

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



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Outline

- Yucca Mountain geology
- Processes for flow
- **Processes for transport**
- Lessons Learned from site characterization
- **Testing update**
- UZ Flow: data feeding models, results, validation
- Tests specific to UZ transport, test predictions for confidence building
- Transport model development: source term, processes and geologic features, modeling tool
- **Transport model results**
- Summary

Yucca Mountain Unsaturated Zone Cross Section and Repository Layout



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YUCCA MOUNTAIN PROJECT

Mountain Scale Flow Patterns



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Processes for UZ Flow

- Present and future climate
- Ambient Infiltration and percolation
- Lateral flow diversion
- Fracture/matrix interactions
 - van Genuchten model
 - Active fracture model
- **Fault Flow**
- Perched water
- **Coupled processes** (TH, THC, THM)





Process for UZ Transport

- All processes pertaining to flow are important to transport
- Drift shadow effect
- Sorption
- Matrix diffusion
 - Active fracture model
- Daughter products of radioactive decay
- Colloidal transport





Site Evaluation and Scientific Investigations

- What has been done?
 - Surface-based Testing and Investigations
 - Underground Testing
 - Laboratory Studies
 - Modeling Activities for Evaluating Repository Performance
- What lessons have we Learned?



Geological Studies

- Extensive surface mapping and trench studies
- Stratigraphy of tuff layers by over 60 deep boreholes
- Detailed line and full periphery maps of fractures on drift walls
- **Lessons Learned:**
- Water flow is associated with faults and a small fraction of fractures
- Detailed fracture mapping is useful mainly for fracture-matrix interaction evaluation





Geophysics Studies

- Electromagnetic (EM) imaging
- Seismic imaging (large scale)
- Radar tomography (ten-meter scale) in ESF and Busted Butte
- **Lessons Learned:**
- EM of limited use due to difficulty to inject current into ground
- Radar tomography successful in detecting saturation changes
- Surface to underground seismic imaging identified intensively fracture zones
- Improvement in geophysical tools needed to detect large hydrological features: perched water bodies, hidden faults





Water Flow Evaluation – Infiltration

- Meteorological stations to measure precipitations and evaporationtranspiration potentials
- Neutron logging of hundreds of shallow boreholes
- Stream gauges to monitor channel runoff
- Water bucket models for wetting front migration
- **Lessons Learned:**
- Difficult to estimate infiltration with conventional approach (above)
- Essential to use geochemical and thermal data to support and constraint the model









Water Flow Evaluation – Matrix Properties

- Saturation and water potential measurements on cores and in boreholes
- Upscaling achieved by inverse modeling
- **Lessons Learned:**
- Water potential is extremely difficult to measure in the range of 0 to –5 bar (may not be important)
- Practically impossible to separate effects of fractures in borehole measurements
- Core drying affects saturation data



Water Flow Evaluation – *Fracture Properties*

Studies:

- Air permeability (K) measured by packer tests (0.3 to 10 m)
- 100 m scale air-K inferred from pneumatic data (damping of atmospheric pressure signals)
- Fracture porosity determined by gas tracer tests and inferred from inverse modeling of seepage and thermal test data

Lessons Learned:

- Pneumatic data extremely useful confirming theoretical upscaling power law (and no air-K upscaling is needed in YM evaluation)
- Fracture porosity is on the order of 0.5% - similar to other rocks





Water Flow Evaluation – Percolation

Studies:

- Site-Scale Model, matched with all available data, is used to determine percolation from redistribution of infiltration
- In addition to hydrological and pneumatic data, temperature and geochemical data (especially total chloride) are used to constraint both flux magnitude and spatial distribution
- **Lessons Learned:**
- Total chloride and temperature data provide most useful constraints for both magnitude and distribution



3-D Calibration Grid; Modified Percolation Flux Map



UZPMR3.8-4REV00



Water Flow Evaluation – Geochemistry

Studies:

- Porewater samples are collected from squeeze and ultracentrifuge
- Gas and perched water samples are collected from pumping
- Systematic and feature-based samples are collected for bomb pulse analyses
- **Lessons Learned:**
- Total chloride, calcite, Sr, Cl³⁶ are very useful to elucidate different flow phenomena
- **Controversy persists on bomb pulse** finding (may not be important)



