanical dispersion is expected to be minimal**
- **Hydrology is the most important factor affecting transport**
- **Sorption and matrix diffusion are the main retardation processes in the transport of sorbing radionuclides**
- **The unsaturated zone of Yucca Mountain appears to be an effective barrier to the transport of strongly sorbing radionuclides (^{90}Sr , ^{226}Ra , ^{229}Th , ^{241}Am , ^{221}Pa , and ^{239}Pu)**



Conclusions

(Continued)

- **Under the conditions of this study, the effectiveness of the unsaturated zone of Yucca Mountain as a natural barrier decreases with (a) a lower sorption affinity of the radioactive solutes and (b) longer half lives. In evaluating the barrier efficiency, the entire radioactive chain must be considered**
- **Under the conditions of this study, the unsaturated zone of Yucca Mountain appears to be an effective barrier to the transport of small colloids. The barrier effectiveness decreases very rapidly with an increasing colloid size**

