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

Engineered Barrier System Environments-Thermal Hydrology & Near-Field Host Rock Chemical Environment

Presented to:
NRC/DOE Technical Exchange on Total System Performance Assessment (TSPA) for Yucca Mountain
San Antonio, Texas

Presented by:
Nicholas D. Francis
Performance Assessment Department
CRWMS M&O/Sandia National Laboratories

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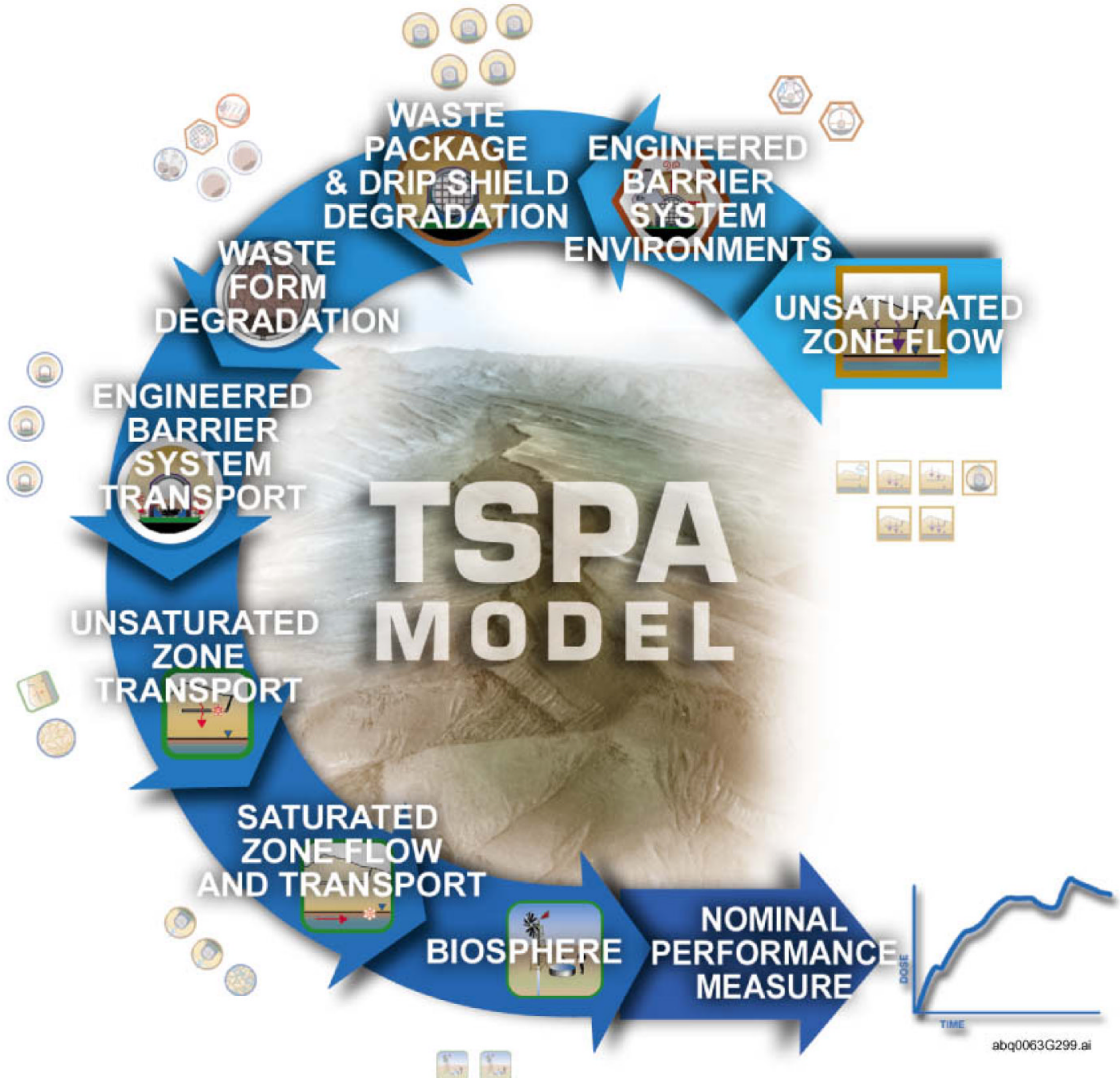
YUCCA MOUNTAIN PROJECT