10-15)

Ratio (x

36CI/CI

sured

Water Flow Evaluation – Perched Water

- Pump testing to determine the spatial extent
- Water sampling to determine ages and chemical mixing
- Lessons Learned:
- **Existence of perched water** bodies infers that fracture permeability below perched water is low
- Partial diversion minimizes contact with zeolitic tuff with strong sorbing capacities
- Model results suggest flow focusing and channeling to faults





Flow Pattern Below Repository

Studies:

- Use information from limited number of deep boreholes
- Site-scale flow model is used to evaluate flow pattern
- **Lessons Learned:**
- Lack of data makes the largescale geological layer structure and features very important
- Modeling results suggest significant diversion to the faults for percolation and radionuclide transport

vertical flux for preq_mA at bottom boundary





Fracture-Matrix Interaction – Conceptual Model

Studies:

• Use double-porosity, dualpermeability, multipleinteracting continuum, and discrete fracture models to evaluate the fracture-matrix interaction Ambient Zone



- Formulate the active fracture model to represent the transition from weak interaction at low fracture saturation (ambient condition) to high saturation (in the condensation zone)
- **Lessons Learned:**
- Transport is more sensitive than flow to the F/M and active fracture representation
- Condensate imbibition into matrix block is better understood than drainage





UZ Testing Update

- Exploratory Studies Facility (ESF) studies
 - Drift Scale Test in the ESF coupled processes
 - Secondary fracture minerals/fluid inclusions/hydrochemistry
- Cross Drift Studies
 - Alcove 8 Niche 3
 - ECRB Moisture monitoring



Drift Scale Test Update (preliminary)

- Cooling continues (since termination of heating in January 2002)
- Air temperature in the Heated Drift is ~ 84°C at end of August 2003
- Highest temperature within rock formation is ~ 95°C





Drift Scale Test Update (2) (preliminary)

- Rewetting of dryout zone is slow and is most prominent in regions where the moisture gradient is largest (at the outer boundary of the dryout zone), as predicted by modeling
- No water has been collected in quarterly sampling trips since August 2002, consistent with modeled results



Reference GPR tomogram of radar velocity at end of heating phase



-0.03 -0.02 -0.01 0.00 0.01 CHANGE IN WATER CONTENT



Testing Update: U-Series Isotope Studies (USGS)

(preliminary)

- **Objective is to determine zones of greater and lesser flow** (water-rock interaction)
- Establishing vertical profile of U-series variations in core from USW SD#9
 - Observing disequilibrium at bulk rock scale in ²³⁴U/²³⁸U and ²³⁰Th/²³⁸U ratios
 - Disequilibrium reflects water-rock interaction on 10³ to 10⁵ year scale
- Lateral variability in U-disequilibria being evaluated in samples from the ESF
- U-series ages range from 3,000 to 140,000 years in recently analyzed sample



Testing Update: Chemical/Isotopic Analyses of Pore Water (USGS)

(preliminary) Vertical variability of dissolved anions and cations in SD-9 pore water probably reflects: evaporation in the PTn, water-rock interactions, and probable microbial activity





Alcove 8-Niche 3 Updates Large Plot Liquid Release











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Seepage rates in Niche 3 from ponded liquid release in Alcove 8 on 8/20/02 (preliminary)





UZ Testing Update: Moisture Monitoring behind Bulkhead (preliminary)

- Terminal section of ECRB from station 22+00 onwards maintained under nonventilated conditions from 11/15/01-2/3/03 and then from 2/5/03-7/7/03
- Observations made on 2/3/03 and 7/7/03 (under nonventilated conditions) show:
 - Water droplets along ventilation tube and cables at various locations.
 - Mold along railway ties and walkway in some locations
 - Wettest area between Stations 25+02 and 25+40







UZ Analysis and Model Reports Relevant for Flow and Transport







Unsaturated Zone Flow

- Present and future climate
- Ambient Infiltration and percolation
- Lateral flow diversion
- Fracture/matrix interactions
 - van Genuchten model
 - Active fracture model
- Fault Flow
- Perched water
- Coupled processes (TH, THC, THM)





