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

Engineered Barrier System Coupled Process Components

Presented to:
Nuclear Waste Technical Review Board

Presented by:
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YUCCA MOUNTAIN PROJECT

Outline

- Overview of Engineered Barrier System (EBS) Environments
- EBS Process Components
  - Thermal-Hydrologic (TH) Environment
  - Chemical Environment
  - Flow and Transport
- Ongoing work
- Summary

Summary of Supplemental EBS Analyses

Key Attributes Of System	Process Model (Section of Yucca Mountain Science and Engineering Report [DOE, 2001])	Topic Of Supplemental Scientific Model Or Analysis	Reason For Supplemental Scientific Model Or Analysis			Section Of Vol. 1
			Unquantified Uncertainty Analysis	Update in Scientific Information	Cooler Thermal Operating Mode Analysis	
Long-Lived Waste Package and Drip Shield	Water Diversion Performance of EBS (4.2.3)	Multiscale thermal-hydrologic model, including effects of rock dryout	X		X T	5.3.1
		Thermal property sets	X	X	T	5.3.1
		Effect of in-drift convection on temperatures, humidities, invert saturations, and evaporation rates	X		X T	5.3.2
		Composition of liquid and gas entering drift	X		X T	6.3.1
		Evolution of in-drift chemical environment	X		X T	6.3.3
		Thermo-Hydro-Chemical model comparison to plug-flow reactor and fracture plugging experiment		X T		6.3.1
		Rockfall		X		6.3.5
	In-Drift Moisture Distribution (4.2.5)	Environment on surface of drip shields and waste packages	X T		T	5.3.2
		Condensation under drip shields	X T			8.3.2
		Evaporation of seepage	X		X T	8.3.1 5.3.2
		Effect of breached drip shields or waste package on seepage	X		X	8.3.3
		Waste package release flow geometry (flow-through, bathtub)	X			8.3.4
	Drip Shield Degradation and Performance (4.2.4)	Local chemical environment on surface of drip shields (including Mg, Pb) and potential for initiating localized corrosion	X		T	7.3.1

T = Thermal Dependence
X = Reason topic was analyzed

Summary of Supplemental EBS Analyses

(Continued)

Key Attributes Of System	Process Model (Section of Yucca Mountain Science and Engineering Report [DOE, 2001])	Topic Of Supplemental Scientific Model Or Analysis	Reason For Supplemental Scientific Model Or Analysis			Section Of Vol. 1
			Unquantified Uncertainty Analysis	Update in Scientific Information	Cooler Thermal Operating Mode Analysis	
Limited Release of Radionuclides from the Engineered Barriers	DHLW Degradation and Performance (4.2.6)	HLW glass degradation rates	X	X	X T	9.3.1
	Dissolved Radionuclide Concentrations (4.2.6)	Solubility of neptunium, thorium, plutonium, and technetium	X	X	X T	9.3.2
	Colloid-Associated Radionuclide Concentrations (4.2.6)	Colloid mass concentrations	X			9.3.4
	In-Package Radionuclide Transport (4.2.6)	Diffusion inside waste package	X	X	X T	10.3.1
		Transport pathway from inside waste package to invert	X	X		10.3.2
		Sorption inside waste package	X	X		10.3.4
	EBS (Invert) Degradation and Performance (4.2.7)	Sorption in invert	X	X		10.3.4
		Diffusion through invert	X		X T	10.3.3
		Colloid stability in the invert	X T			10.3.5
		Microbial transport of colloids	X	X		10.3.6

T = Thermal Dependence
X = Reason topic was analyzed

Engineered Barrier System Environments

- Thermal loading and ventilation
- Natural convection
- Incoming water and gas modified by fluid-rock interactions
- Chemical interactions among water, gas, and emplaced EBS materials
- Water flow through the EBS
- Drip shield (DS) and waste package (WP) degradation
- Waste form degradation
- Radionuclide transport
- Rock fall

In-Drift Thermal Hydrologic Environment

Thermal Hydrologic Environments

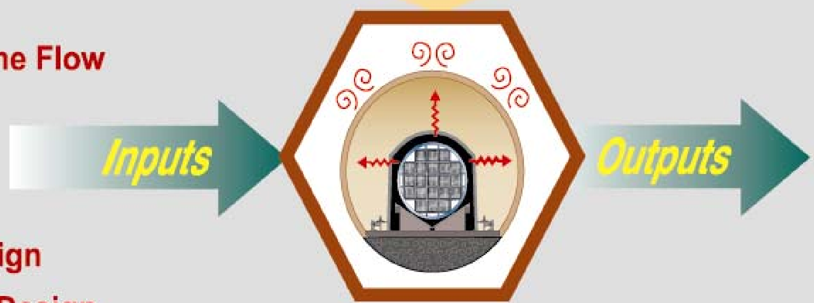
- *Both Drift-Scale and Mountain-Scale Effects Included*
- *Waste Package Variability*
- *Dual-Permeability Flow Model*
- *Active Fracture Model*

