



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

# Unsaturated Zone Flow and Transport

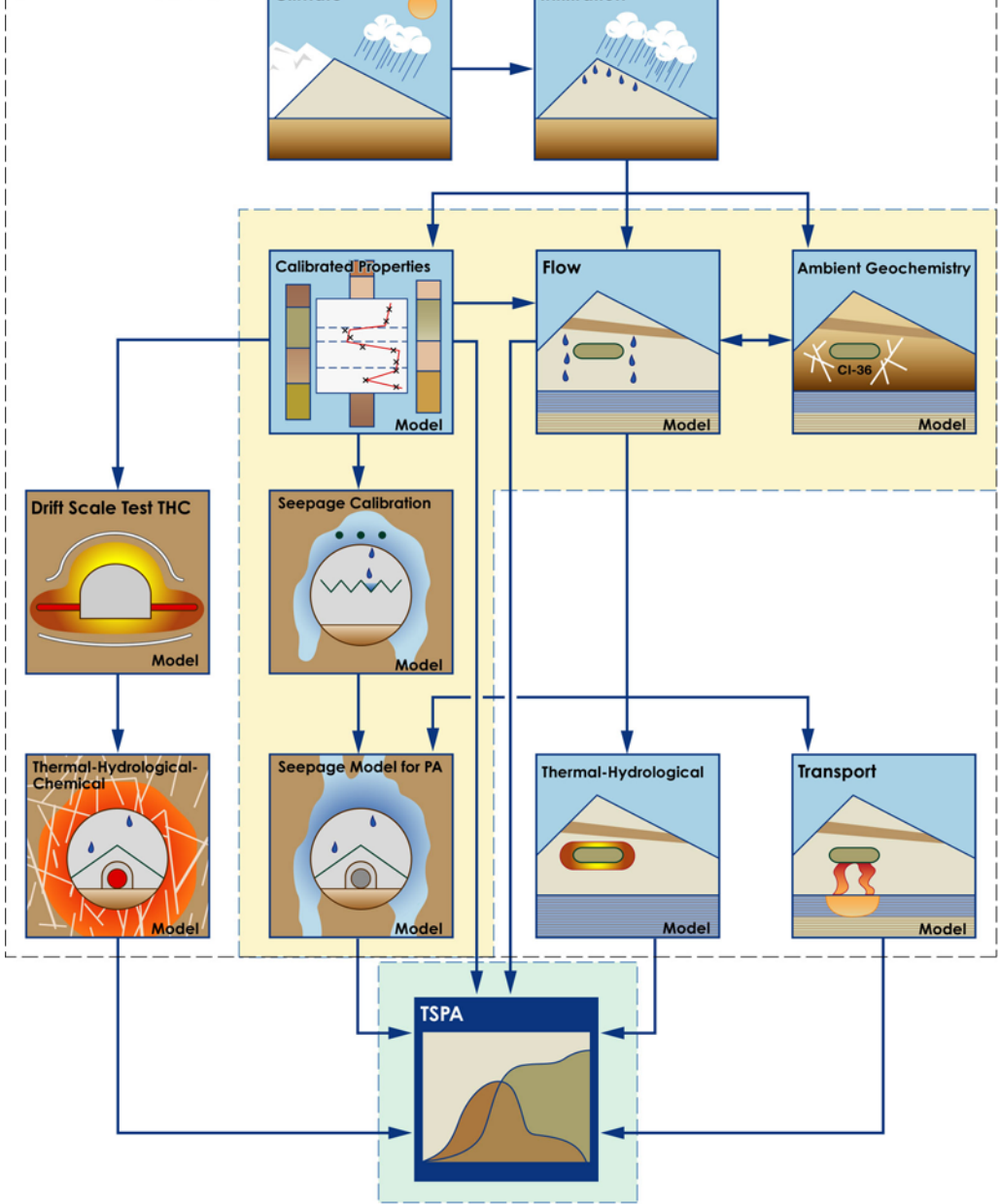
Presented to:  
**Nuclear Waste Technical Review Board**

Presented by:  
**G. S. Bodvarsson**  
**Lawrence Berkeley National Laboratory**  
**Yucca Mountain Site Characterization Office**  
**U.S. Department of Energy**

**August 1, 2000**

**YUCCA  
MOUNTAIN  
PROJECT**

**UZ PMR Models**



UZPMR1-2REV00

# UZ Flow and Transport Process Model Factors

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Water Contacting Waste Package	Climate	<ul style="list-style-type: none"> <li>• Climate states</li> <li>• Timing and sequence</li> </ul>
	Net Infiltration	<ul style="list-style-type: none"> <li>• Probabilities for different infiltration scenarios</li> <li>• Infiltration Rate</li> </ul>
	Unsaturated Zone Flow	<ul style="list-style-type: none"> <li>• Flow fields for different infiltration scenarios and climate states</li> <li>• Percolation flux at repository</li> </ul>
	Coupled Effects on UZ Flow	<ul style="list-style-type: none"> <li>• Percolation flux affected by TH</li> </ul>
	Seepage into Emplacement Drifts	<ul style="list-style-type: none"> <li>• Seepage flux and seepage fraction as a function of percolation flux</li> <li>• Percolation flux -- f (multiple locations, waste type, time, climate)</li> </ul>
	Coupled Effects on Seepage	<ul style="list-style-type: none"> <li>• Seepage flux and seepage fraction as a function of percolation flux</li> <li>• Seepage composition affected by THC</li> </ul>

# UZ Flow and Transport Process Model Factors

(Continued)

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Transport Away from the Engineered Barrier System	UZ Radionuclide Transport	<ul style="list-style-type: none"> <li>• Fracture aperture and spacing in different units</li> <li>• Flow fields for different infiltration scenarios and climate states</li> <li>• <math>K_d</math> for all elements included in TSPA</li> <li>• Matrix diffusion coefficients – f (isotopes, units)</li> <li>• <math>K_c</math> and/or kinetic colloid parameters for Pu, Am, Th etc.</li> <li>• Colloid filtration factor</li> </ul>
	SZ Radionuclide Transport	<ul style="list-style-type: none"> <li>• Breakthrough curves – f (radionuclide, region)</li> <li>• Climate change flux multiplication factor</li> <li>• Capture zones and release locations within each zone.</li> <li>• Flow fields</li> <li>• Flowing interval spacing</li> <li>• Effective porosity for all units except the volcanic units</li> <li>• Dispersivity (longitudinal, horizontal transverse, vertical transverse)</li> <li>• Boundary definition of the alluvium</li> <li>• <math>K_d</math> for isotopes included in TSPA</li> <li>• Flowing interval porosity</li> <li>• Matrix porosity</li> <li>• Effective diffusion coefficient</li> <li>• <math>K_c</math> colloid parameters</li> <li>• Colloid filtration factor</li> </ul>
	Wellhead dilution	<ul style="list-style-type: none"> <li>• Annual groundwater usage</li> </ul>
	Biosphere Dose Conversion Factor	<ul style="list-style-type: none"> <li>• Biosphere dose conversion factor – f (radionuclide, irrigation time)</li> </ul>

# Climate and Infiltration Models

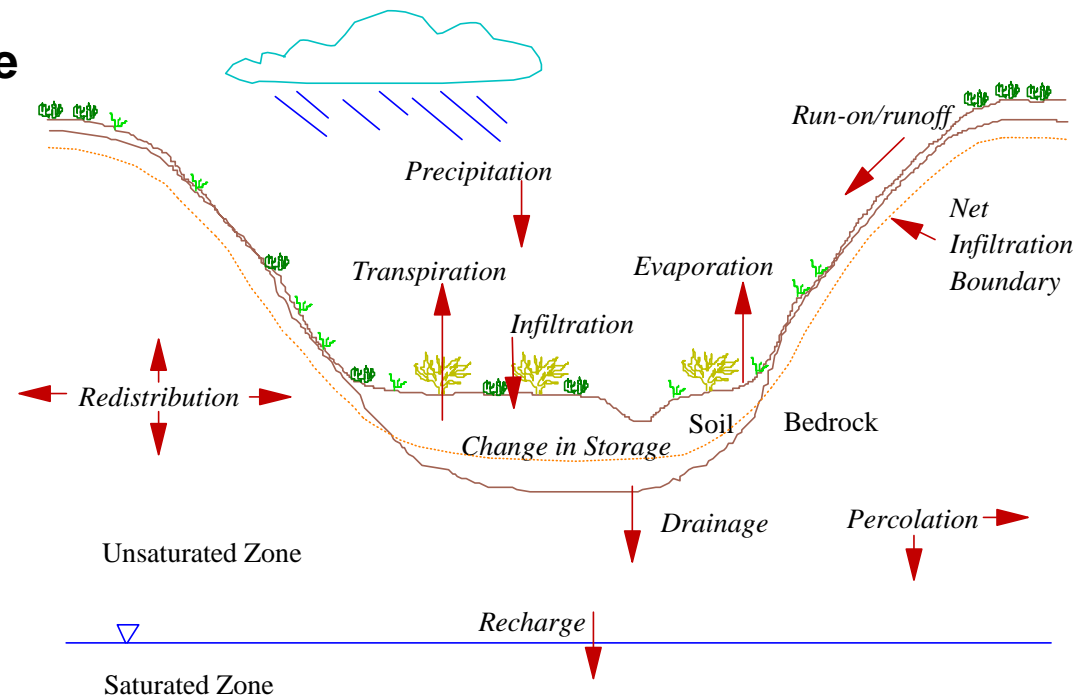
## Objectives

### • Climate

- Analysis of potential future climate conditions-10,000 years
- Estimate mean, upper and lower bounds for precipitation and air temperature
- Provide input for Infiltration Model

### • Infiltration

- Provide spatially-distributed time-averaged estimates of net infiltration
- Upper boundary of UZ Flow and Transport Model



# Climate and Infiltration Models

(Continued)