Data That Feed Unsaturated Zone Flow Model(s)

- Geological layering
- Surface infiltration
- Water saturation and water potential on cores and in boreholes
- Pneumatic data
- **Temperature profiles from boreholes**
- Geochemical data: total chloride, calcite, strontium, Cl₃₆



UZ Flow Model: Plan View of 3D Numerical Grid and Infiltration Map



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Numerical Tools for Flow Predictions: TOUGH2 Family of Simulators

TOUGH: Transport Of Unsaturated Groundwater and Heat

- multidimensional
- multiphase
- multicomponent
- nonisothermal
- flow and transport
- fractured-porous media

- 1D, 2D, 3D
- liquid, gas, NAPL
- water, air, VOC, radionuclides
- heat
- multiphase Darcy law
- dual-f, dual-k, MINC, ECM

EOS: Accurate description of thermophysical properties



Numerical Tools for Geochemical Transport Predictions: *TOUGH/REACT*

- Multiphase fluid flow:
 - TOUGH2
- Transport of aqueous and gaseous species:
 - Advection
 - Diffusion
- Reactions:
 - Any number of chemical species present in liquid, gas and solid phases
 - Chemical equilibrium and kinetics
 - Aqueous complexation
 - Mineral dissolution/precipitation
 - Gas dissolution/exsolution
 - Cation exchange
 - Surface complexation
 - Chemical heterogeneity





Selected Calibration Examples

- Pneumatic Pressure
- Liquid Saturation and Water Potential
- Temperature
- Chloride along ESF
- Calcite in WT-24



Calibration to Pneumatic Data in Borehole SD-7 and SD-12 (3D Numerical Simulation)





Calibration to Liquid Saturation and Water Potential (3D Model)





Calibration to Temperature Data in Boreholes (3D Numerical Simulation)





Use of Chloride Profile along ESF to Calibrate Percolation

Observation

ESF

 Pore water chloride from samples along ESF

Modeling

- 3D UZ flow fields
- Present day and glacial transition infiltration scenarios



Distance from the North Portal Entrance (m)


Use of Calcite Data to Constrain Percolation

- Observation
 - Total calcite abundance (ppmV or 10-6 volume fraction in deep boreholes WT-24
- Modeling Approach
 - 1D geochemical transport simulation under different infiltration rates
 - Compare simulated total calcite abundance (matrix plus fracture) with data
- Results
 - Over a range of 2–20 mm/yr infiltration rates, the simulated abundances generally fall within the range of calcite observed





Elevation (m)

Model Results: Percolation Fluxes at the Repository Horizon and Water Table

vertical flux for preq_mA at repository layer

vertical flux for preq_mA at bottom boundary





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Validation of UZ Flow Models

- Observed ECRB geology consistent with predictions
- Construction water migration
- Predictions of Chloride concentration in ECRB
- Carbon 14 on pore water age



Observed ECRB Geology Well Represented by Predictive Report

- Faults encountered were of the type, size, and offset anticipated by the Predictive Report.
 - A small number of minor faults were encountered (as expected)
- **Characteristics of predicted faults were nearly** identical to what was presented in the Predictive Report
 - The Solitario Canyon Fault (SCF) was encountered within a few meters of the predicted location. Orientation of the structure and offset along the fault were essentially identical to predictions



Use of Measured Chloride Concentration along ECRB to Validate 3D Geochemical Model

ECRB



Distance from the ECRB Entrance (m)



Adapted from J. Contaminant Hydrology 38 (1999) 107-156



UZ Transport

- All process pertaining to flow are important to transport
- Drift shadow effect
- Suite of radionuclides
 - Sorbing and non-sorbing, different k_d's
- Sorption
 - Vitric and zeolitic
- Matrix diffusion
 - Active fracture model
- Daughter products of radioactive decay
- Colloidal transport



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Testing Specific to UZ Transport Model Predictions Provide Confidence for Validity of UZ Transport Model