TSPA-SR Nominal Scenario



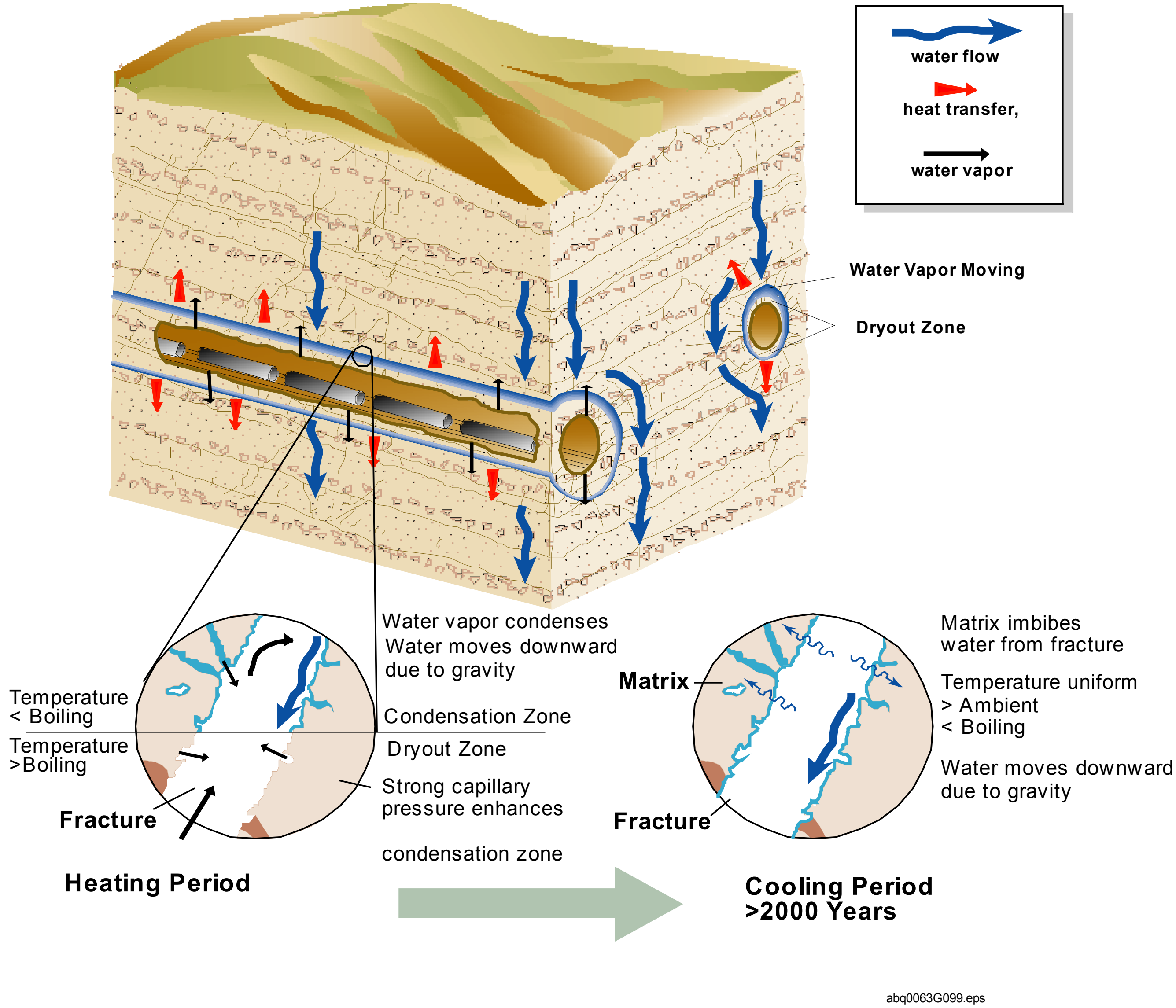
Key Technical Issues

- Relevant Integrated Subissues from the Total System Performance Assessment and Integration Issue Resolution Status Report Rev. 2 include:
  - Quantity and Chemistry of Water Contacting Waste Packages and Waste Form
- Other relevant acceptance criteria may be found in the following Issue Resolution Status Reports:
  - Thermal Effects on Flow
  - Evolution of the Near-Field Environment
- The Engineered Barrier System Degradation, Flow, and Transport Process Model Report (PMR) and Near-Field Environment PMR address acceptance criteria related to this topic and will be discussed at a Technical Exchange scheduled for September 7, 2000.