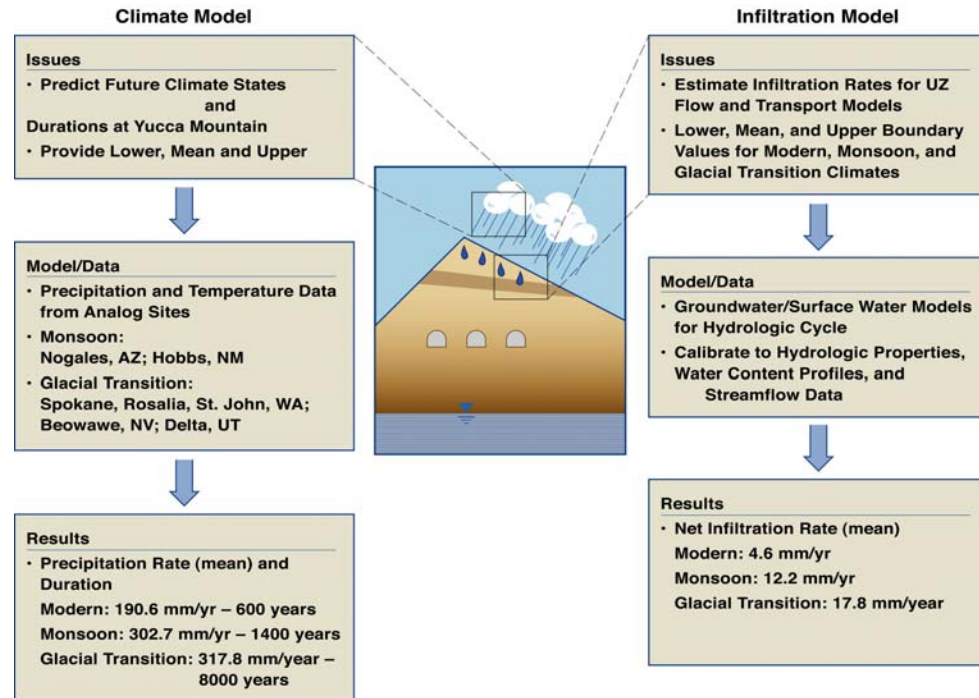
## Assumptions

### Climate

- Analysis based on examining paleoclimate records
- Climate is cyclical with several alternating glacial and interglacial periods

### Infiltration

- Model infiltration through root-zone only
- Simplified "bucket-model" used to simulate infiltration process



UZPMR3.5-1REV00



# Climate and Infiltration Models

(Continued)

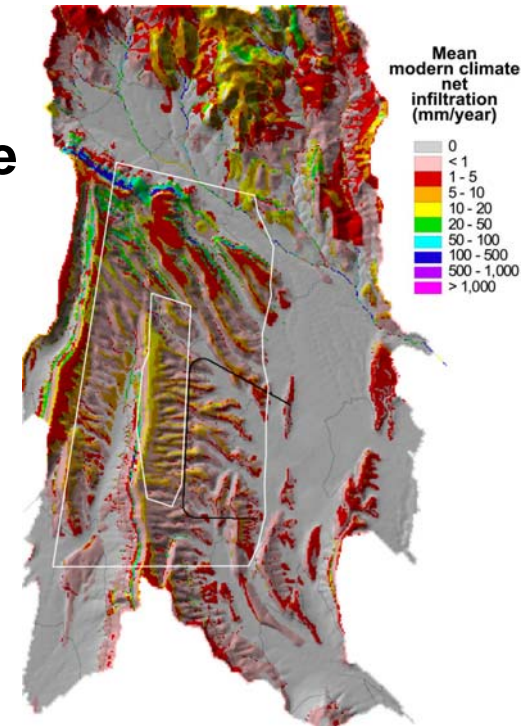
## Results

### ● Climate

—	Duration	Mean Precipitation Rate
— Modern:	400-600 years	190.6 mm/yr
— Monsoon:	900-1400 years	302.7 mm/yr
— Glacial Transition:	800-8700 years	317.8 mm/yr

### ● Infiltration

—	Mean Infiltration Rate
— Modern:	4.6 mm/yr
— Monsoon:	12.2 mm/yr
— Glacial transition:	17.8 mm/yr



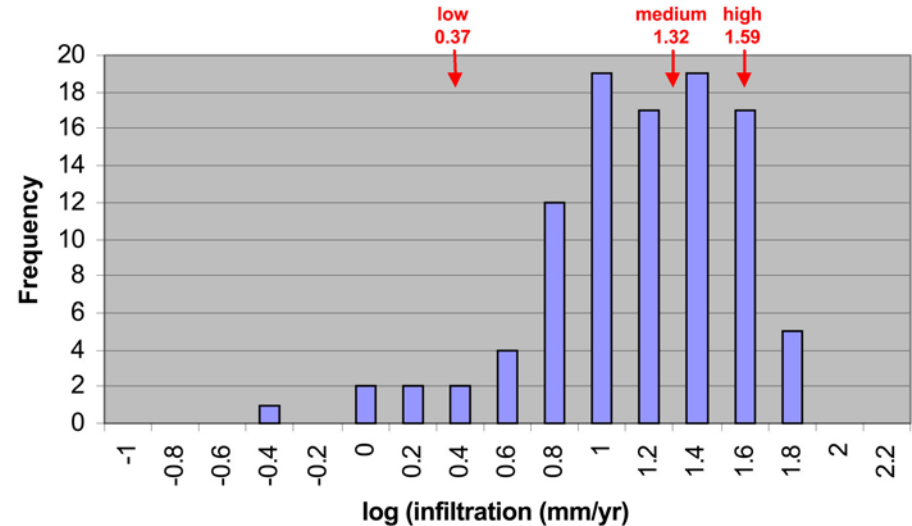
# Climate and Infiltration Models

(Continued)

## Uncertainty

### ● Climate

- Not included in base TSPA simulations-indirectly through effects on UZ Flow Model
- Future work: vary climate change times



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### ● Infiltration

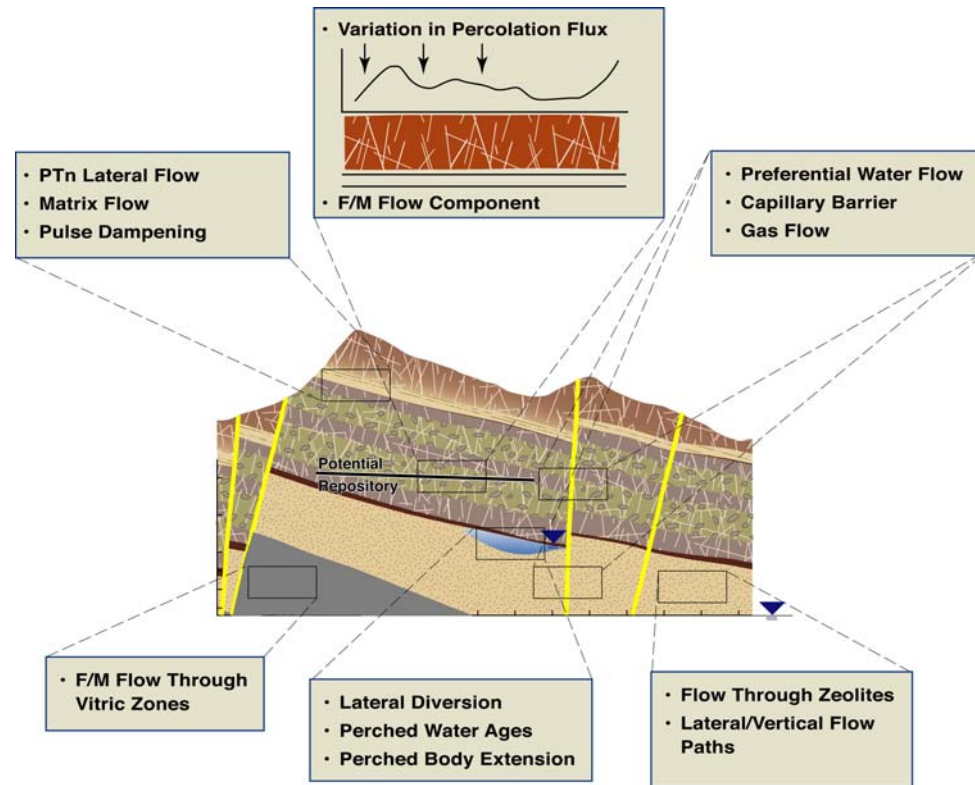
- Included indirectly in TSPA simulation as boundary condition on UZ Flow Model
- Monte Carlo simulation varying parameters in Infiltration Model-generate infiltration histogram for each climate scenario
- Weight climate scenario histograms for sampling in TSPA simulations



# UZ Flow Model

## Objectives

- To integrate the available data from the UZ system into a comprehensive 3-D model
- To develop several submodels for detailed studies of percolation and perched water through different units
- To quantify the flow of moisture, heat, and gas through the UZ, under present-day and estimated future climate scenarios
- To contribute model parameters and model input to other specific studies or models
- To provide TSPA with 3-D steady-state flow fields



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# UZ Flow Model

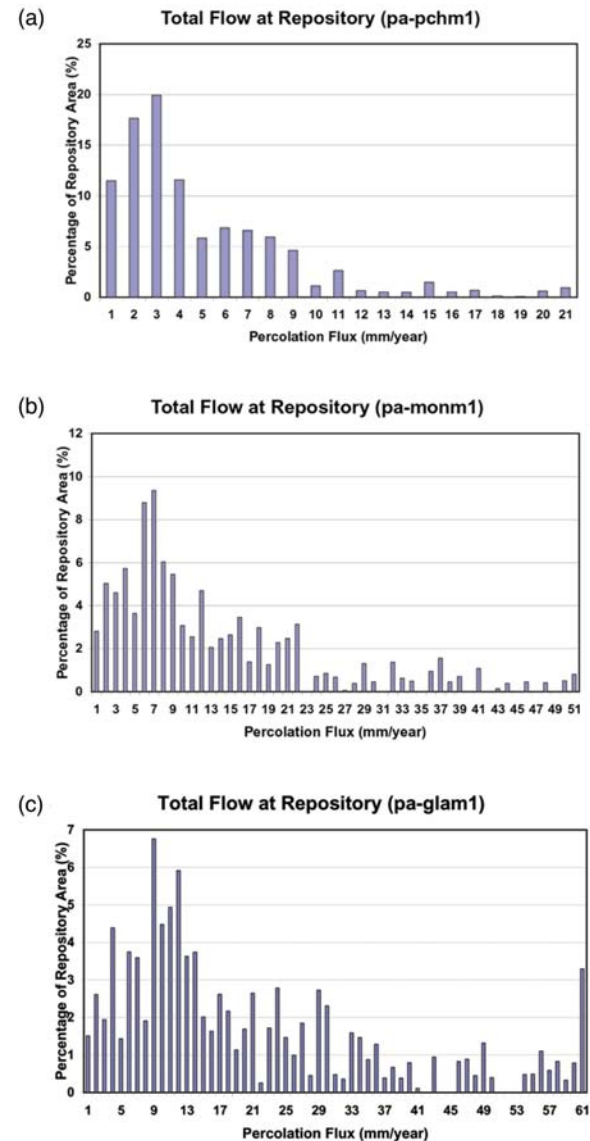
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## Results

- Model Calibration completed
- Several submodels developed for PTn, faults, and CHn/perched water
- Percolation fluxes, flow patterns and fracture-matrix flow components predicted using nine infiltration scenarios