- Alcove 1 in ESF
 - From surface through fractured Tiva Canyon welded tuff
- Alcove 8 ECRB-Niche 3 ESF
 - Crossing Topopah Spring welded upper lithophysal and middle nonlithophysal unit interface
- Busted Butte
 - Calico Hill outcrop



Solute Transport – **Alcove 1 Infiltration Study on the Bedrock**

Test Studies:

- Apply infiltration rates below run-off threshold on the ground surface
- **Collect seepage at** Alcove 1, 30m below, for water and tracer collection

Modeling:

- Predict seepage
- Predict tracer breakthrough
- **Results:**
- Matrix diffusion is important in order to interpret delay in tracer breakthrough





Alcove 1 Test Predictions (preliminary)

Phase 1 calibration, phase 2 predictions

Tracer breakthrough Seepage 800 600 applied tracer concentration observed seepage tracer concentration 700 dispersivity=0.0, tortuosity = 0.75 Data 500 dispersivity=30.0, tortuosity = 0.75 Simulation dispersivity=0.0, tortuosity = 0.5 Seepage rate [L/day] 400 300 200 200 100 100 0 0 800 0 200 400 600 200 30 Time (days) 100 300 Time [day]



400

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500

Alcove 8/Niche 3 Fault Test







THE TESTBED

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Alcove 8-Niche 3 First Arrival along Fault and Evidence of Matrix Diffusion

Studies:

(preliminary)

- Infiltrate water along a fault at Alcove 8 in the ECRB Cross Drift, and collect seepage in Niche 3 in the ESF Main Drift, ~20 m below
- Inject two tracers with different sizes to evaluate matrix diffusion effects
- **Observations:**
- First arrival was along the fault, with subsequent seepage also through fracture network
- **Clear observation of matrix** diffusion dependence on tracer size, with large molecules staying more in the fractures







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Busted Butte Transport Test

Studies:

- Inject multi-tracer solutions into borehole arrays in and above Calico Hills vitric tuff
- Track plume migrations with periodic Ground Penetrating Radar imaging between borehole pairs





Solute Transport – Busted Butte Transport Test



Tracers:

Lithium Bromide Sodium Fluorecein Microspheres etc.



Observation:

Layout of Boreholes in the Busted Butte Test Area

Earth Sciences Division

- Calico Hills vitric tuff has simple porous medium characteristics with well-defined plume pattern
- Different tomographic techniques are useful to monitor plume migration





1.4

Unsaturated Zone Transport Model Development

- Radionuclide source term: drift shadow concept
- Geological attributes that are key to transport
- Numerical tools
- Selective UZ transport model results



Radionuclide Source Term: Drift Shadow Concept

- Drift Shadow (zone of lower water saturation and flux) from seepage diversion is expected to exist in 50 to 90% of drifts
- Radionuclides primarily enter the rock matrix by diffusion



Drift Shadow: Impact on Radionuclide Transport – (preliminary)





Transport time (to 45 m below emplacement drift) of thousands of years calculated, compared with a few years for release into the unperturbed flow



Vitric and Zeolitic in CH Play Dominant Role in Radionucllide Transport



NSP Easting (m)







Numerical Tools Specific to **UZ Transport Modeling**

TOUGH2 family of codes

- TOUGH2 V1.11 Module EOS9nT simulates flow and the transport of multiple radioactive solutes and/or colloids (parents and daughters)
- TOUGH2 V1.4 (Module EOS9 V1.4)
- T2R3D V1.4 simulates flow and the coupled transport of a single radioactive solute tracer
- DCPT V1.0 and V2.0 involves the particle-tracking method to simulate transport in a single radioactive tracer
- FRACL V1.0 provides semianalytical solutions to the problem of 2-D transport of multiple radioactive solutes and /or colloids



Breakthrough at Water Table (Present-Day Infiltration scenarios) (preliminary) ⁹⁹Tc



Non-sorbing Radionuclide: Relative Mass Fraction of ⁹⁹Tc in the Fractures Immediately above the Water Table (preliminary)

100 years

1000 years





Sorbing Radionuclide: Relative Mass Fraction of ²³⁷Np in the Fractures Immediately above the Water Table





Parent-Daughter Decay Transport: Mass Fractions of Each Member of the ²⁴⁰Am Chain (preliminary)