Unsaturated-Zone Flow

- Climate
- Infiltration
- Hydrologic properties

Subsurface Design

Waste Package Design



Chemical Environments (EBS environments subcomponent)

- Temperature and relative humidity at:
  - Drift wall
  - Drip shield
  - Waste package
  - Invert
- Water flow rate, water saturation, and water evaporation rate at invert
- Water evaporation rate at drip shield/waste package

Unsaturated Zone Flow

- Percolation flux above the drift

Waste Package and Drip Shield Degradation

- Temperature and relative humidity at:
  - Drip shield
  - Waste package

Waste Form Degradation

- Temperature at waste package

Engineered Barrier System Transport

- Liquid saturation in invert

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Supplemental Thermal Hydraulic Analysis

- **High temperature operating mode (HTOM) and low temperature mode (LTOM) have been analyzed**
- **Main difference between high temperature operating mode (HTOM) and Total System Performance Assessment for Site Recommendation (TSPA-SR) Base Case is an updated estimate of thermal conductivity for lithophysal hydrogeologic units**
- **Several uncertainties have been identified and evaluated using multi-scale TH submodels to determine their significance**

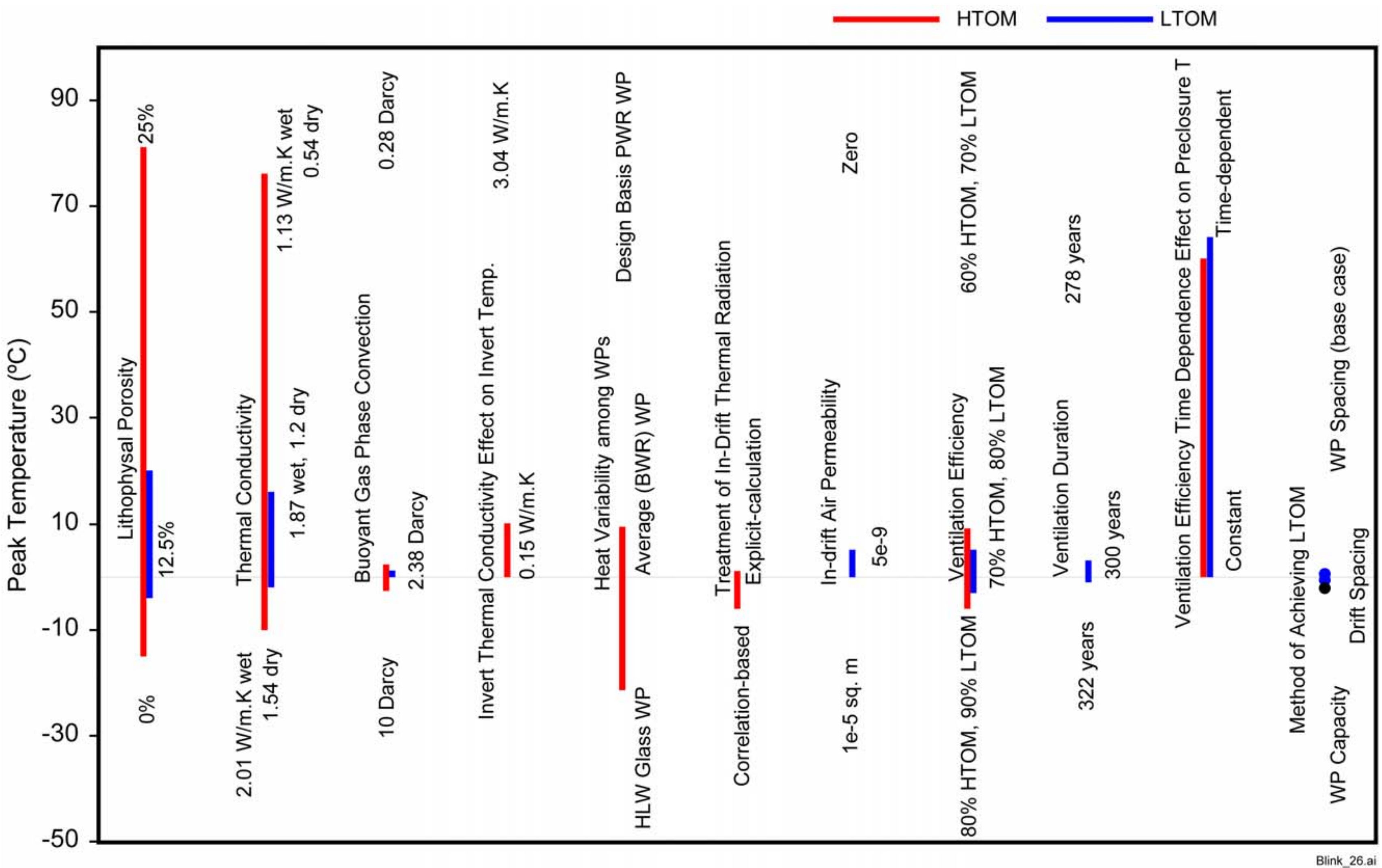
Key Thermal-Hydrologic Environment Uncertainties Evaluated in SSPA Vol. 1