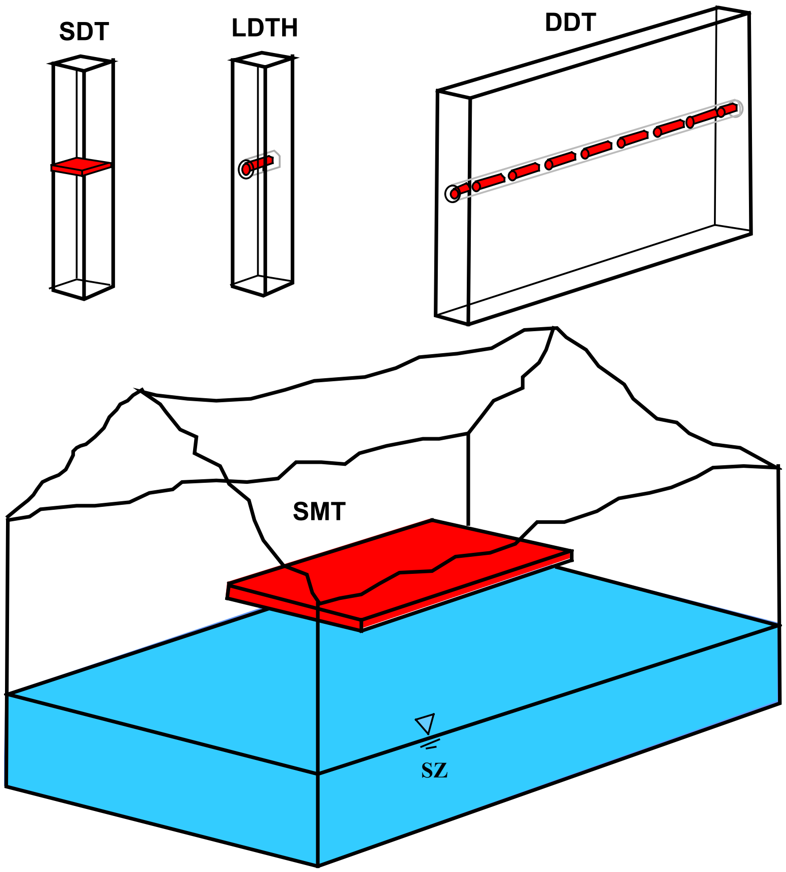
TSPA-SR Nominal Scenario

- **Primary Attributes of Repository Performance Addressed in Engineered Barrier System Environment**
  - Water Contacting Waste Package
    - Percolation Flux Affected by Thermal-Hydrological (TH) Process
    - Seepage Composition Affected by Thermal-Hydrological-Chemical (THC) Process
  - Waste Package Lifetime
    - Temperature and Relative Humidity on Drip Shield and Waste Package
    - Evaporation Rate at Drip Shield and in Invert
    - Volume Flow of Water at Drip Shield and in Invert