Colloidal Transport: Relative Mass Fraction in the Fracture Immediately above the Water Table for 6 nm PuO₂ (preliminary)



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Colloidal Transport: Relative Mass Fraction in the Fracture Immediately above the Water Table for 450 nm PuO₂ (preliminary)



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Colloidal Transport Declogging Models (preliminary)

Similarity of Normalized Release at the Water Table for Case 1 - No Declogging, and Case 2 - Strong Kinetic Declogging Indicates Dominant Role of the Fractures



UZ Transport Model Uncertainties

- Uncertainties in the flow conceptual model and the corresponding parameters
- **Climate uncertainties**
 - assessed by estimating transport under nine climatic scenarios
- Uncertainties in matrix diffusion
- **Uncertainties in sorption**
- **Uncertainties in filtration**



Example of Model Uncertainty: Active Fracture Model Parameter γ

Halving the calibrated γ does not affect saturation (flow)

alibrated AFP

Smaller AFP for under repository Model unit interface

0.5

Saturation

0.75

0.25

1400

1300

1200

1100

1000

900

800

700 L

Elevation (m)

PT

Odel Parameter γ Breakthrough (transport) is greatly affected by halving the calibrated γ



Conclusions – UZ Flow

- Available data, including geophysical, geochemical and hydrological data, provide significant constraints on the UZ flow model
- The UZ flow model is well calibrated using pneumatic, saturation/moisture tension, perched water, total chloride, strontium, calcite and temperature data
- The UZ flow model is validated using data from the Cross Drift (ECRB), in particular geology, fault and total chloride data
- The global water flow is well represented in the UZ flow model, and there is much confidence in those models results
- The local (detailed) water flow patterns (spacing and magnitude distribution) are poorly understood (represented by the active fracture model and flow focusing)
- Other major uncertainties relate to the van Genuchten formulation and fault properties and their effect on flow, especially below the repository horizon



Conclusions – UZ Transport

- On-going and completed tests provide input data that constrain the UZ transport model and allow the Project to take substantial credit for this important barrier
- Tracer tests using Alcove 1 and Alcove 8/Niche 3 provide clear evidence of matrix diffusion and provide essential data for the calibration of the UZ transport model
- Tracer tests conducted in the Busted Butte facility have clearly confirmed the porous medium nature of the vitric Calico Hills and verified sorption values for some important radionuclides
- Colloidal transport is significantly affected by the colloid size, but not much by kinetic declogging (reverse filtering)
- Daughter products of some important radionuclides, such as ²³⁹Pu and ²⁴¹AM must be considered in the UZ transport model
- Greatest uncertainties in the UZ transport model relate to the detailed characteristics of flow, the active fracture model and the efficiency of matrix diffusion. It is expected that significant additional benefits of this barrier can be achieved by full implementation of the shadow zone in the process models and TSPA.



Back-up Slides



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Vitric/Zeolitic: Geology Important for Transport to the Water Table



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Lessons Learned from Site Characterization Studies



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Testing Update: Geochemical Studies of Fracture Minerals (USGS) (preliminary)

- Conducting microbeam analyses of calcite at UCLA to determine carbon and oxygen isotope variability and implications for subsurface influence of **Pleistocene/Holocene climate changes**
- **Continued microdigestion and TIMS analyses of** youngest opal to evaluate depositional rates in the latest Pleistocene and Holocene
 - U-series ages range from 3,000 to 140,000 years in recently analyzed sample



Use of Construction Water Migration to Validate Fast Flow through Fractures

Observation

- Ponded release of construction water (tagged with LiBr)
- Br/CI ratios with distance from water source
- **Modeling Approach**
- Heterogeneous fracturematrix system (MINC)
- Interpretation of geochemical data
- Variability and uncertainty
- Results
- Fast flow through fractures
- Saturation changes consistent with Br/CI ratios


Use of Carbon-14 Age to Evaluate Active Fracture Model – Model Confidence Building





Transport Simulations for Suite of Radionuclides: *Different Lab-Determined k_d*'s