## Factors/Conservatisms/Optimisms

- Surface net infiltration rates
- Heterogeneity of the hydrogeological system
- Characterization of faults



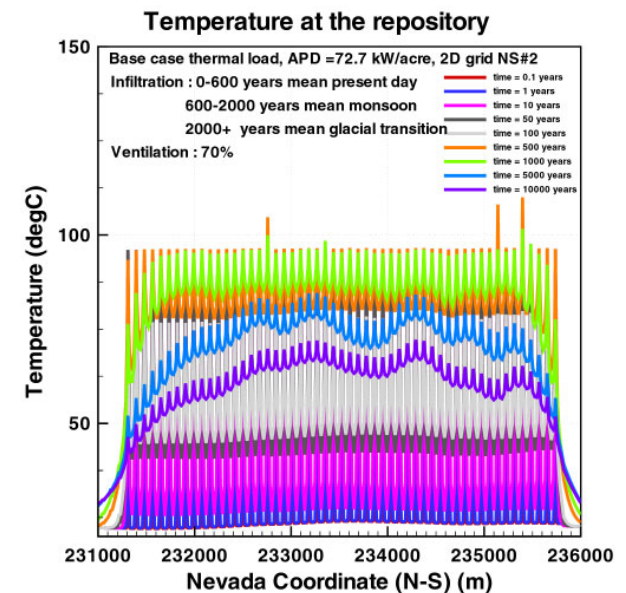
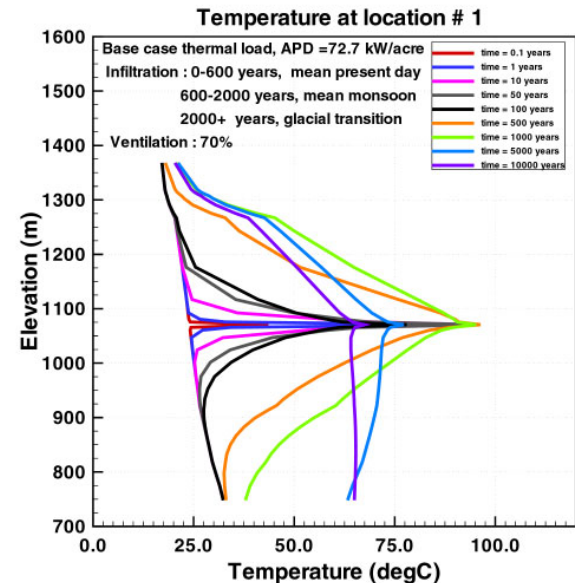
# Mountain Scale Coupled Processes - TH Mode

## Objectives

- Evaluate temperature changes over the Mountain size of the 2-phase zone, temperature at Repository PTn, CHn, and water table
- Evaluate the effects of heat on liquid and gas distribution.
- Evaluate the effects of heat on liquid and gas flow the far field; close to drifts; drainage in the pillars

## Assumptions

- Uniform heat distribution at repository; ventilation removes only heat
- Layer constant flow properties; not effected by thermal load; no hysteresis
- Fixed temperature top and bottom boundary conditions
- Modeling approach supported by:
  - Geothermal natural analog continuum mode
  - Drift Scale Heater Test





# Mountain Scale Coupled Processes: TH Model

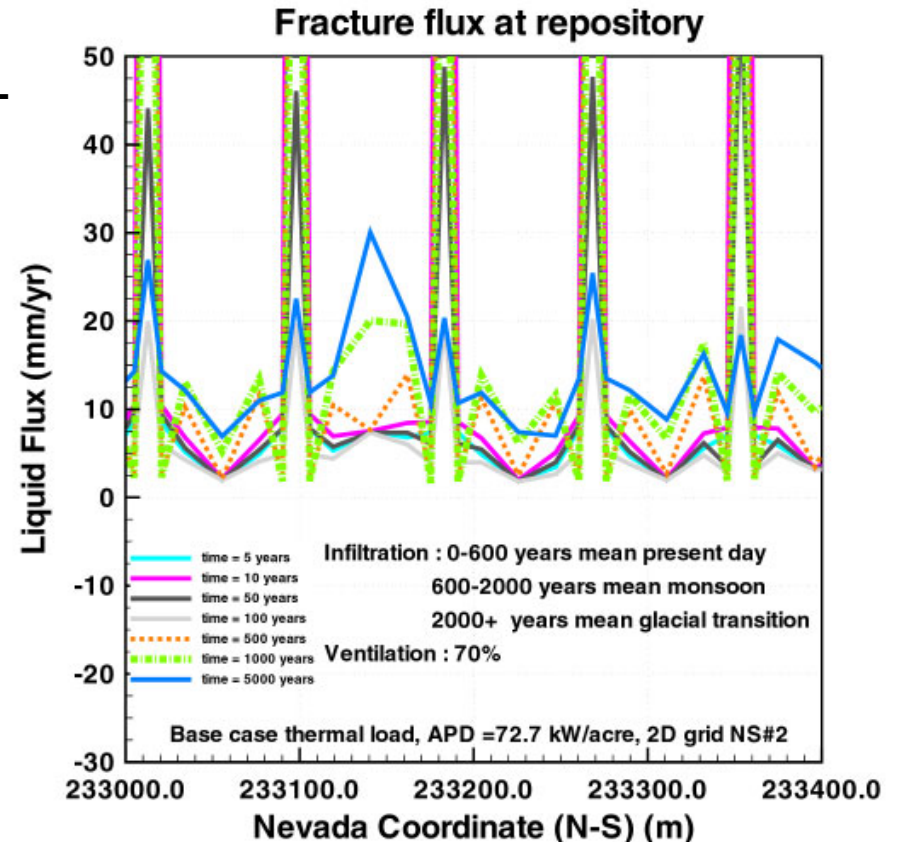
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## Results

- The two-phase zone is confined to less than 10-20 m from drifts
- Temperatures at the repository drifts rises to above boiling conditions ( $>97\text{ }^{\circ}\text{C}$ )  
Temperatures of pillars is  $80\text{-}85\text{ }^{\circ}\text{C}$ ,  $70\text{-}75\text{ }^{\circ}\text{C}$  CHn and  $67\text{-}70\text{ }^{\circ}\text{C}$  at water table
- High fracture permeabilities allow for easy and rapid drainage in pillars between drifts
- Liquid flux towards the drifts may exceed 400 mm/year, but is all vaporized by repository heat. Drainage between the drifts is enhanced by condensate water

## Factors that may impact predictions

- Lateral variation properties across layers; focussed and channelized flow of condensate through fractures and heterogeneous features
- Changes in long term distribution of ambient surface infiltration and effects of climate



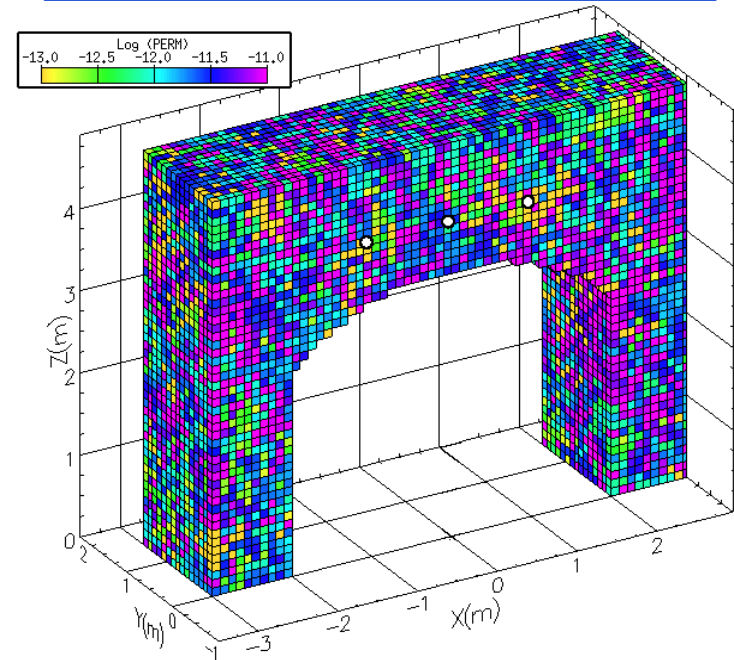
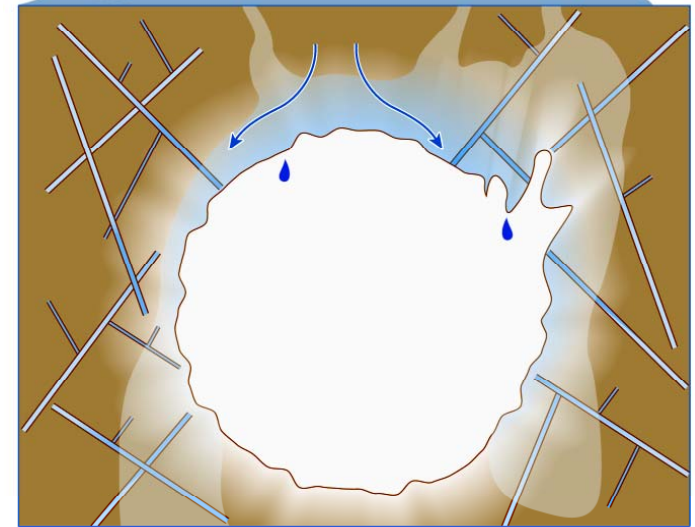
# Drift Seepage Models

## Objectives

- Determine fraction of waste packages affected by seepage
- Determine seepage flux

## Assumptions

- Heterogeneous fracture continuum
- Flow focusing
- No evaporation/condensation
- Partial drift collapse
- Large variability and parameter uncertainty



# Drift Seepage Models

(Continued)