Conceptualization



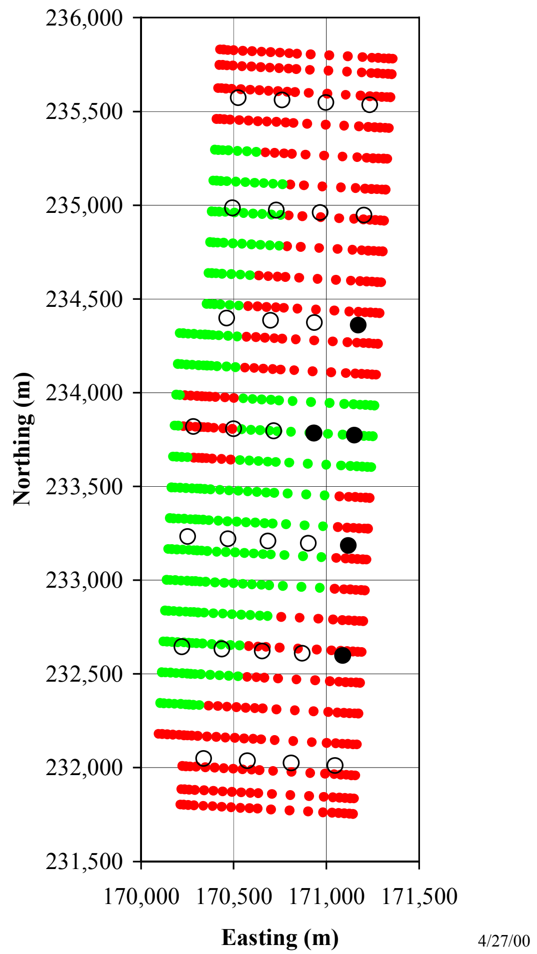
Multiscale TH Model Components



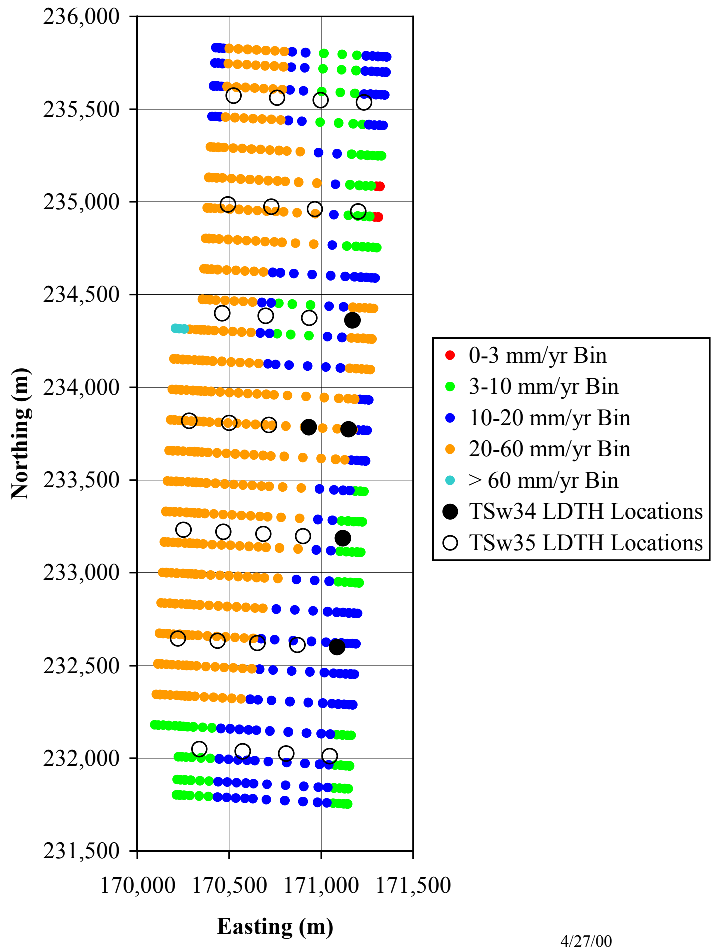
SDT =	**Smeared-Heat-Source Drift-Scale Thermal-Conduction Submodel**
LDTH =	**Line-Averaged-Heat-Source Drift-Scale Thermal Hydrologic Submodel**
DDT =	**Discrete-Heat-Source Drift-Scale Thermal-Conduction Submodel**
SMT =	**Smeared-Heat-Source Mountain-Scale Thermal-Conduction Submodel**

TSPA-SR Abstraction-TH

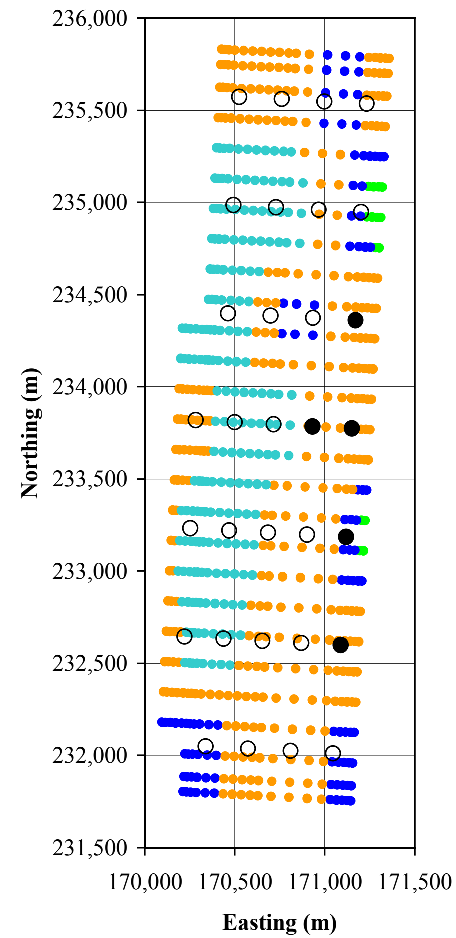
610 Low Glacial Infiltration Bin Locations



610 Medium Glacial Infiltration Bin Locations

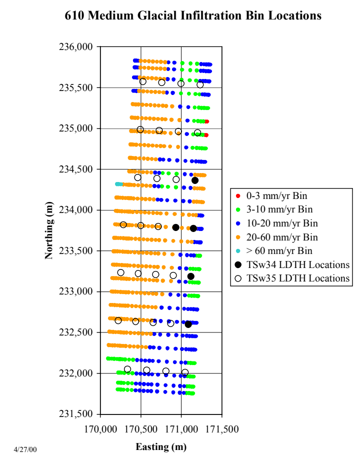


610 High Glacial Infiltration Bin Locations



TSPA-SR Abstraction-TH (continued)

- **610 Location Dependent Results Abstracted Directly from the Multiscale TH Model**
  - **Temperature and Relative Humidity at**
    - **Drip Shield**
    - **Waste Package**
  - **Percolation Flux Above the Crown**



