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

Engineered Barrier System Supporting Models and Analyses for TSPA-SR

Presented to:
Nuclear Waste Technical Review Board

Presented by:
Dr. Ernest L. Hardin
Civilian Radioactive Waste Management System
Management and Operating Contractor

August 1, 2000

YUCCA MOUNTAIN PROJECT

Areas Addressed by EBS Models/Analyses

- **Temperature, Relative Humidity, and Seepage During the Thermal Period**
- **Water Composition During the Thermal Period**
- **Flow Modes and Types of Breaches in the Drip Shield/Waste Package**
- **EBS Radionuclide Transport**
- **Overview of TSPA Abstractions - In-Drift Environment**
- **Evaluation of Features, Events, & Processes (FEPs)**
  - **Condensation Under the Drip Shield**
  - **Rockfall**

(Not Discussed Here: *Microbial Effects, Introduced Materials, Ex-Container Produced Colloids*)

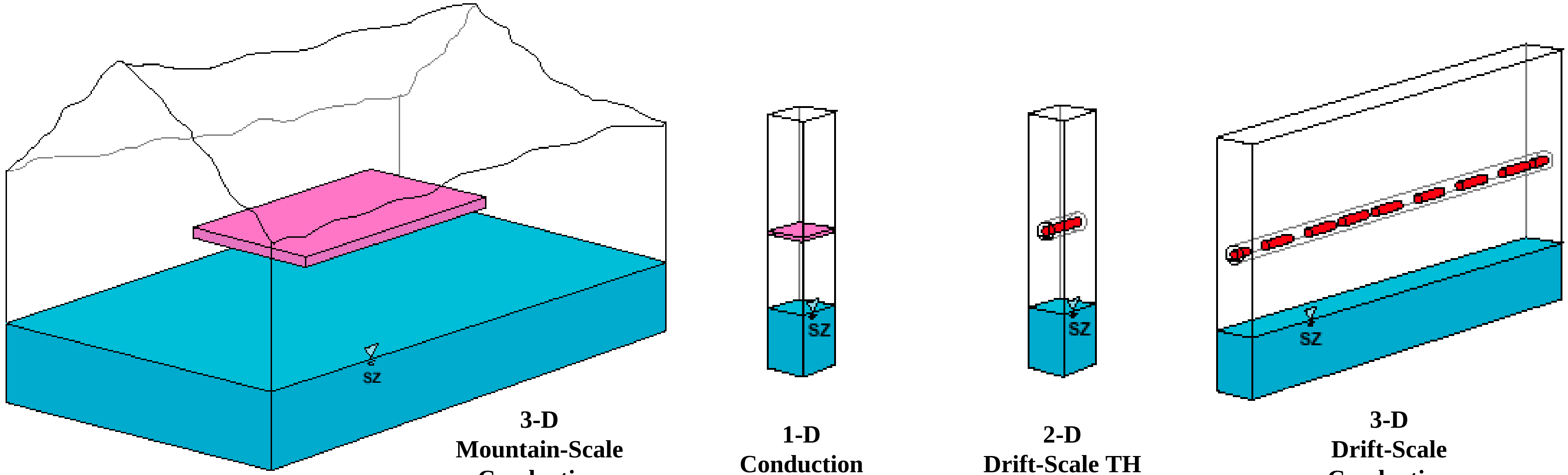
Process Model Factors Affecting Waste Package Lifetime- Engineered Barrier System Environments

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Waste Package Lifetime	In-Drift Physical and Chemical Environments	• Rock volume and mass distribution • Temperature and RH on the drip shield and waste package surface – f (multiple locations, waste type, time, climate) • Fugacity of CO_2 • pH – f (region, time) • Chloride – f (region, time) • Mass of microbes
	In-Drift Thermal-Hydrologic Environment	• Seepage flux through the drip shield • Fraction of drip shield and waste package surface that is wet

Process Model Factors Affecting Radionuclide Release From the Engineered Barriers

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Radionuclide Mobilization and Release from the Engineered Barrier System	In Package Environments	• pH – f (region, time) • Total dissolved carbonate (CO_3^{2}) – f (region, time) • Oxygen fugacity – f (region, time) • Ionic strength – f (region, time) • Fluoride – f(region, time) • CO_2 fugacity • Volume of water in the waste package/waste form cell
	Cladding Degradation and Performance	• Fraction of surface area of Zircaloy-clad CSNF exposed as a function of time
	CSNF Degradation and Performance	• CSNF intrinsic dissolution rate
	DSNF Degradation and Performance	• DSNF intrinsic dissolution rate
	HLW Degradation and Performance	• HLW intrinsic dissolution rate • Specific surface area
	Dissolved Radionuclide Concentration	• Concentration limits (solubilities) for all isotopes
	Colloid-Associated Radionuclide Concentrations	• Types of waste form colloids • Concentration of colloids • K_d and/or K_c for various colloid types • Fraction of inventory that travels as irreversibly attached onto colloids
	In-Package Radionuclide Transport	• Porosity of corrosion products – f (time) • Saturation of corrosion products – f (time) • Evaporation – f (temperature, relative humidity, composition)
	EBS (Invert) Degradation and Performance	• Thermally perturbed saturation in the invert – f (waste type, region, time, climate) • Porosity of the invert • Diffusion coefficient • Volumetric flux through the invert – f (climate, time) • Saturation in the invert after thermal pulse – f (time)

Multiscale Thermal-Hydrology (TH) Model



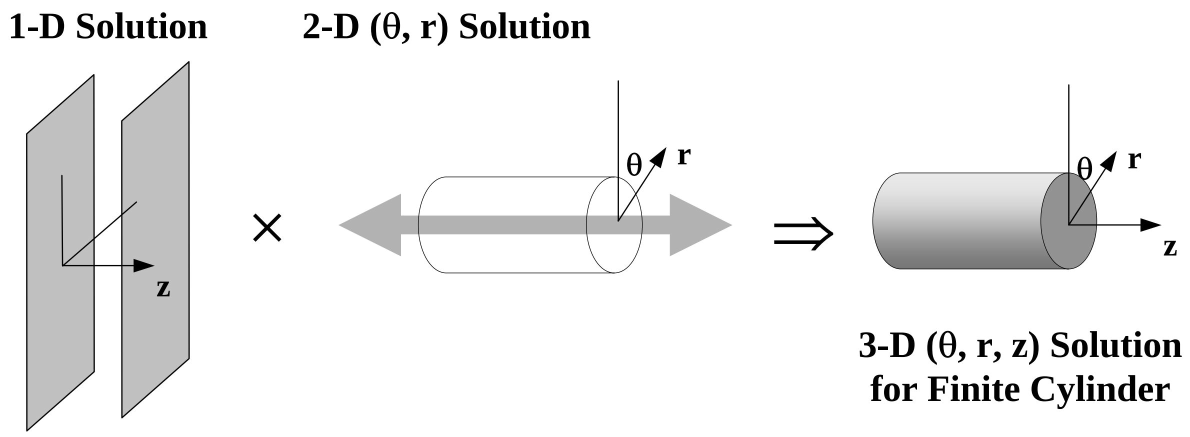
3-D Mountain-Scale Conduction (DDT) Model