## Results

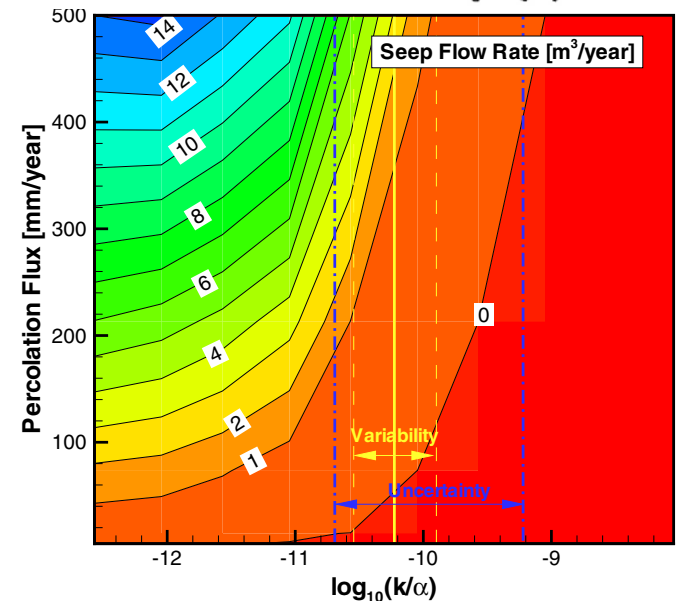
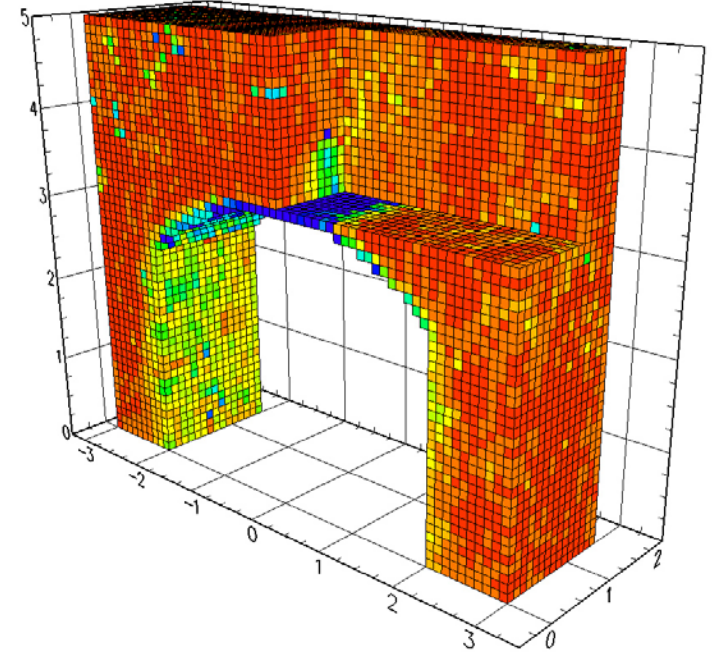
- Seepage-relevant parameters determined from seepage experiments
- Calculated seepage fraction and seepage flux for large range of parameters

## Factors

- Percolation flux
- Channeling effect
- Effective capillary strength of fractures
- Fracture permeability

## Conservatisms/Optimisms

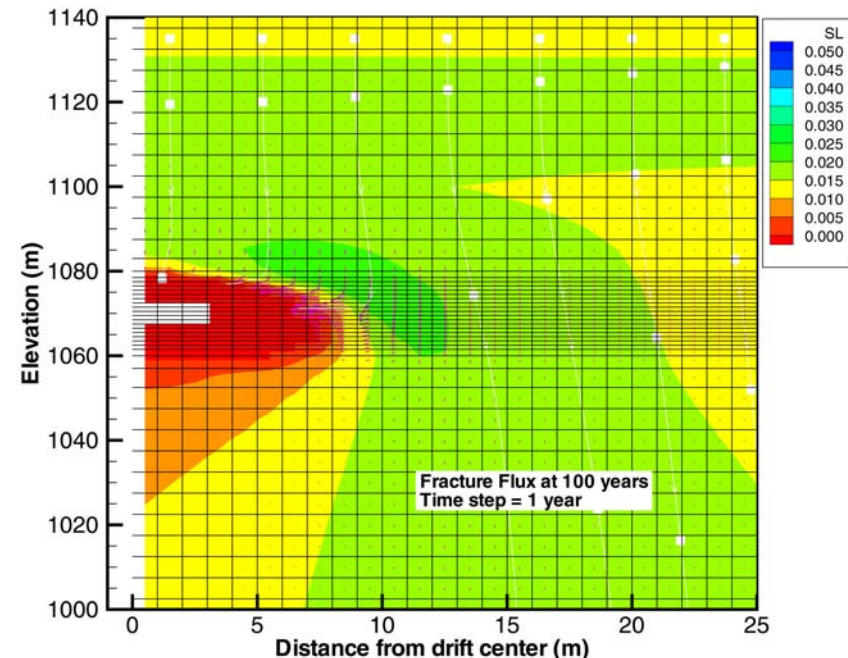
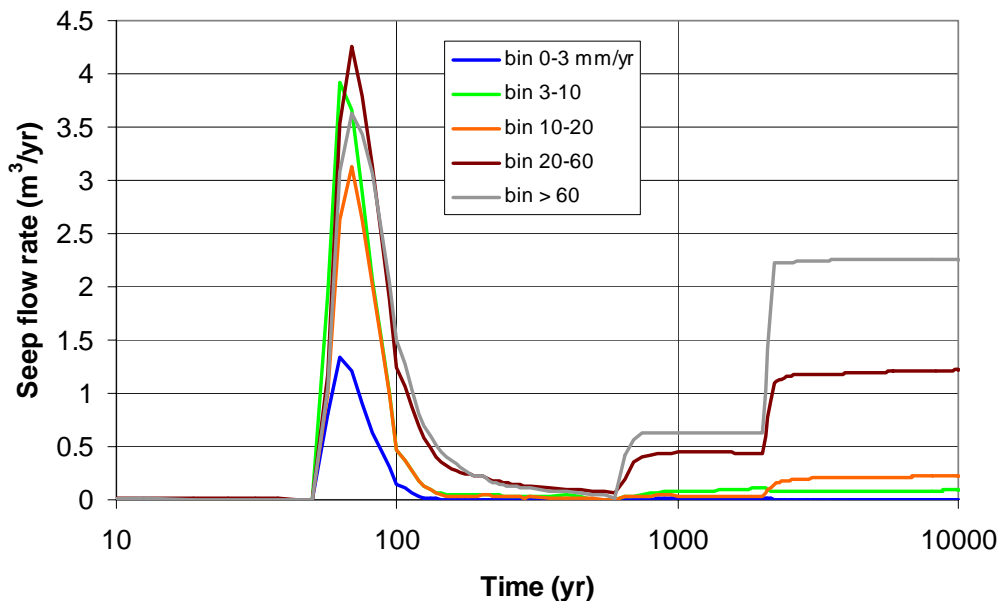
- Conservative parameter values
- Ignore ventilation/ evaporation
- Ignore in-drift condensation





# Seepage During Thermal Period

- Percolation flux 5 m above the drift is used in seepage calculations
- Capillary driven flow towards drifts produces a pulse of seepage at around 100 years. This abstraction is conservative and has little effect on TSPA results
- Recent model simulations using heterogeneous fracture properties show no seepage and efficient drainage in pillars



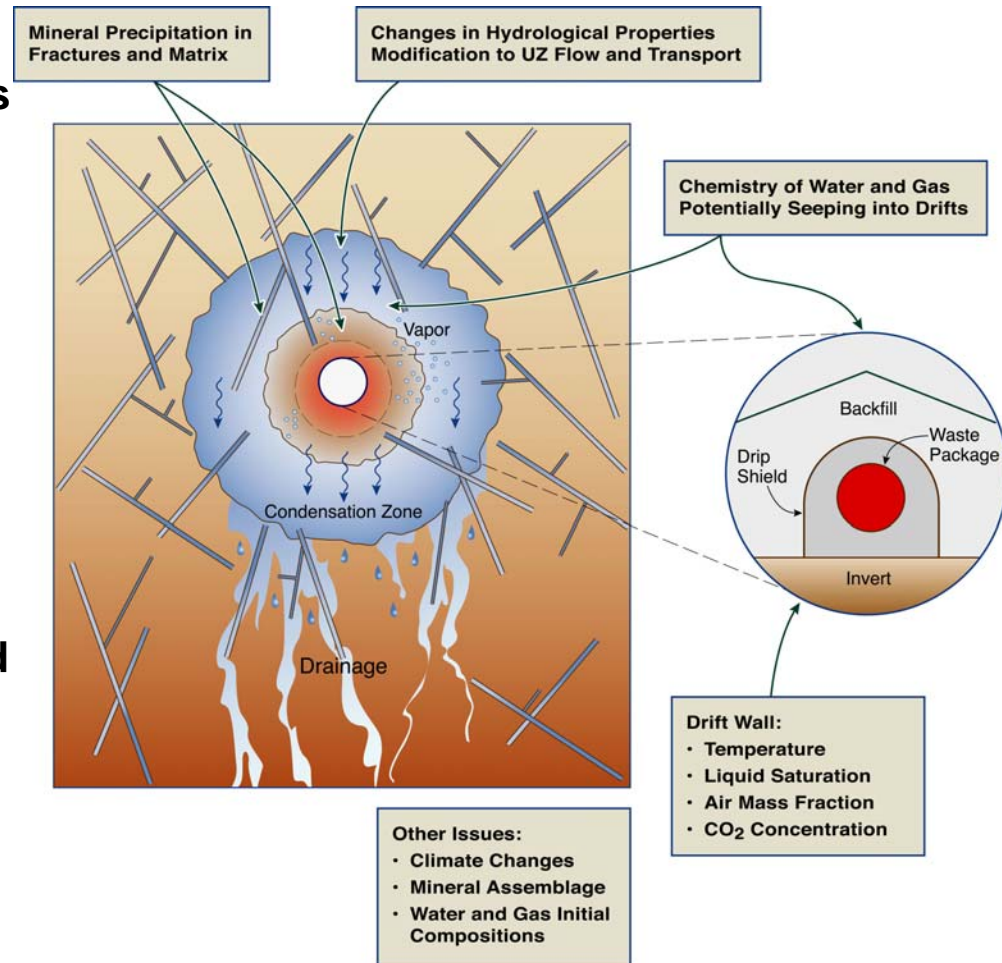
# Drift Scale THC Models

## Objectives

- Predict the chemistry of water and gas that will seep into drifts
- Evaluate changes in hydrological properties due to mineral precipitation/dissolution
- Calibrate/validate model using the chemical evolution of water, gas, and minerals in the Drift Scale Test

## Assumptions

- Dual-permeability model
- Initial water chemistry in fractures and matrix pore water is the same
- Geochemical systems considered adequately capture the ambient system