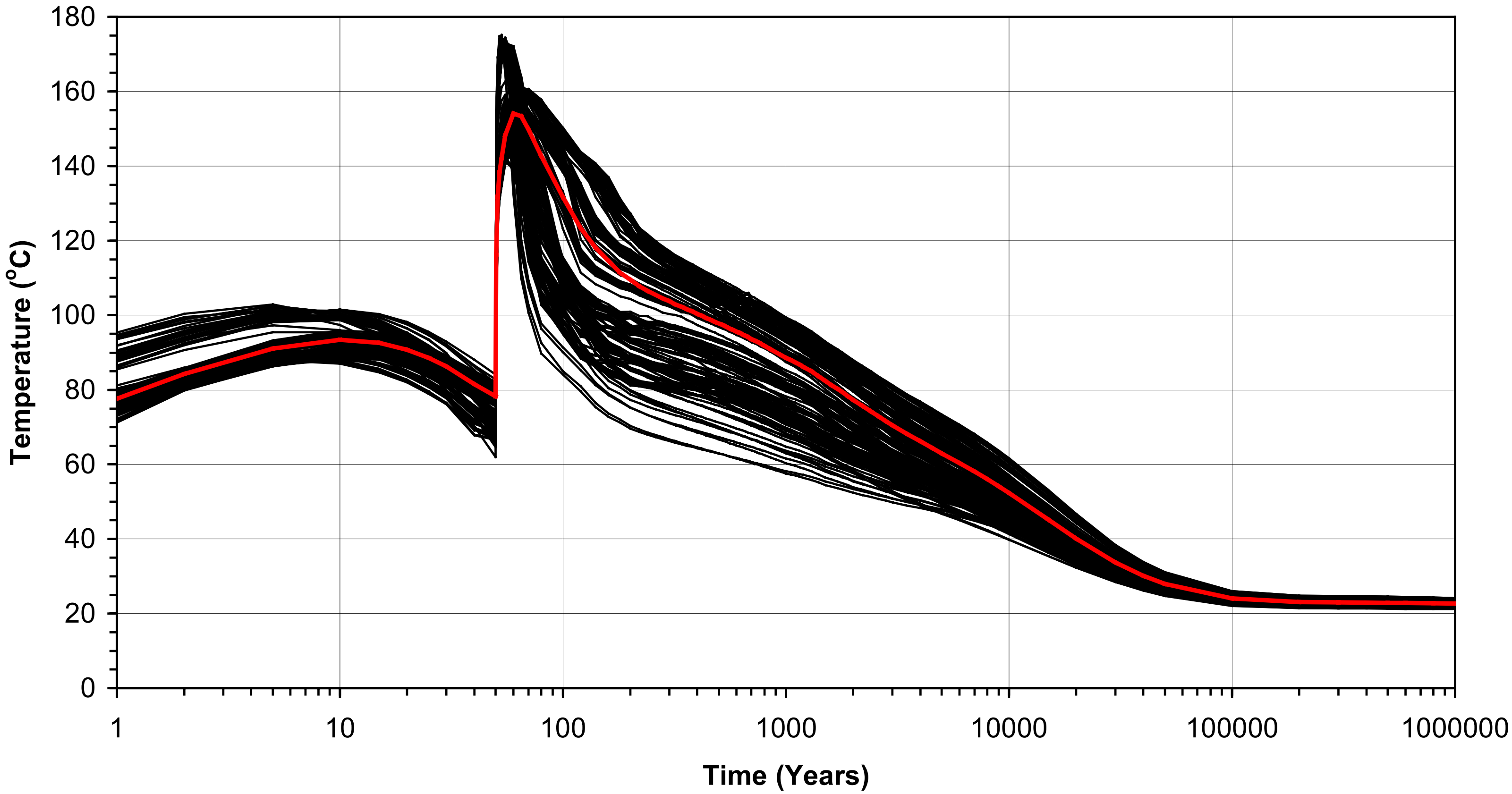
- **TH Process Model Features**
  - **Repository Edge and Center Proximity**
  - **Infiltration Rate Variability and Uncertainty**
  - **Two Future Climate States**
  - **Repository Design without Backfill**

TSPA-SR Abstraction-TH (continued)

- **Infiltration Rate Bin Averaged Results Computed from the Multiscale TH Model Results**
  - Temperature and Relative Humidity at
    - Drift Wall
    - Drip Shield
    - Waste Package
    - Invert
  - Water Flow Rate and Evaporation Rate
    - Invert
  - Infiltration Bin Maximum Waste Package Temperature (not an average)
  - Liquid Saturation in Invert