Model (Conceptual) Uncertainty	Process Uncertainty	Input Data Uncertainty
Use of effective thermal conductivity and thermal radiation approaches		
Porous media approximation of comprehensive fluid dynamics processes	Hysteresis of imbibition	Invert properties
Use of single continuum versus DKM approach for invert materials	THM and THC changes to hydrologic properties	Host rock bulk permeability
Neglecting dryout during ventilation		Host rock thermal conductivity
Coupling of submodels		Host rock heat capacity
Localized effects of seepage		Heat output of waste packages
Neglecting fracture heterogeneity impacts on seepage		Impacts of lithophysal porosity on thermal conductivity
Neglecting effects of mountain-scale gas-phase convection		Wet and dry thermal conductivity
Effects of lithophysal porosity on vapor storage		Duration of ventilation

NOTE: DKM = dual permeability model; THM = thermal-hydrologic-mechanical; THC = thermal-hydrologic-chemical.

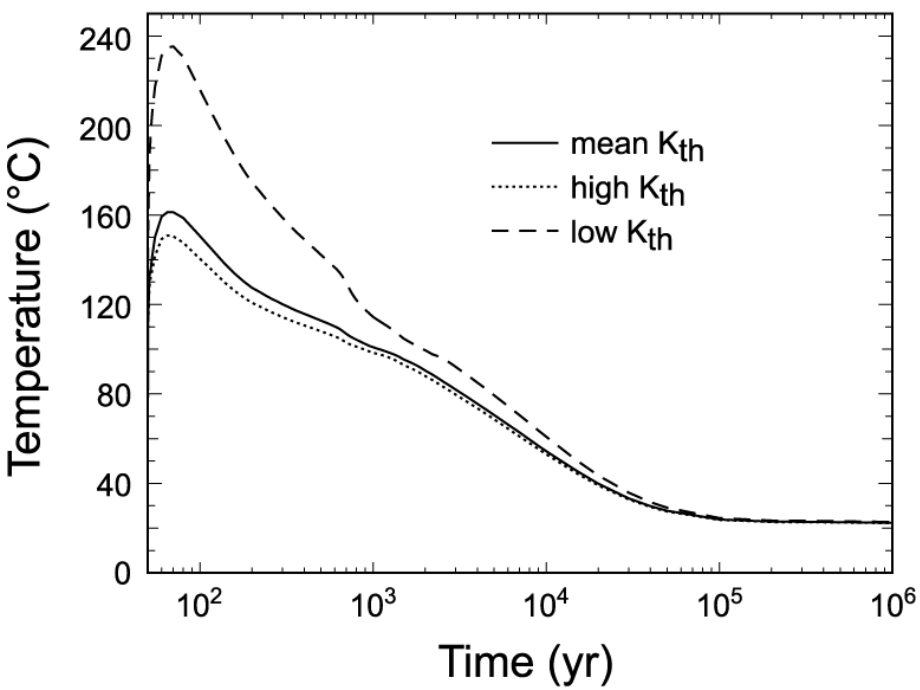
Sensitivity of In-Drift Thermal-Hydrologic Performance to Uncertainties