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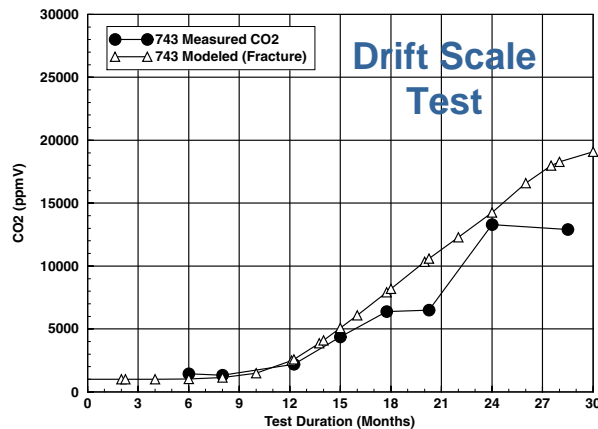
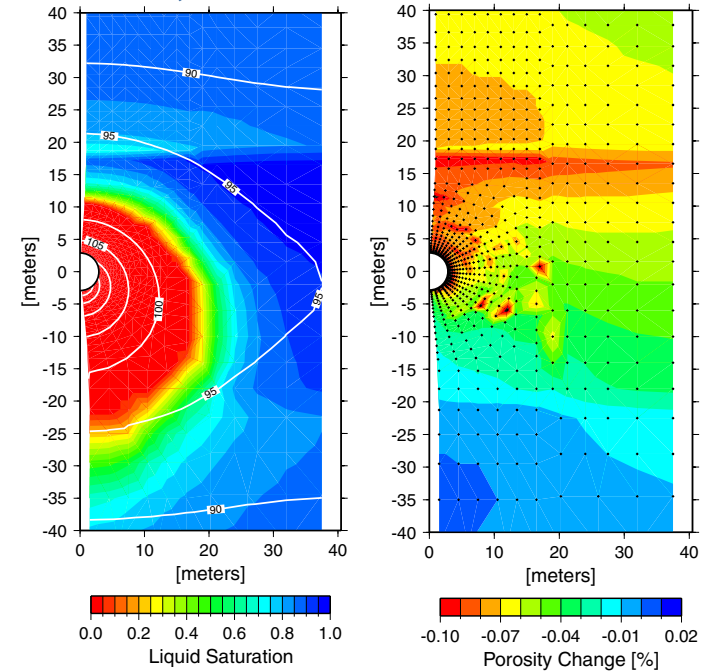
# Drift-Scale THC Models

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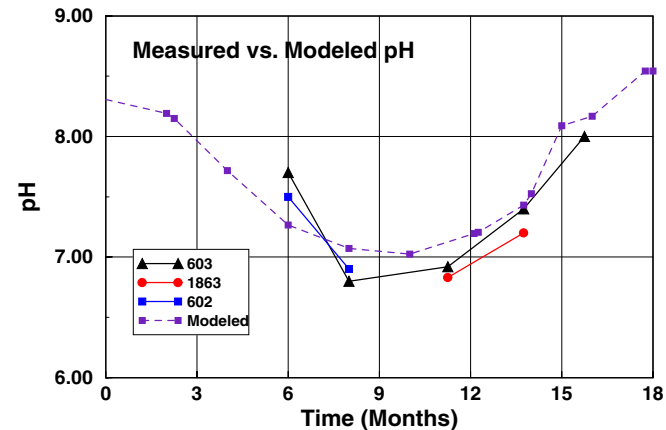
## Results and Validation

- A large zone of increased gaseous CO<sub>2</sub> concentrations was predicted in the DST and has been confirmed by analyses
- Modeled fracture water chemistry in the DST shows a similar trend in pH over time to waters collected from boreholes
- The pH of water flowing in fractures to the drift wall during the rewetting period is near neutral to slightly alkaline (~ 7.5 to 9) and is not strongly concentrated in salts
- Porosity and permeability changes over the first 10,000 years are small and effects on flow fields minimal

## 10,000 Year Predictions



## Drift Scale Test



# Drift-Scale THC Models

(Continued)

## Conservatisms/Optimisms

- Initial water chemistry is more concentrated in many components than the average UZ pore water, and thus would give a conservative estimate on salt concentrations and mineral precipitation from boiling alone
- Changes in permeability that are based on porosity changes are likely to be underestimated (optimistic), because mineral precipitation/dissolution may be localized

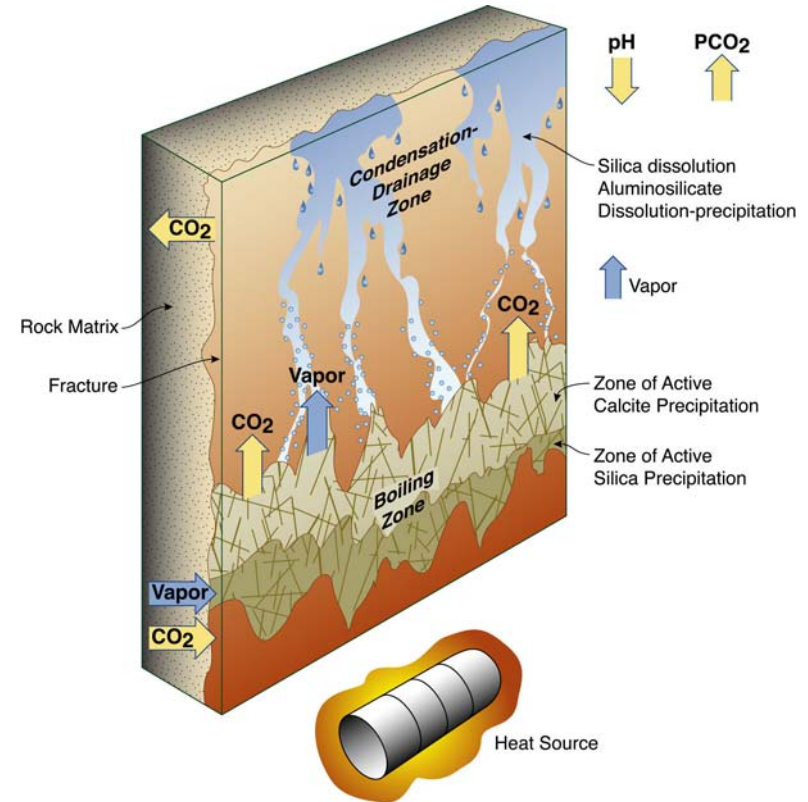
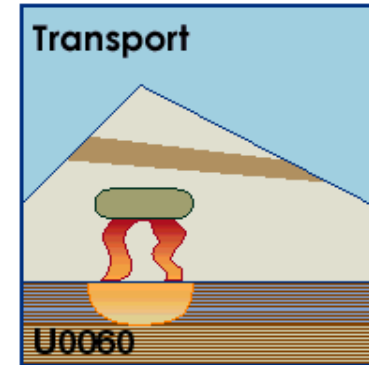


Diagram Showing THC Processes

# UZ Transport Model

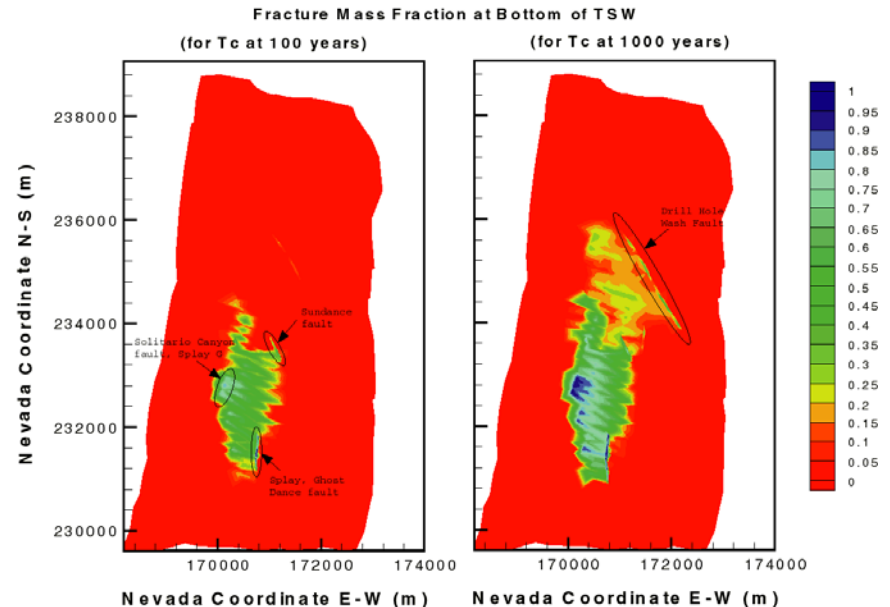
## Objectives

- Develop a model for investigating radionuclide solute and colloid transport in UZ to support PA abstraction for TSPA



## Assumptions

- Flow component the same as for the UZ Flow Model
- Governing transport processes (advection, dispersion, diffusion, sorption, radioactive decay, colloid filtration, and colloid-assisted transport)



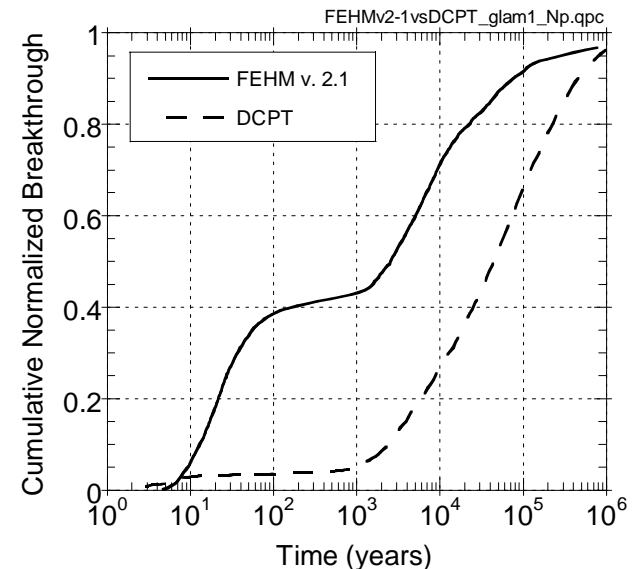
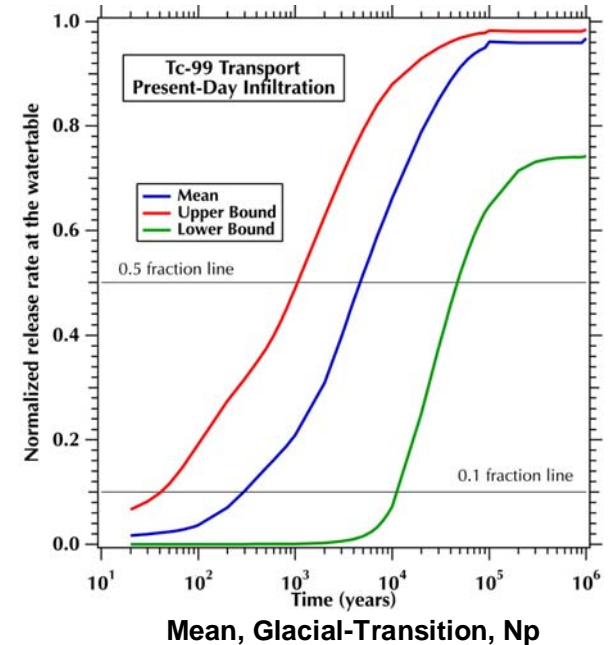