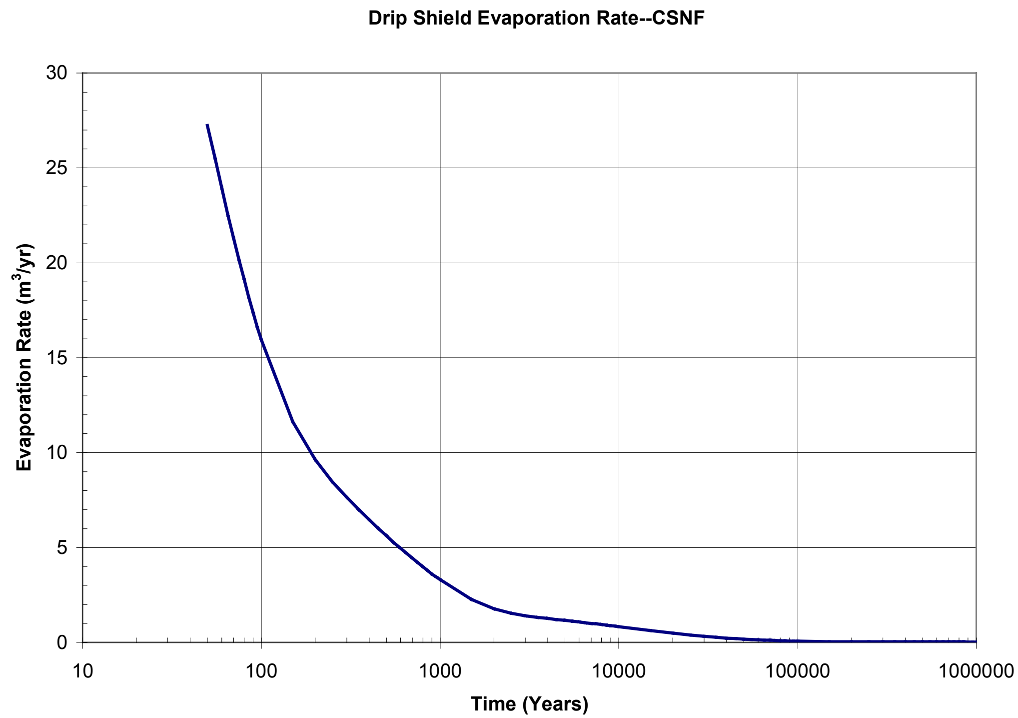
TSPA-SR Abstraction-TH
(continued)

Waste Package Surface Temperature
No Backfill, Medium Infiltration Flux Case
Infiltration Rate Bin 10 to 20 mm/yr
(170 of 610)



TSPA-SR Abstraction-TH
(continued)

- **Heat Balance Applied at the Drip Shield Upper Surface to Determine Maximum Potential Seepage Water Evaporation Rate**
  - **Average commercial spent nuclear fuel (CSNF)**
  - **Average high level waste**