1-D Conduction (SDT) Model

2-D Drift-Scale TH (LDTH) Model

3-D Drift-Scale Conduction (DDT) Model

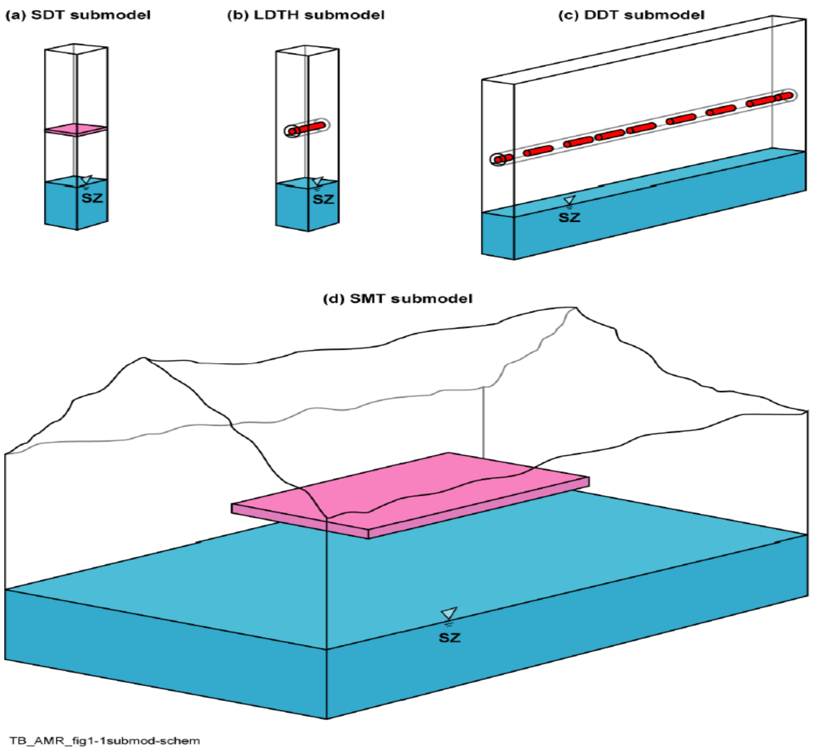
Models are Combined in a Manner Analogous to a Product Solution in Heat Conduction Theory:



T & RH at the Drip Shield and Waste Package

Multiscale Thermal-Hydrology (TH) Model Methodology

- Represent 3-D Heat Flow at Mountain Scale and Drift-Scale
- Radiative Coupling of Waste Package and Drip Shield
- Hydrologic Effects are Limited to 2-D in TSPA-SR Model