# UZ Transport Model

(Continued)

## Results/Important Factors

- Faults dominate and control transport
- Matrix diffusion and sorption are main retardation mechanisms
- $^{239}\text{Pu}$  decay chain products are important
- Colloidal transport could be important
- Current PA transport model may be very conservative



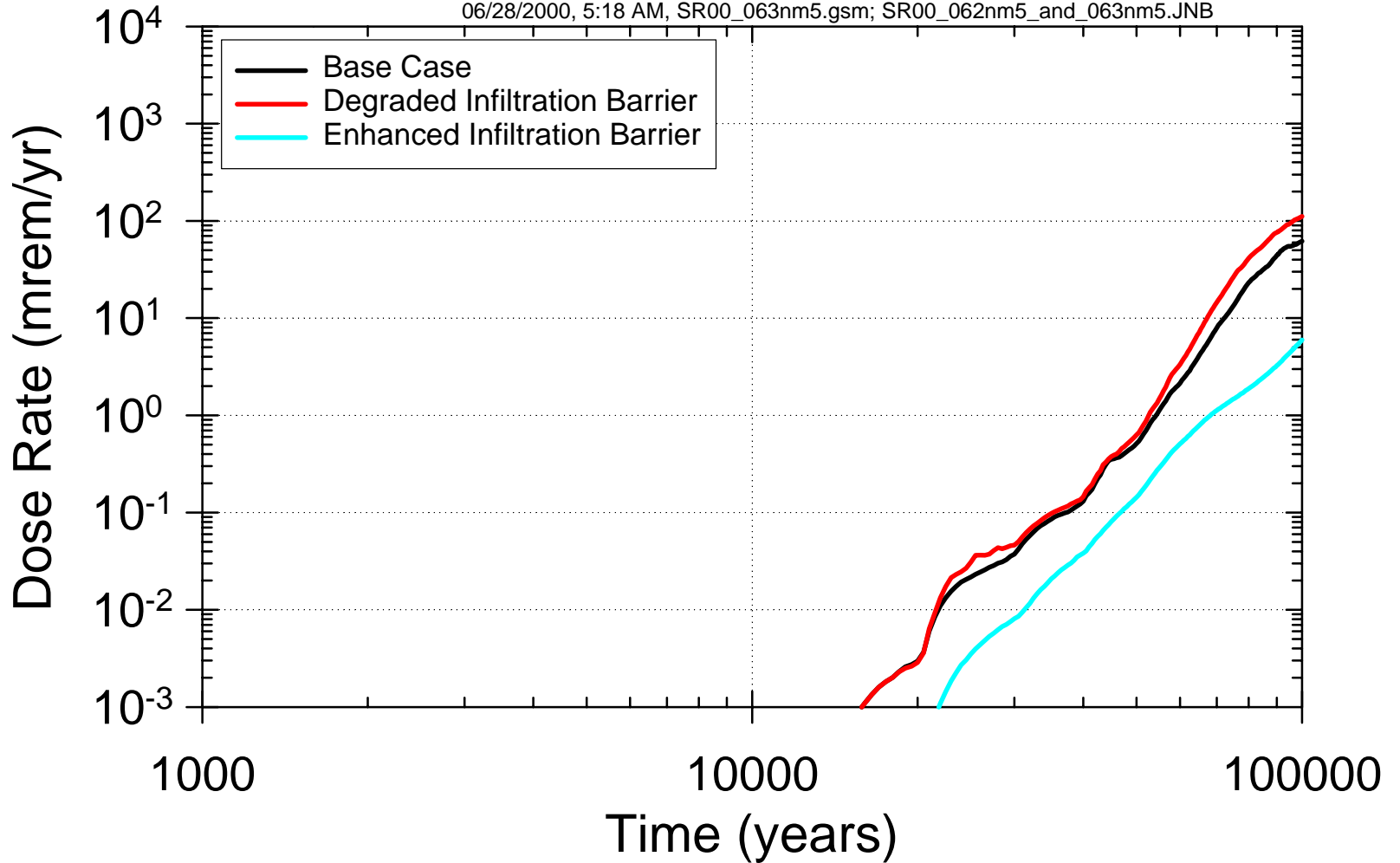
# Infiltration Barrier Sensitivity

- **Degraded Barrier**
  - High infiltration case throughout the model
- **Enhanced Barrier**
  - Low infiltration case throughout the model



# Preliminary Infiltration Barrier Sensitivity

06/25/2000, 1:33 PM, SR00\_047nm5.gsm; 06/28/2000, 1:40 AM, SR00\_062nm5.gsm;  
06/28/2000, 5:18 AM, SR00\_063nm5.gsm; SR00\_062nm5\_and\_063nm5.JNB



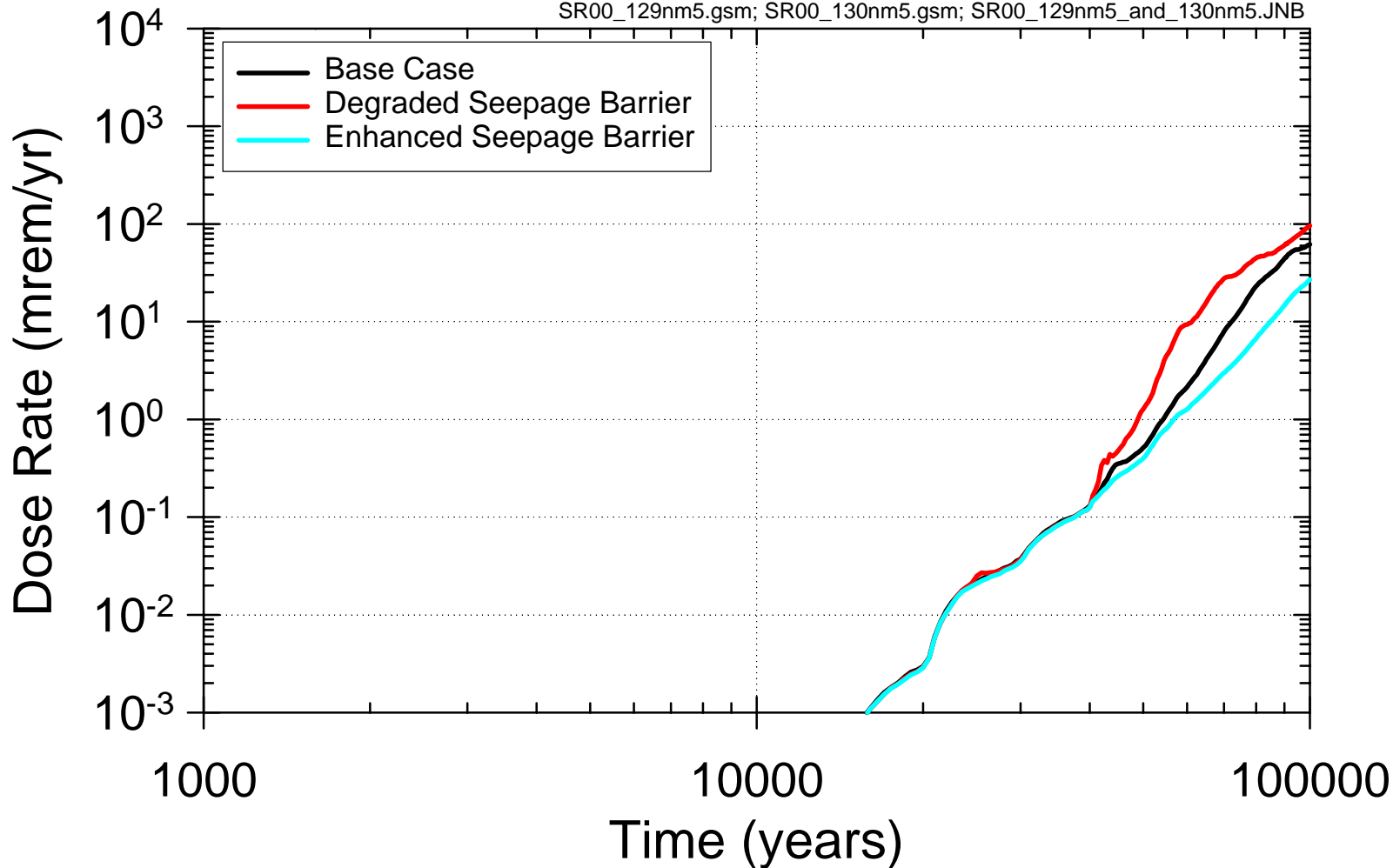
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# Seepage Barrier Sensitivity

- **Degraded Barrier**
  - **95th %tile flow focus factor**
  - **95th %tile seepage uncertainty index (implies 95th %tile seepage fraction, 95th %tile mean seepage flux, & 95th %tile seepage flux standard deviation)**
- **Enhanced Barrier**
  - **5th %tile flow focus factor**
  - **5th %tile seepage uncertainty index (implies 5th %tile seepage fraction, 5th %tile mean seepage flux, & 5th %tile seepage flux standard deviation)**

# Preliminary Seepage Barrier Sensitivity

06/25/2000, 1:33 PM, SR00\_047nm5.gsm;  
SR00\_129nm5.gsm; SR00\_130nm5.gsm; SR00\_129nm5\_and\_130nm5.JNB