Change from Base Case (HTOM or LTOM) Peak Postclosure Temperature, C

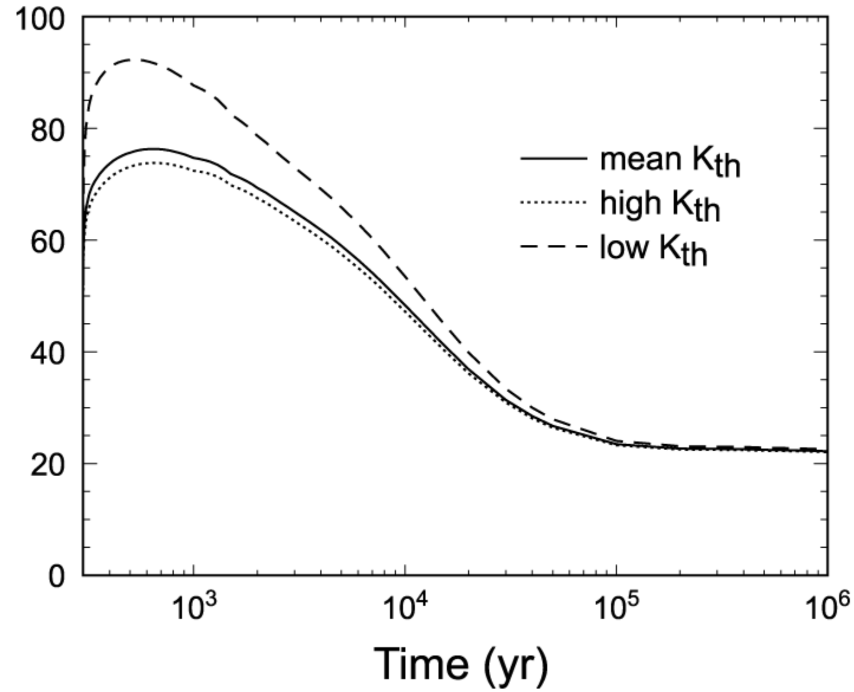


Impact of Uncertainty in Thermal Conductivity on Drip Shield Temperature