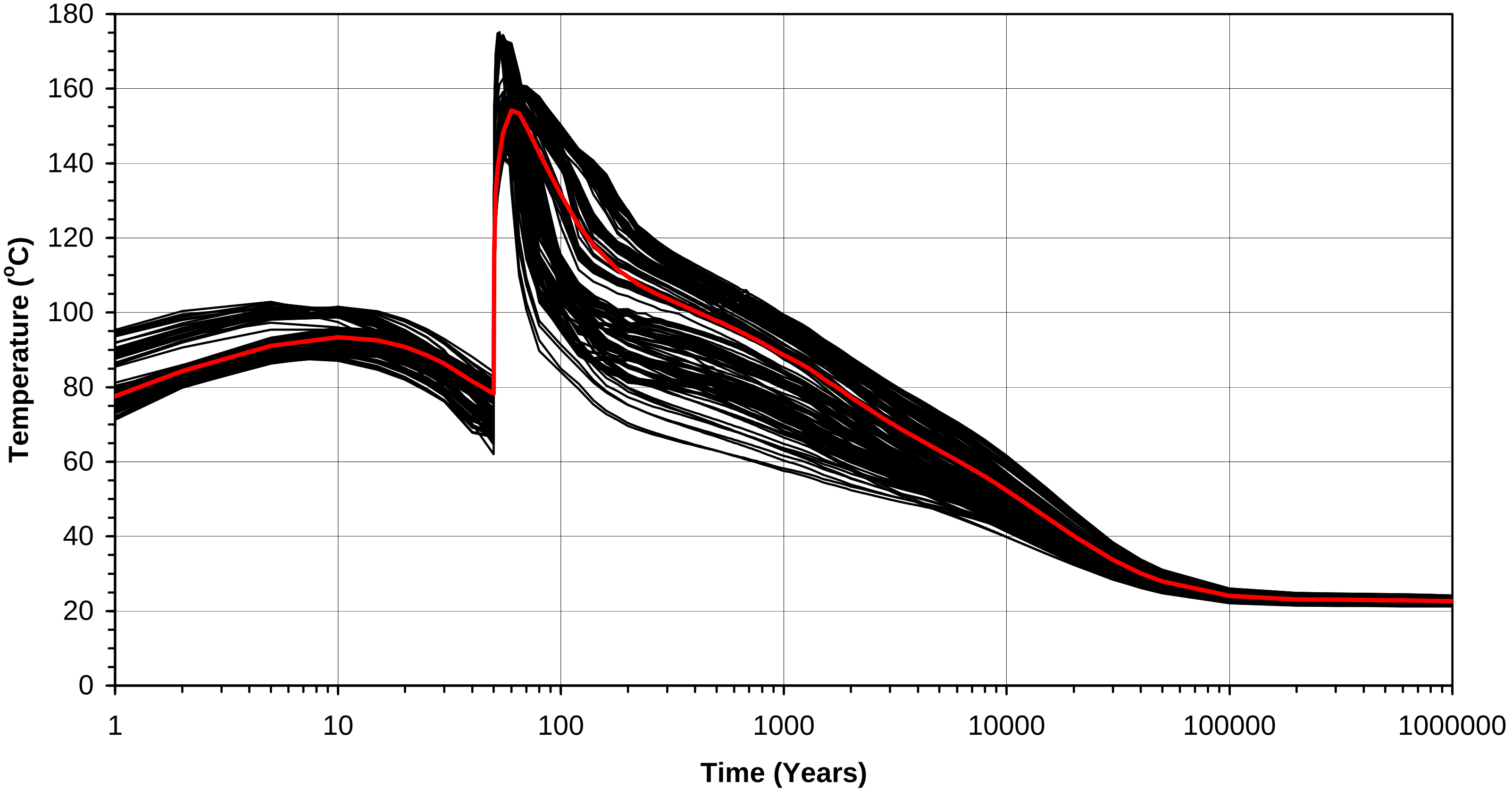


Source: Multiscale Thermohydrologic Model AMR (ANL-EBS-MD-000049 REV 00)

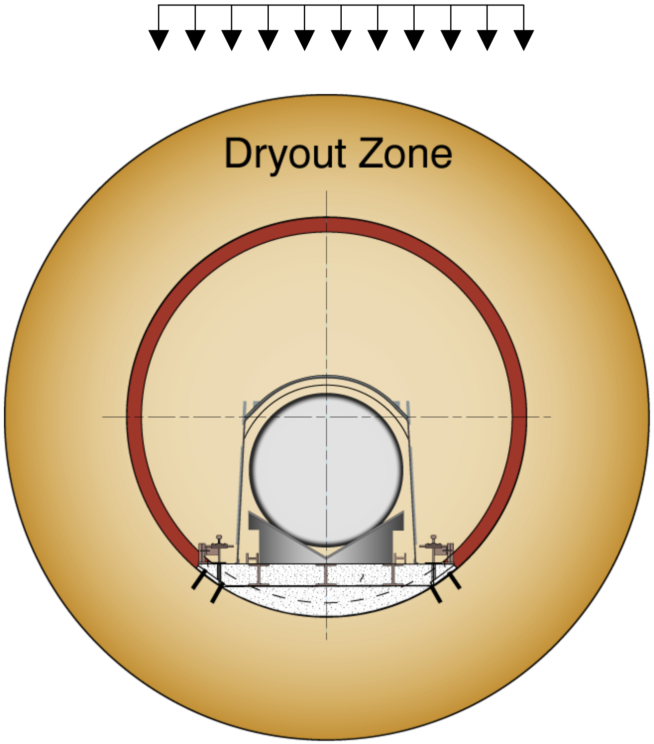
Example Multiscale TH Calculations

Average Surface Temperature of Waste Packages (No-Backfill, Mean Infiltration Case)

170 Locations With Infiltration in the Range 10 to 20 mm/yr
(610 Locations Represent the Repository Layout)



Abstraction of Thermally Perturbed Seepage

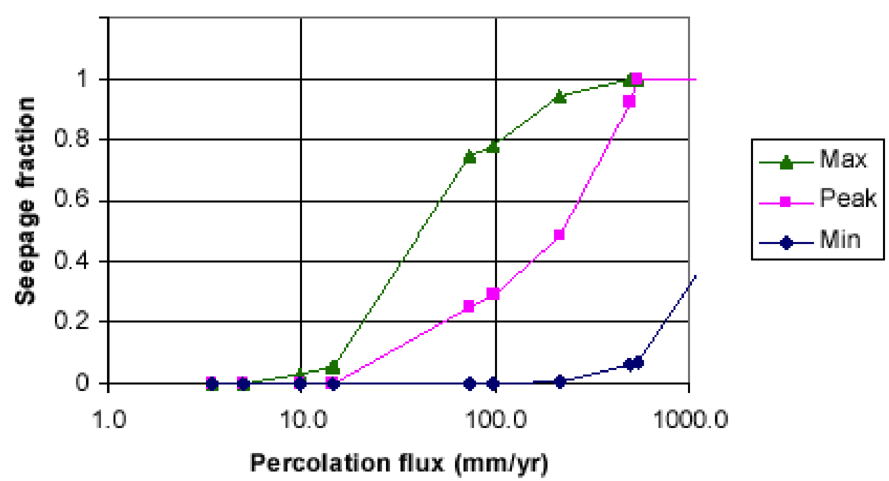


EBS Schematic
Cross-Section View

Multiscale TH Model Prediction
Liquid Flux 5 m Above the Emplacement Drift Opening

Seepage Fraction vs. Percolation

Source: Figure 2 of Drift Seepage Abstraction AMR (ANL-NBS-MD-000005 Rev. 00)