Species	Unit/Analysis	Distribution	Coefficients describing distribution [®] (ml/g)
U	Zeolitic	Cumulative	(Kd value, probability) (0, 0) (0.5 , 0.5) (30, 1.0)
	Devitrified	Cumulative	(Kd value, probability) (0, 0) (0.2 , 0.5) (4, 1.0)
	Vitric	Cumulative	(Kd value, probability) (0, 0) (0.2 , 0.5) (3, 1.0)
Np	Zeolitic	Cumulative	(Kd value, probability) (0, 0) (0.5 , 0.5) (6, 1.0)
	Devitrified	Cumulative	(Kd value, probability) (0, 0) (0.5 , 0.5) (6, 1.0)
	Vitric	Cumulative	(Kd value, probability) (0, 0) (1.0 , 0.5) (3, 1.0)
Pu	Zeolitic	Cumulative	(Kd value, probability) (10, 0) (100 , 0.5) (200, 1.0)
	Devitrified	Cumulative	(Kd value, probability) (10, 0) (70 , 0.5) (200, 1.0)
	Vitric	Cumulative	(Kd value, probability) (10, 0) (100 , 0.5) (200, 1.0)
Am	Zeolitic	Uniform	Range = 100- 1000 (500)
	Devitrified	Uniform	Range = 100- 2000 (1,000)
	Vitric	Cumulative	(Kd value, probability) (100, 0) (400 , 0.5) (1,000, 1.0)
Pa	Zeolitic	Uniform	Range = 1000 – 20,000 (10,000)
	Devitrified	Uniform	Range = 1000 – 20,000 (10,000)
	Vitric	Uniform	Range = 1000 – 20,000 (10,000)
Cs	Zeolitic	Cumulative	(Kd value, probability) (425, 0) (5,000 , 0.5) (20,000, 1.0)
	Devitrified	Uniform	Range = 1 – 15 (7.5)
	Vitric	Cumulative	(Kd value, probability) (0, 0) (2 , 0.5) (100, 1.0)
Sr	Zeolitic	Uniform	Range = 50 – 2000 (1000)
	Devitrified	Uniform	Range = 10 – 70 (40)
	Vitric	Uniform	Range = 0 – 50 (25)
Ra	Zeolitic	Uniform	Range = 1000 – 5,000 (2,500)
	Devitrified	Uniform	Range = 100 – 1,000 (500)
	Vitric	Uniform	Range = 50 – 600 (300)
Th	Zeolitic	Uniform	Range = 1,000 - 30,000 (15,000)
	Devitrified	Uniform	Range = 1,000 - 10,000 (5,000)
	Vitric	Uniform	Range = 1,000 - 10,000 (5,000)

Output-DTN: LA0302AM831341.002 TDIF: 314028 (UZ)

NOTE:^a The numbers in boldface were used in the simulations.



(preliminary)

UZ Transport Model Summary (1)

- Transport is dominated and controlled by faults (e.g. Drillhole Wash fault and Pagany Wash fault)
 - Provide fast paths to downward migration
 - Limit lateral migration across the fault walls into the formation
- Faster transport over a larger area in the northern part of the repository
 - Consistent with the geological model for UZ, which is characterized by the highly fractured zeolitic CHZ layers in that area



UZ Transport Model Summary (2)

- Transport patterns follow the infiltration and percolation distributions
 - Water flow pattern dictates the advective transport pattern
- Fractures are the main pathways of radionuclide transport
- Diffusion from the fractures into the matrix is one of the main retardation processes in radionuclide transport



UZ Transport Model Summary (3)

- Transport to the water table is strongly dependent on the sorption affinity of the radionuclide to the geohydrologic units it encounters in the UZ
 - Lower k_d (quantifying weaker sorption) leads to faster radionuclide transport
- In considering transport of ²³⁹Pu and ²⁴¹Am, contribution to the breakthrough of daughter products is important



UZ Transport Model Summary (4)

- For continuous colloid release under a mean presentday infiltration regime, the transport of radioactive true colloids is not appreciably influenced by the kinetic declogging(reverse filtering).
- The colloid size has a significant effect on transport.
- The UZ of Yucca Mountain is an effective barrier to the transport of the strongly sorbing radionuclides