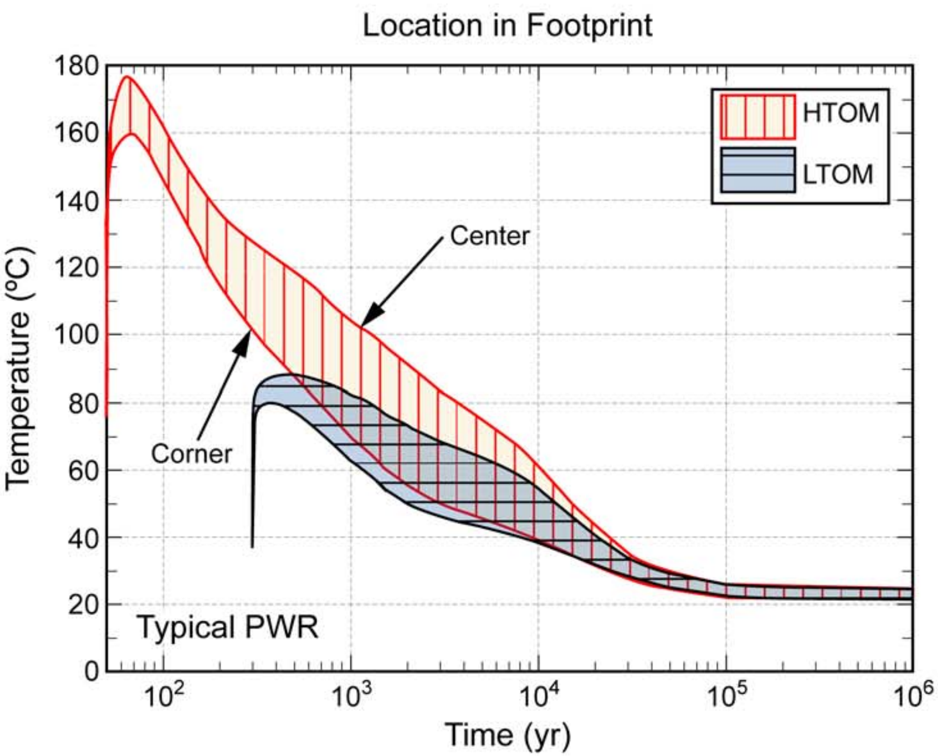
HTOM

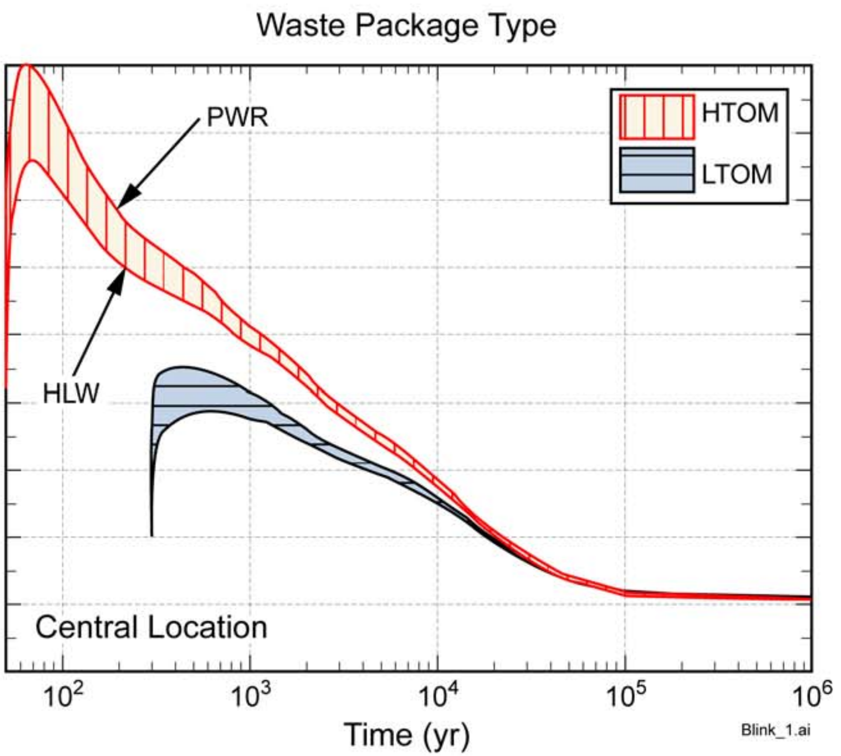


LTOM

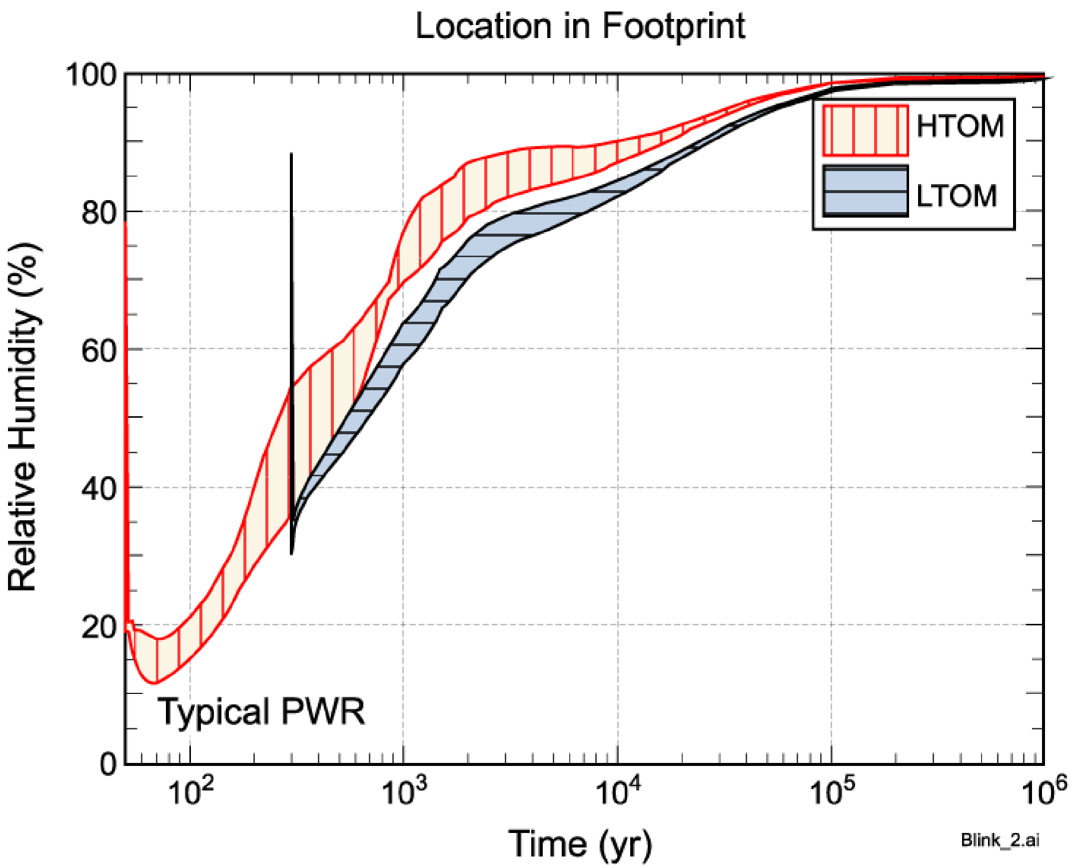