Coupled Thermal Chemical Effects on Water Composition

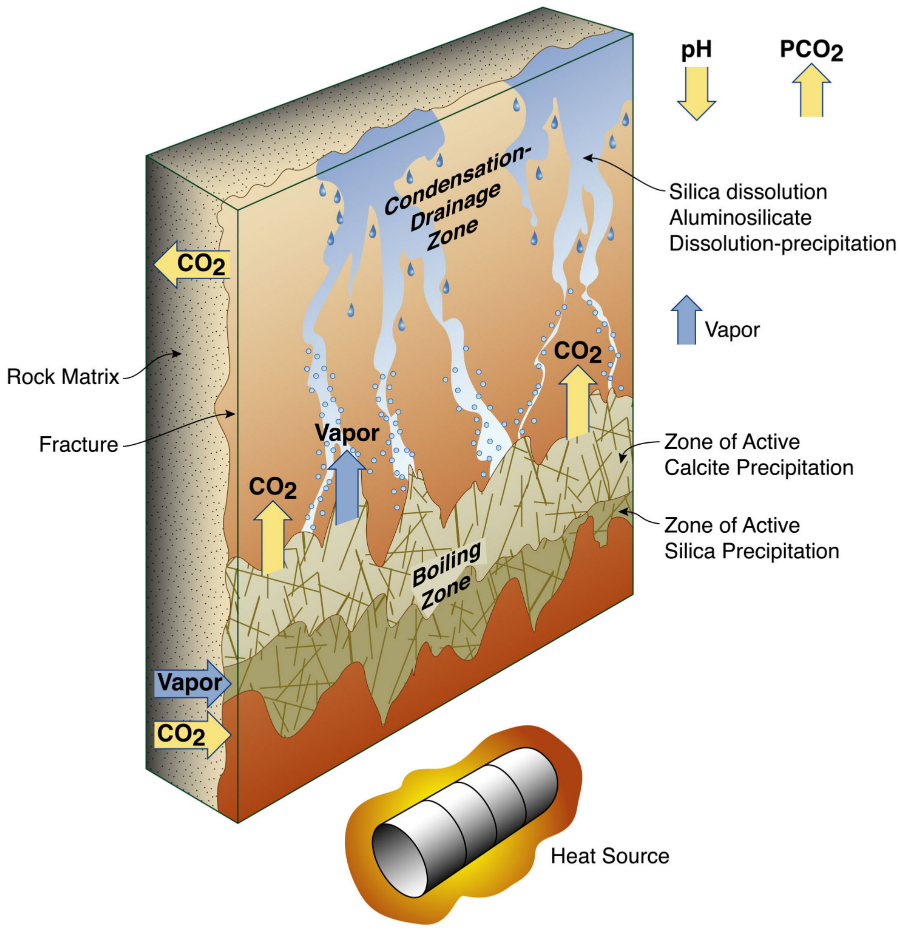


Diagram Showing THC Processes

- 2-D Drift-Scale Coupled THC Model
  - Low, Medium, High Flux Cases
- Incoming Water and Gas Composition Derived from Coupled THC Model at the Drift Wall for a Range of Infiltration Rates
- Aqueous Chemical Attributes Include pH, HCO^-_3, and Cl^-
- Gas Composition Considers CO_2

Coupled Thermal Chemical Effects on Water Composition (continued)

Aqueous Species	Gaseous Species	Minerals	
Both models:	Both models:	Both models:	
H^+	CO_2	Calcite	Amorphous Silica
Ca^{+2}		Tridymite	Gypsum
Na^+		α–Cristobalite	Glass
H_2O		Quartz	
SiO_2		Complex model only:	
Cl^-		Hematite	K-Smectite
HCO_3^-		Fluorite	Illite
SO_4^{-2}		Goethite	Kaolinite
Complex model only:		Albite	Sepiolite
Mg^{+2}		Microcline	Stellerite
K^+		Anorthite	Heulandite
AlO_2^-		Ca-Smectite	Mordenite
$HFeO_2$		Mg-Smectite	Clinoptilolite
F^-		Na-Smectite	

Source: CRWMS M&O (2000, U0110, Tables 7, 8)

Coupled Thermal Chemical Effects on Water Composition (continued)

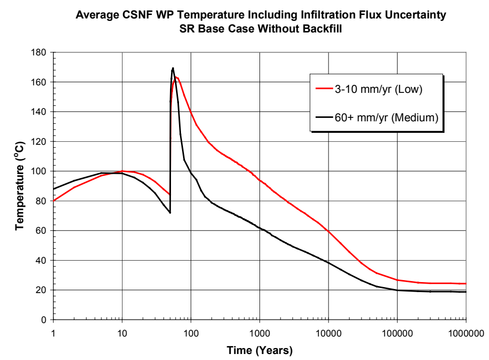
	Preclosure	Boiling	Transitional Cool-Down	Extended Cool-Down
	Period 1	Period 2	Period 3	Period 4
Parameter	**Abstracted Values**	**Abstracted Values**	**Abstracted Values**	**Abstracted Values**
Time	**0 - 50 years**	**50 - 1000 years**	**1000 - 2000 years**	**2000 - 100,000 years**
Temperature, °C	80	96	90	50
log CO_2, vfrac	-2.8	-6.5	-3.0	-2.0
pH	8.2	8.1	7.8	7.3
Ca^{2+}, molal	1.7E-03	6.4E-04	1.0E-03	1.8E-03
Na^{+}, molal	3.0E-03	1.4E-03	2.6E-03	2.6E-03
SiO_2, molal	1.5E-03	1.5E-03	2.1E-03	1.2E-03
Cl^{-}, molal	3.7E-03	1.8E-03	3.2E-03	3.3E-03
HCO_3^{-}, molal	1.3E-03	1.9E-04	3.0E-04	2.1E-03
SO_4^{2-}, molal	1.3E-03	6.6E-04	1.2E-03	1.2E-03
Mg^{2+}, molal	4.0E-06	3.2E-07	1.6E-06	7.8E-06
K^{+}, molal	5.5E-05	8.5E-05	3.1E-04	1.0E-04
AlO_2^{-}, molal	1.0E-10	2.7E-07	6.8E-08	2.0E-09
$HFeO_2$, molal	1.1E-10	7.9E-10	4.1E-10	2.4E-11
F^{-}, molal	5.0E-05	2.5E-05	4.5E-05	4.5E-05