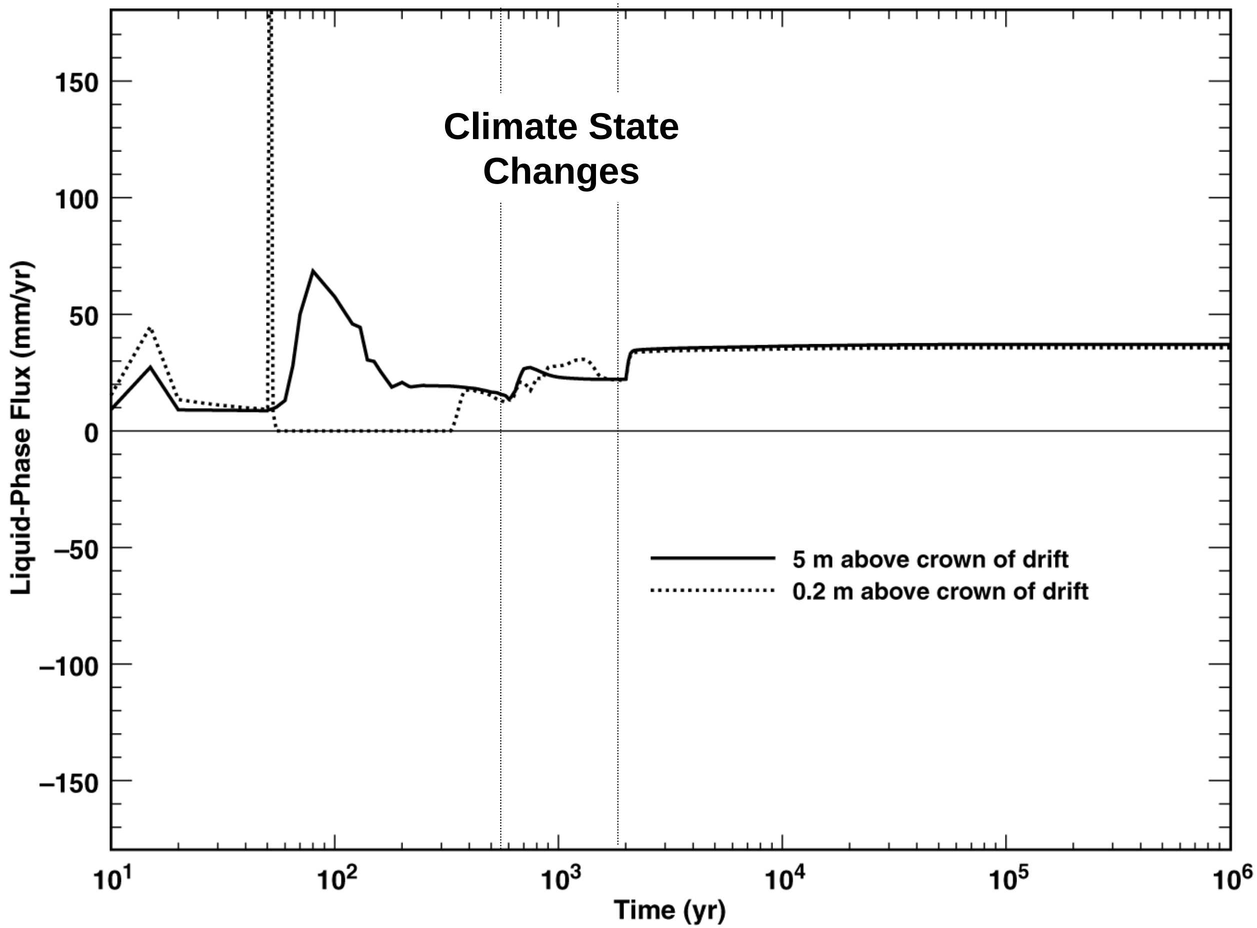


"Seepage fraction" = Proportion of WP locations that will be exposed to seepage.

Thermally Perturbed Seepage
(continued)

- **Thermally Elevated Liquid Flux in the Host Rock Yields Higher Seepage Than Ambient**
  - **All locations/cases: Flux ranges from 40 to 120 mm/yr (with additional WP-to-WP variability)**
  - **(Ambient percolation flux ranges from 0.7 to 38 mm/yr, at 31 model locations through the repository, in this time period)**
- **Approach Does Not Incorporate**
  - **Dryout within 5 meters of drift openings**
  - **Potentially *greater* flux closer to drifts**
- **Thermally Perturbed Seepage Will Be Insignificant After 600 yr**
- **Dose-Rate TSPA Impact Would Require WP *and* DS Failures**

Thermally Perturbed Seepage
(continued)

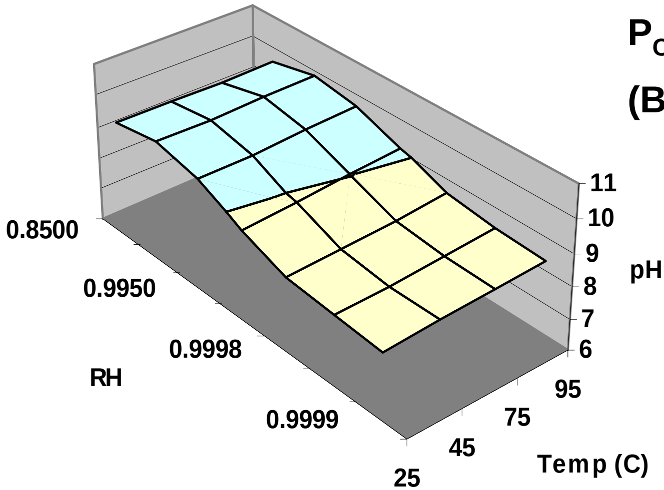


Liquid Flux at the Indicated Positions Above the Drift Crown Center of Repository Layout; Mean Infiltration Case
(Source: Figure 3-18 of NFE PMR Rev. 00)

Modeling Water Composition vs. T & RH

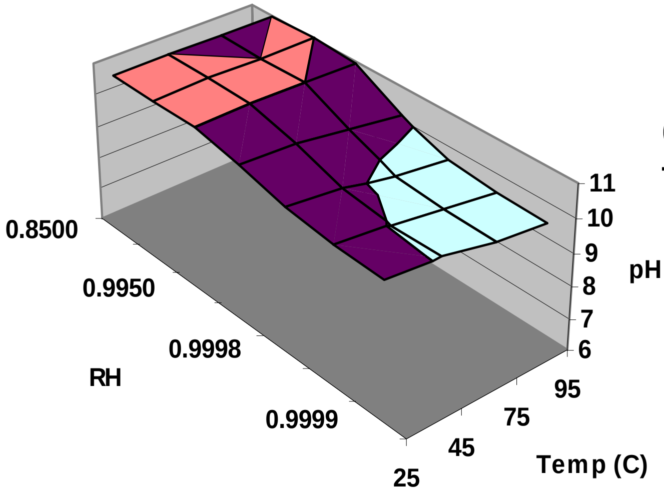
- **Available Chemical Models Dictate Approach**
  - **Empirical Approach (for RH from 50 to 85%)**
    - **Supported by laboratory evaporation tests**
  - **Pitzer Formulation (for RH > ~85% RH)**
    - **Supported by tabulated solubility data**
  - **Debye-Huckel Type Models (for RH > 98%)**
    - **Supported by laboratory evaporation tests**
- **Chemical Parameters for TSPA: pH, Ionic Strength, & Chloride Conc., Over Ranges of T, RH, & P_{CO2}**
- **Includes RH Effect (No Seepage) and Evaporative Concentration (Seepage)**

Modeling Water Composition vs. T & RH



P_{CO2} = 10^{-3} atm

(Background)



P_{CO2} = 10^{-6} atm

(Decreased by thermal effect)

Evolution of Sodium-Bicarbonate (J-13) Water From RH 85% to 99+%

Example Results from Approximate Pitzer Model (EQ3/6 with PT4 Database)