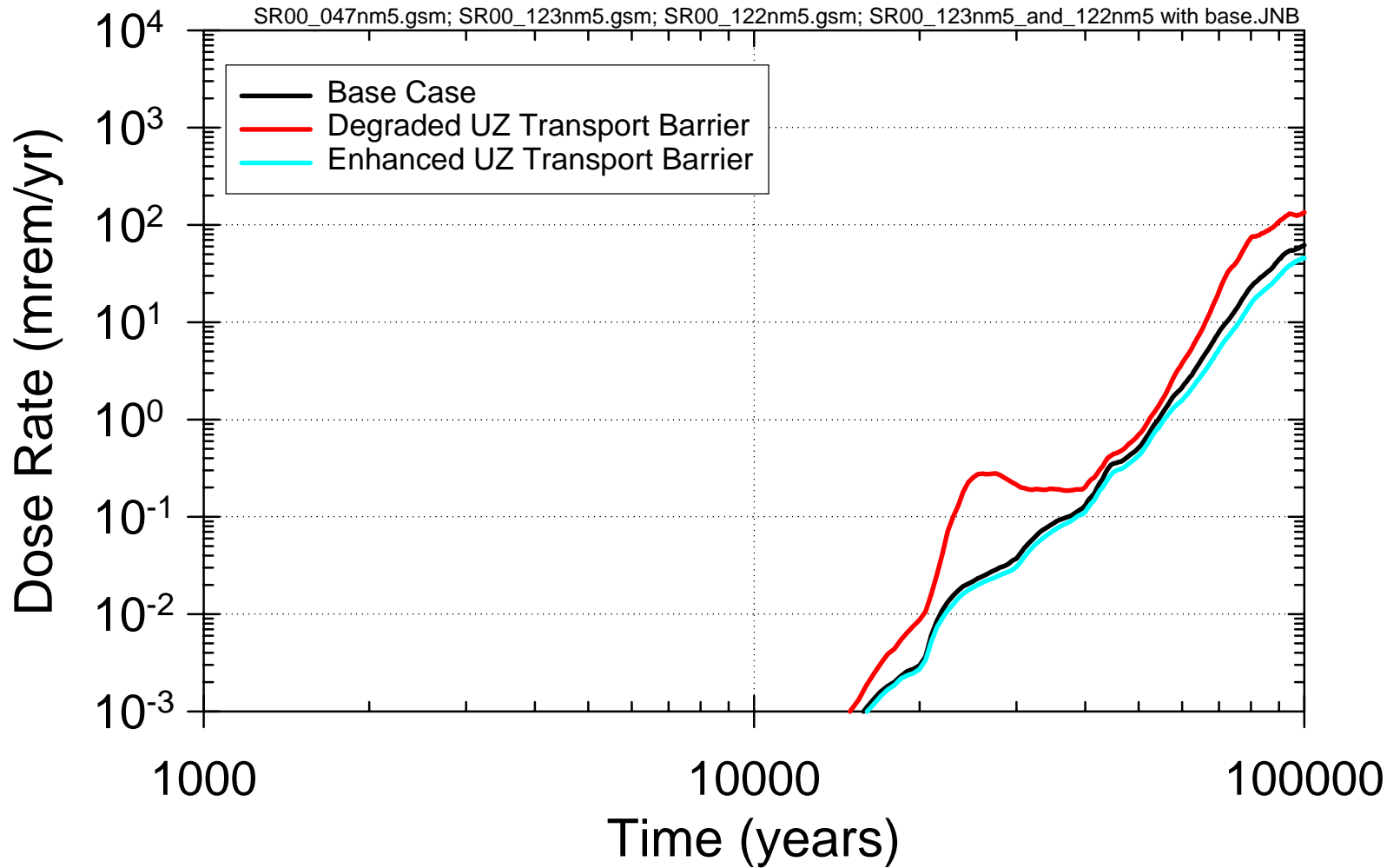


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# UZ Transport Barrier Sensitivity

- **Degraded Barrier**
  - 5th %tile matrix Kds for all radionuclides
  - 95th %tile Kc for reversible colloids
  - 5th %tile anion/cation matrix diffusion coefficients
  - 95th %tile fracture apertures for all units
- **Enhanced Barrier**
  - 95th %tile matrix Kds for all nuclides
  - 5th %tile Kc for reversible colloids
  - 95th %tile anion/cation matrix diffusion coefficients
  - 5th %tile fracture apertures for all units

# Preliminary UZ Transport Barrier Sensitivity



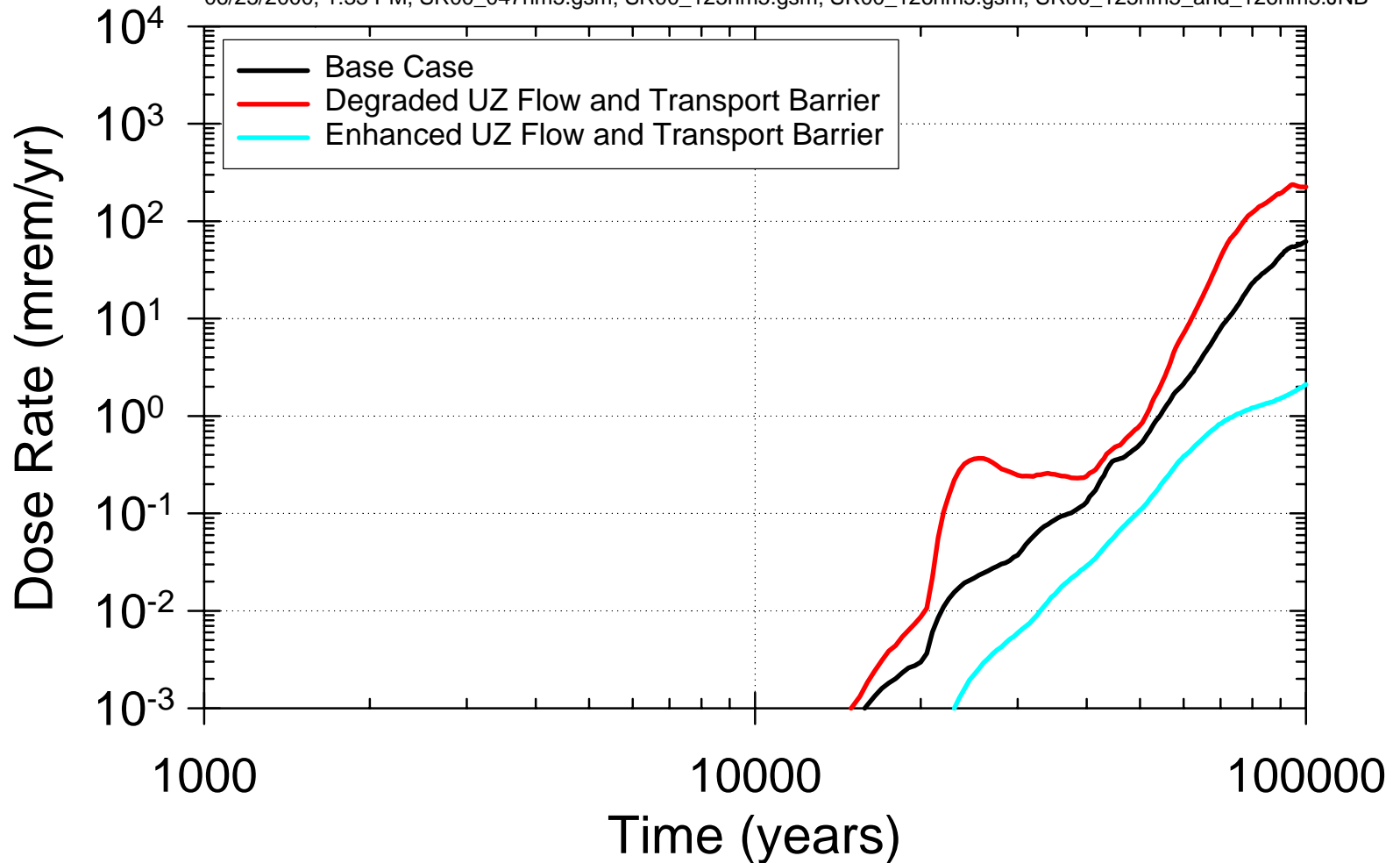
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# UZ Flow and Transport Barrier Sensitivity

- **Degraded Barrier**
  - Degraded UZ transport barrier
  - Degraded Infiltration barrier
- **Enhanced Barrier**
  - Enhanced UZ transport barrier
  - Enhanced Infiltration barrier

# Preliminary UZ Flow and Transport Barrier Sensitivity

06/25/2000, 1:33 PM, SR00\_047nm5.gsm; SR00\_125nm5.gsm; SR00\_126nm5.gsm; SR00\_125nm5\_and\_126nm5.JNB



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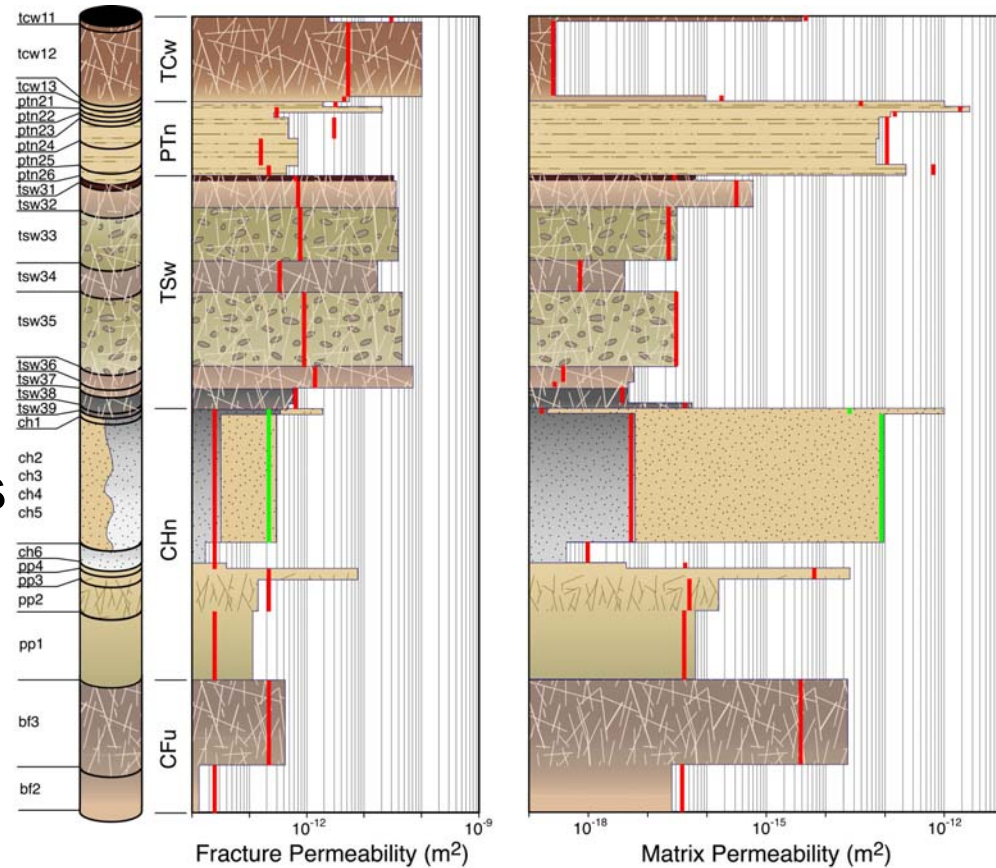
# Backup



# Calibrated Properties Model

## Objectives

- Mountain-scale, calibrated parameters for entire UZ F&T Model
- Drift-scale, calibrated parameters for repository horizon and adjacent layers
- Fault, calibrated parameters for entire UZ F&T Model
- Thermal parameters (uncalibrated) for entire UZ F&T Model
- Estimate uncertainties for the parameters