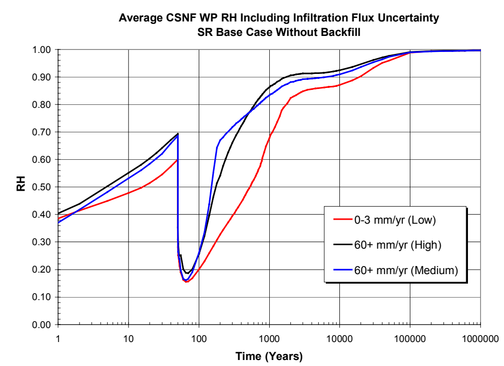
Comparison to TSPA-VA Models and Abstraction

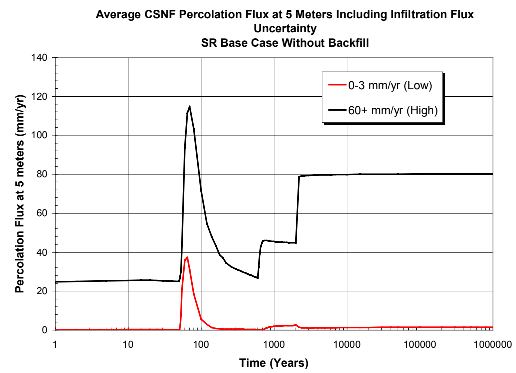
- **TH Abstraction**
  - Utilizes Infiltration Rate Binning Instead of Subregion Binning
    - 5 Infiltration Rate Bins Instead of 6 Subregion Bins
  - Provides More Spatial Resolution to TSPA
    - 610 Location Dependent Results Instead of 180 Maximum Possible Different Results
- **THC Abstraction**
  - Uses Host Rock Water and Gas Composition Obtained from a Fully Coupled Process-Level THC Model
    - Two Geochemical Systems Compared to Drift Scale Test results in order to consider alternative modeling approaches consistent with available data and current understanding
- **Process model comparison of near-field host rock flow and state variables between TH-only and fully coupled THC models**

Model and Abstraction Uncertainty

- **The TH and THC Model Uncertainty Included in the Abstraction of TH Data for the Near-Field Environment Component of TSPA is Specified by the UZ Flow and Transport Component of TSPA**
  - Ground Surface Infiltration Rates
    - Low, Medium, High
  - Fracture Hydrologic Properties
    - Low, Medium, High
  - Initiation of Future Climate States
    - Monsoonal (600 Years), Glacial-Transition (2000 Years)







Conclusions

- **TH and THC Abstractions Provide Direct Inputs to TSPA Models that Result in an Assessment of Attributes of Repository Performance**
  - Water Contacting Waste Package
  - Waste Package Lifetime
- **TSPA Models Applying TH and THC Abstractions**
  - Chemical Environments (EBS Environments Subcomponent)
  - Unsaturated Zone Flow
  - Waste Package and Drip Shield Degradation
  - Waste Form Degradation
  - Engineered Barrier System Transport

Conclusions

- **TH and THC Models and Abstractions Include**
  - Drift-Scale (TH and THC) and Mountain-Scale (TH only) Effects
  - Waste Package Variability (TH only)
  - Dual-Permeability (Active Fracture) Flow Model (TH and THC)
- **Model Confidence**
  - Thermal Properties from Lab Measurements
  - Comparison to ESF Thermal Tests and Large Block Test
    - Property Set Testing
    - Conceptual Model Validation

Conclusions
(continued)

- **Integration**
  - **Both Models (TH and THC) Apply:**
    - **Low Areal Mass Loading (AML) Repository Design Features Including Ventilation**
    - **Active Fracture Conceptual Flow Model to Ensure Fracture Flow During Heating**
    - **Identical Infiltration Flux Cases (Including Future Climate States)**
    - **Results of the Thermal Tests and LBT to Assess Conceptual Models**
  - **Abstractions Apply:**
    - **Methods that Maintain the Ranges of Results from the Process Models Through**
      - » **Direct use of Data**
      - » **Appropriate Averages Based on Data Fitting Similar Characteristics**

BACKUP

References

- **Multiscale Thermohydrologic Model**
  - **ANL-EBS-MD-000049**
- **Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux**
  - **ANL-EBS-HS-000003**
- **Drift-Scale Coupled Processes (DST and THC Seepage) Models**
  - **MDL-NBS-HS-000001**
- **Abstraction of Drift-Scale Coupled Processes**
  - **ANL-NBS-HS-000029**
- **Features, Events, and Processes in Thermal Hydrology and Coupled Processes**
  - **ANL-NBS-MD-000004**