Colors Correspond to Integer Values of pH

Source DTN MO9912SPAISP45.004

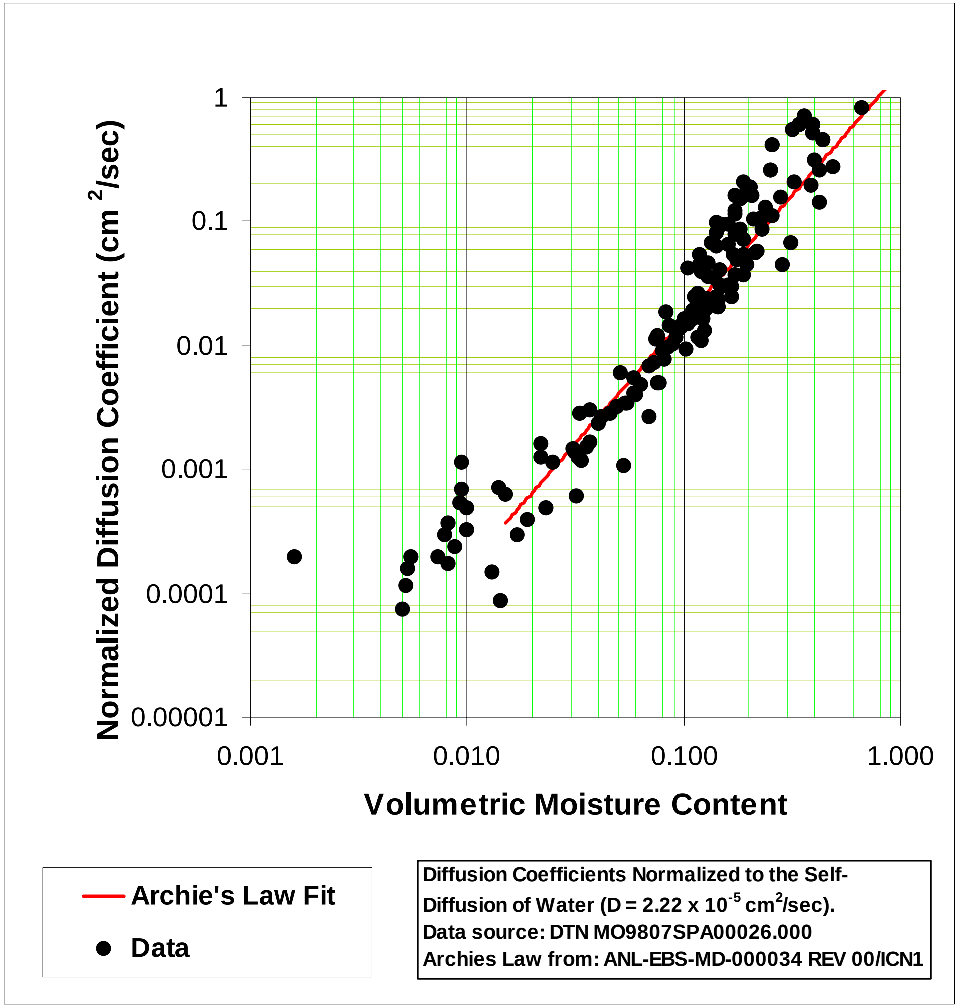
Flow Modes and Types of Breaches

- **Occurrence of Water in the EBS:**
  - **Thin films of moisture on surfaces**
  - **Capillary/droplet flow from condensation or dripping seepage**
- **Types of Breaches**
  - **Stress Corrosion Cracks (WP):**
    - **Advective liquid flow will be negligible, but water vapor movement and radionuclide diffusion can occur through cracks**
  - **General Corrosion (WP and DS):**
    - **Capillary/droplet flow through "patches"**

EBS Transport Model

"Diffusion Barrier"

- **1-D Flow Paths**
  - **WP Surface to Host Rock, Through Invert Ballast**
  - **Use When Advective Flow is Negligible**
- **Colloid-Facilitated Radionuclide Transport**
  - **Advection and Diffusion**
  - **(Waste Form Colloid Source Term)**



Chemical Processes Considered

- **Included in TSPA:**
  - **Gas-Water Interaction (CO_2)**
  - **Evaporation/Condensation of Water**
  - **Precipitation/Dissolution of Salts**
  - **Colloid-Water Interactions**
  - **Advective-Diffusive Radionuclide Transport**
- **Excluded Influences on Bulk Chemical Environment (Low Consequence):**
  - **Microbial Effects**
  - **Cement-Water Interactions**
  - **Corrosion Products**

Inputs to TSPA from TH, THC, & Seepage Models Used in Assessment of the Nominal Scenario

Multiscale Model:

Percolation Flux

Temperature

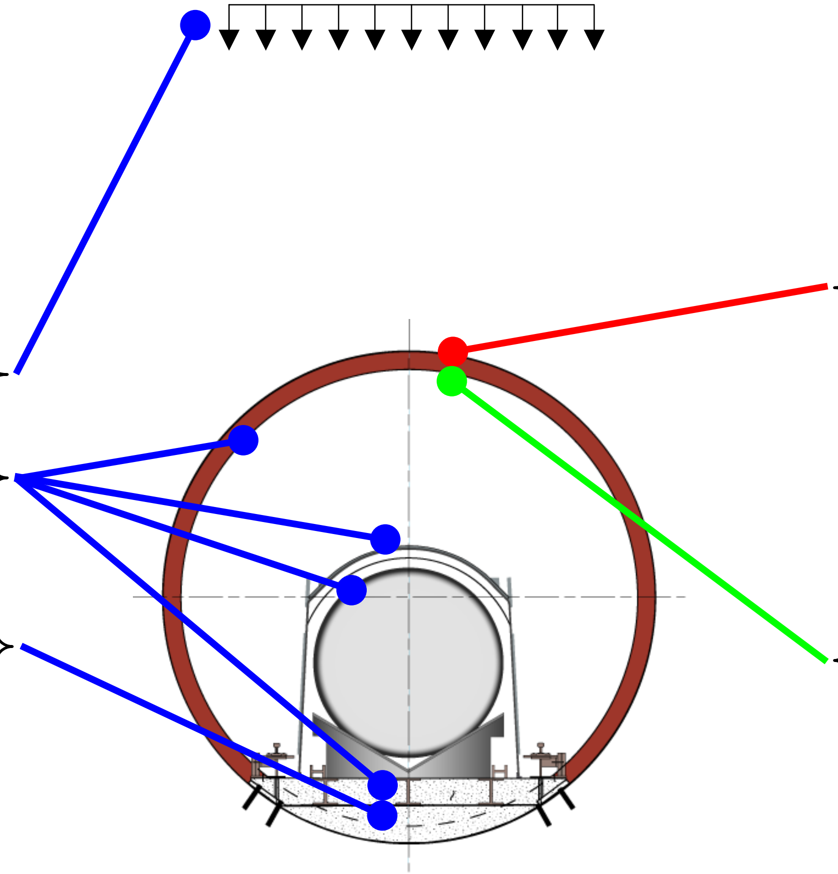
Relative Humidity

Flux

Liquid Saturation

Evaporation Rate

(610 Locations;
EBS PMR)