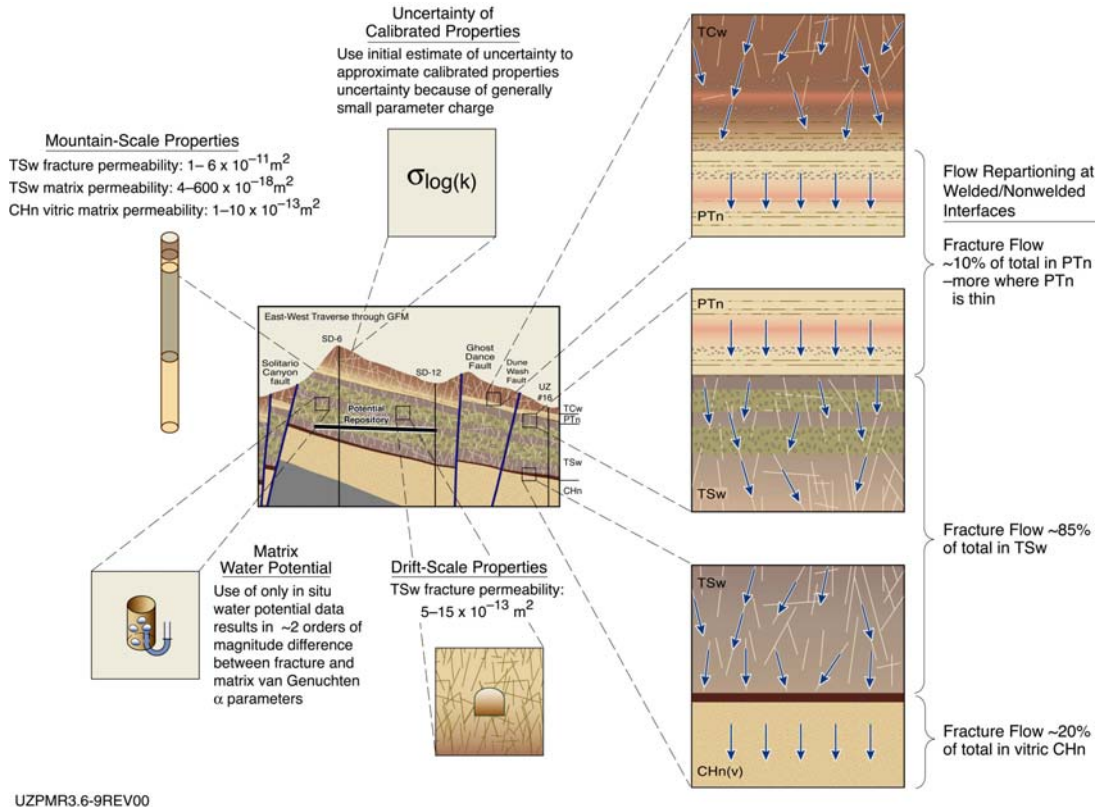
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# Calibrated Properties Model

(Continued)

## Assumptions

- Heterogeneity is controlled by hydrogeologic layering (i.e. properties are homogeneous within a layer)
- Liquid flow under ambient conditions is steady-state
- Flow is simulated using a dual-permeability model
- van Genuchten model is used for liquid relative permeability and water potential
- Brooks-Corey model is used for gas relative permeability
- An active fracture model is used to represent the effect of non-flowing fractures

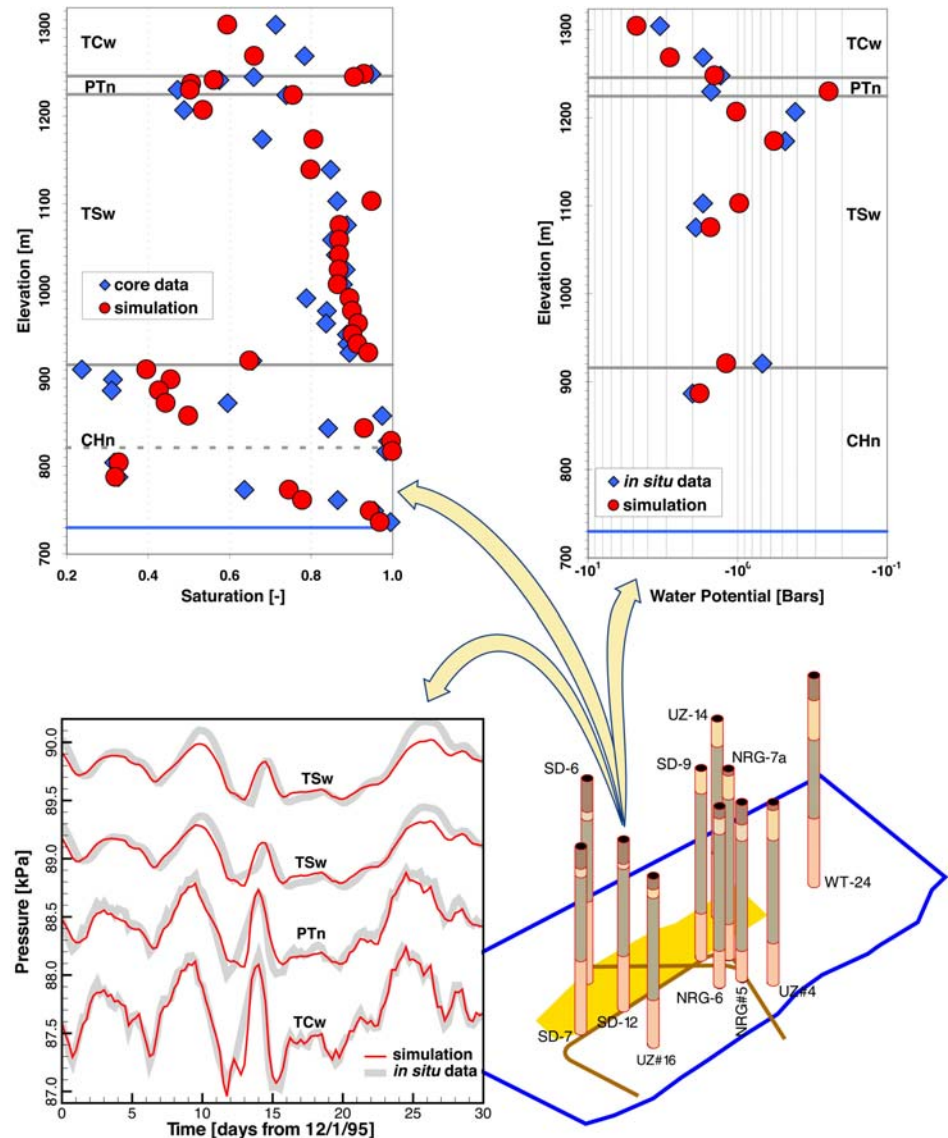


# Calibrated Properties Model

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## Results

- Simulated and measured saturation, water potential, and pneumatic pressure match well
- Calibrated hydrologic parameters and uncalibrated thermal parameters are validated against data not used for estimation and calibration
- iTOUGH2 code rigorously treats parameter sensitivities and uncertainties



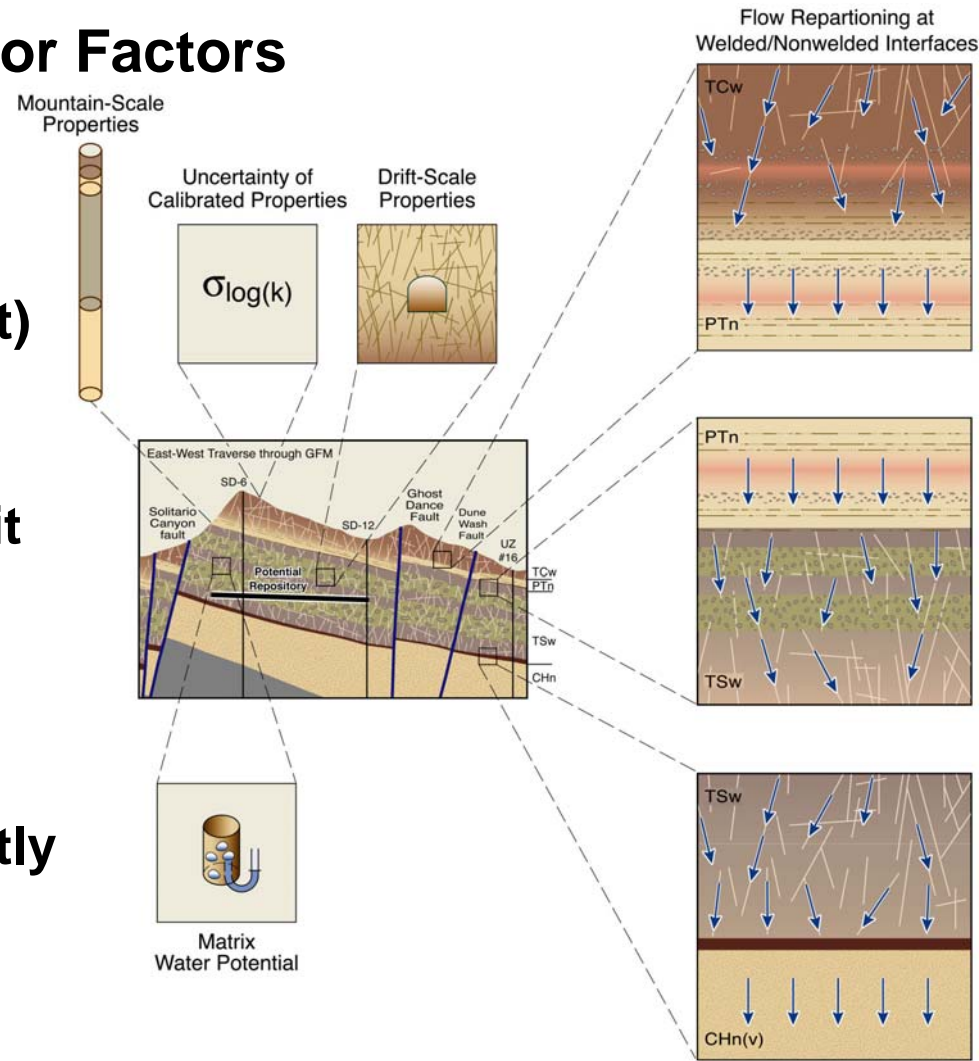
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# Calibrated Properties Model

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## Conservatism/Optimism and Major Factors

- Continuous fracture pathways are assumed to exist from the mountain surface to the water table (conservative for transport)
- Calibrated parameters are controlled by limited dates especially in the Calico Hills unit
- At major hydrogeologic unit interfaces (e.g. TCw to PTn), calibrated parameters are controlled by the assumption of flow transition from dominantly fracture to dominantly matrix (or vice-versa)



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