Seepage Model:

Seepage Rate vs.
Percolation Flux

(UZ PMR)

THC Model:

Incoming Water
Composition

Gas Composition

(UZ PMR)

TH, THC, and Seepage Abstractions

(continued)

Improvements to In-Drift Chemical Environment Abstractions (Nominal Scenario)

- Aqueous Solution Chemistry
  - Pitzer approach
- Colloids Model
  - New data for WF colloids
  - Ionic strength effect
- Transport Model
  - Improved invert diffusion model

Condensation Under the Drip Shield (FEPs)

Approach:
Use NUFT (porous medium simulator; radiative coupling)

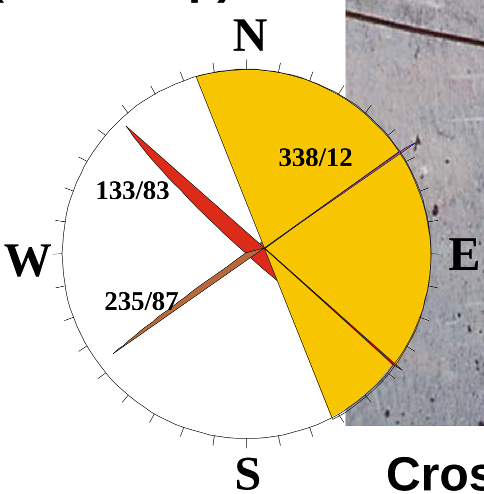
Compare to Analytical Solution; Develop Pseudo Properties for Air

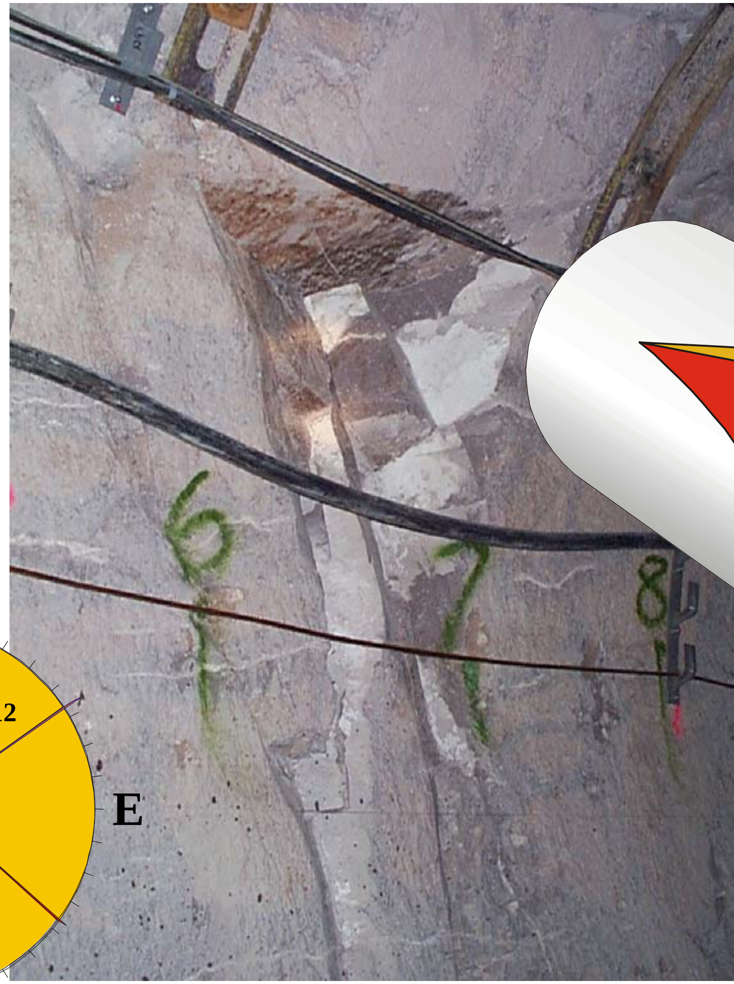
Perform TH Simulations (Range of Infiltration Rates)

Results Applied to TSPA:
- **Condition for condensation under DS: elevated invert saturation associated with liquid water influx**
- **Condensation will become increasingly unlikely as thermal output decays**
- **(Condensate would have no impact on corrosion)**

Key Block Occurrence at Yucca Mountain (FEPs)

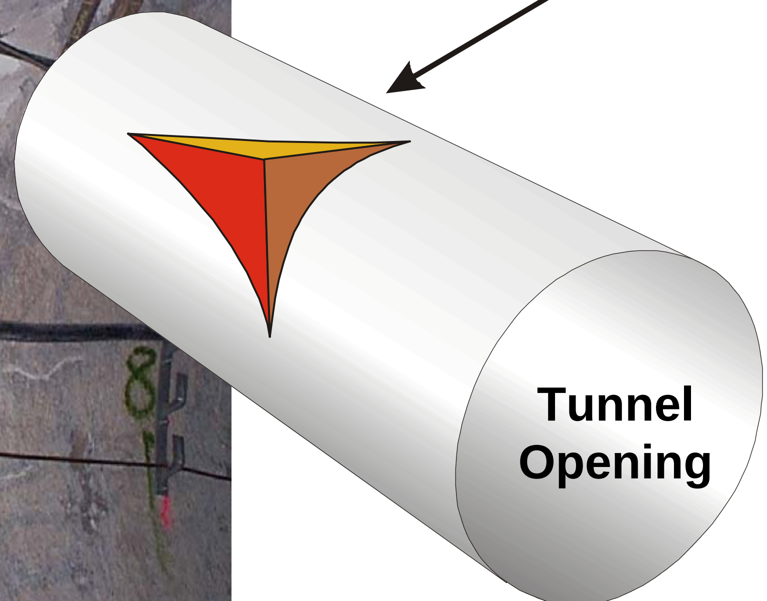
Stereographic Projection of Key-Block Forming Fracture Planes (strike/dip)





Cross Drift Station 11+55 m

Key Block Formed by the Intersection of the Opening with Three Fracture Planes

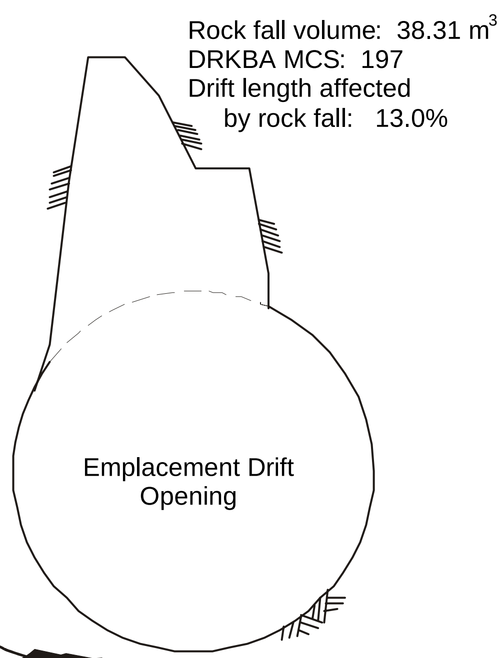


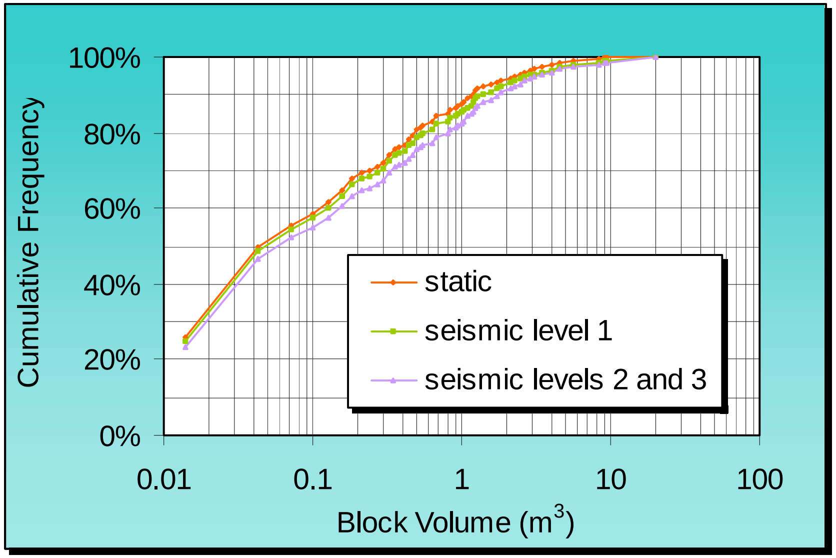
Rockfall FEPs:
- **Include for Seepage**
- **Exclude for Damage to DS & WP**

Probabilistic Rockfall Analysis Contribution to Design

- **Output**
  - **Maximum size key blocks**
  - **Number of potential key blocks**
  - **Distribution of block sizes**
  - **Stability of key blocks**
  - **Progressive block failure / final drift profile**

Lithologoic Zone	Percent Length of Drift in Lithologic Zone	Number of Key Blocks per Kilometer: Static	Static Plus Seismic: Level 1 (1,000-yr)	Level 2 (5,000-yr)	Level 3 (10,000-yr)
Tptpul	0%	15	15	17	17
Tptpmn	7%	37	38	40	40
Tptpll	78%	3	3	3	3
Tptpln	15%	3	3	5	5

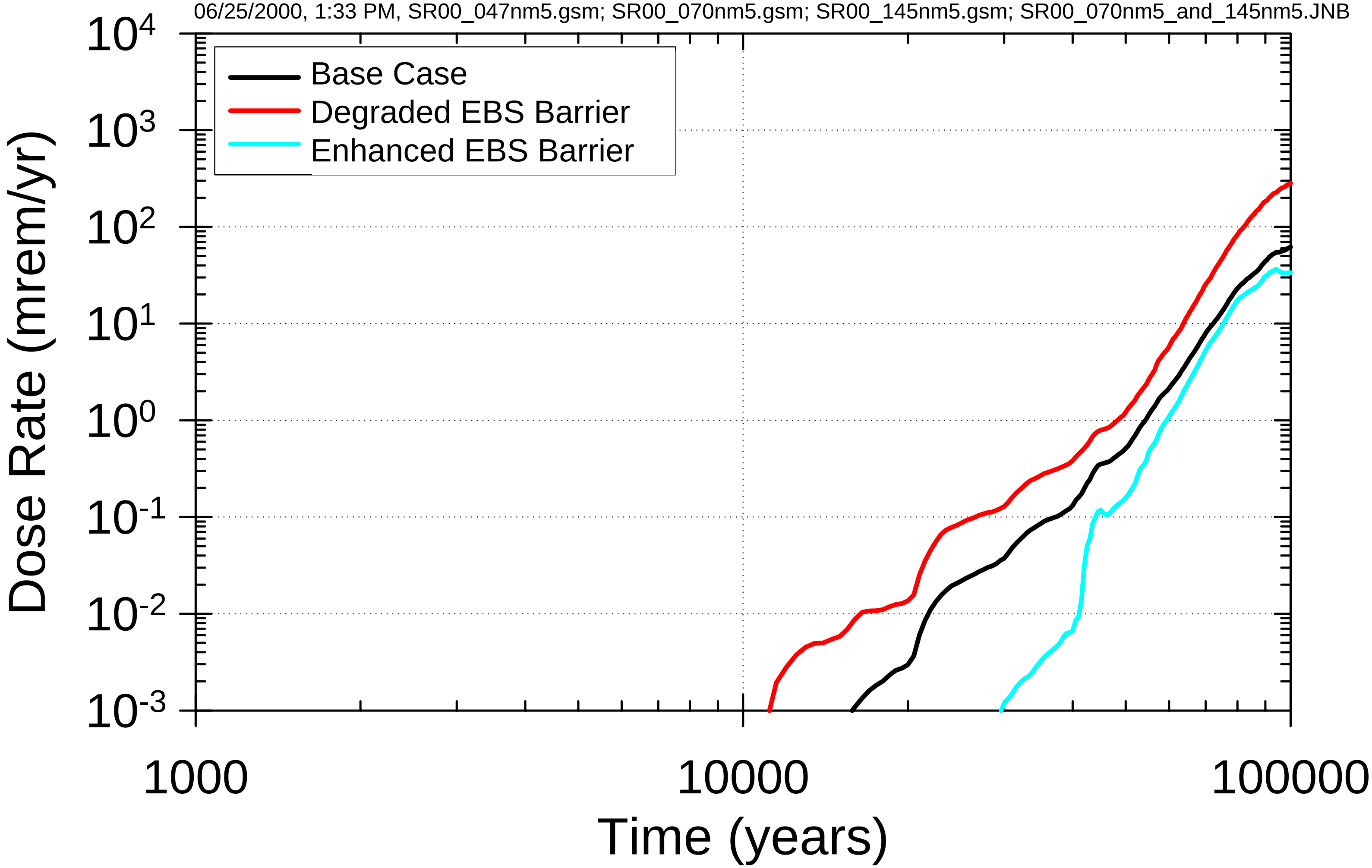




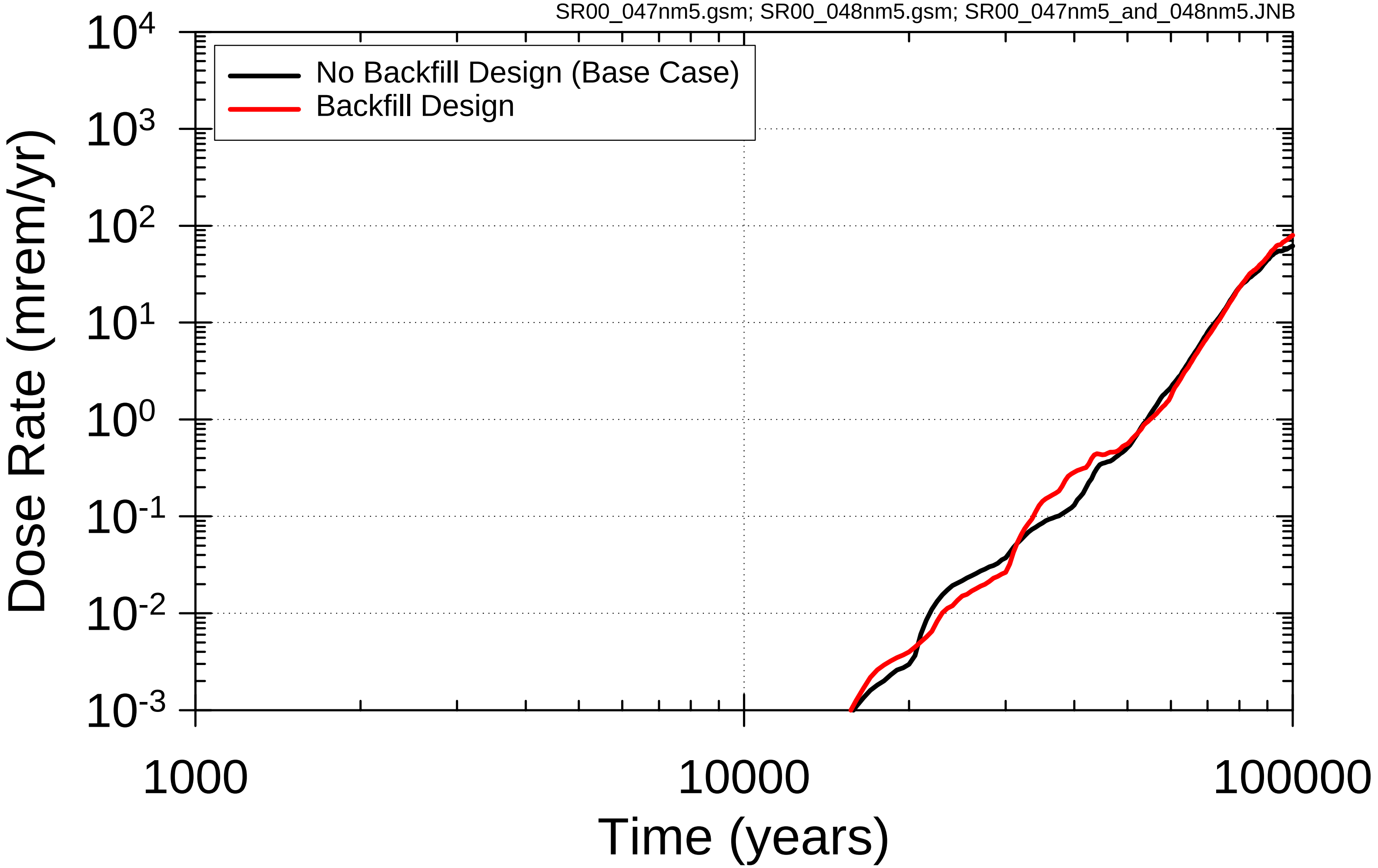
EBS Transport Barrier Sensitivity

- **Degraded Barrier**
  - **High Diffusion Model, $D_{inv} \sim \phi S$ (Base Case diffusion model uses $D_{inv} \sim \phi^{1.3} S^{1.85}$)**
  - **Degraded Concentration Limits Model**
    - **95th %tile solubilities,**
    - **Use WP chemistry in invert**
    - **maximum colloid stability**
    - **95th %tile K_d for sorption onto colloids**
- **Enhanced Barrier**
  - **Low Diffusion Model, $D_{inv} = 10^{-11}$ cm^2/sec**
  - **Enhanced Concentration Limits Model**
    - **5th %tile solubilities,**
    - **Use invert chemistry in invert**
    - **minimum colloid stability**
    - **5th %tile K_d for sorption onto colloids**

Preliminary
EBS Transport Barrier Sensitivity



Preliminary
Backfill Sensitivity



This information was prepared for the 8/00 NWTRB meeting for illustrative purposes only and is subject to revision; not appropriate for assessing regulatory compliance.

Summary of Major Points

- T & RH are Principal Variables That Depend Mainly on Location and Percolation Flux
  - Uncertainty and Variability are Represented
- In-Drift Models Quantify Water Composition at the DS, WP, Waste Form, and Invert
  - Combining TH, THC, and Seepage Inputs
- Water Compositions Will Vary from Brines to Dilute Waters, and Will Be Temporally and Spatially Heterogeneous
  - Bounding Compositions Are Identified