Waste Package Temperature Sensitivity to Location and Waste Package Type



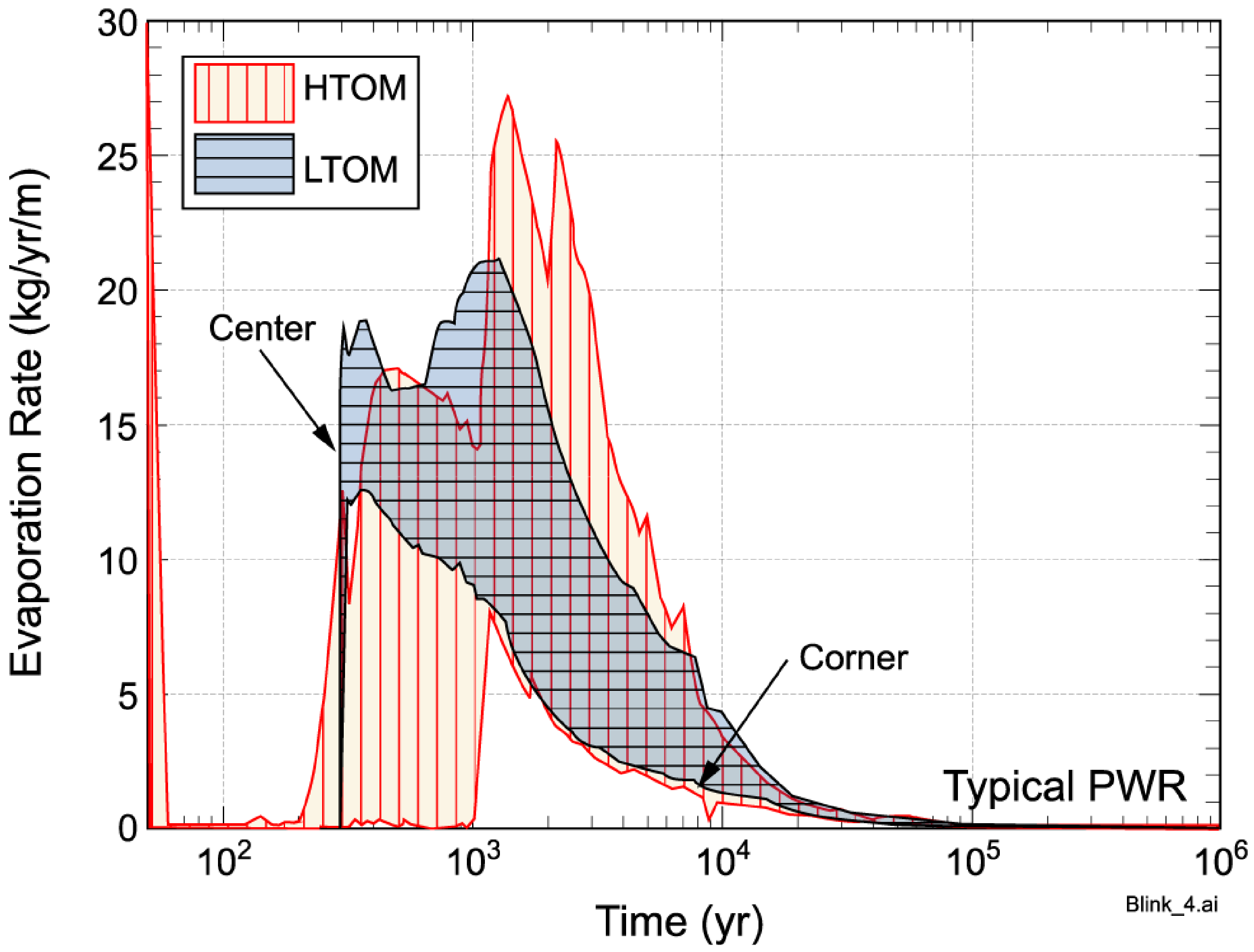


Relative Humidity Sensitivity to Location



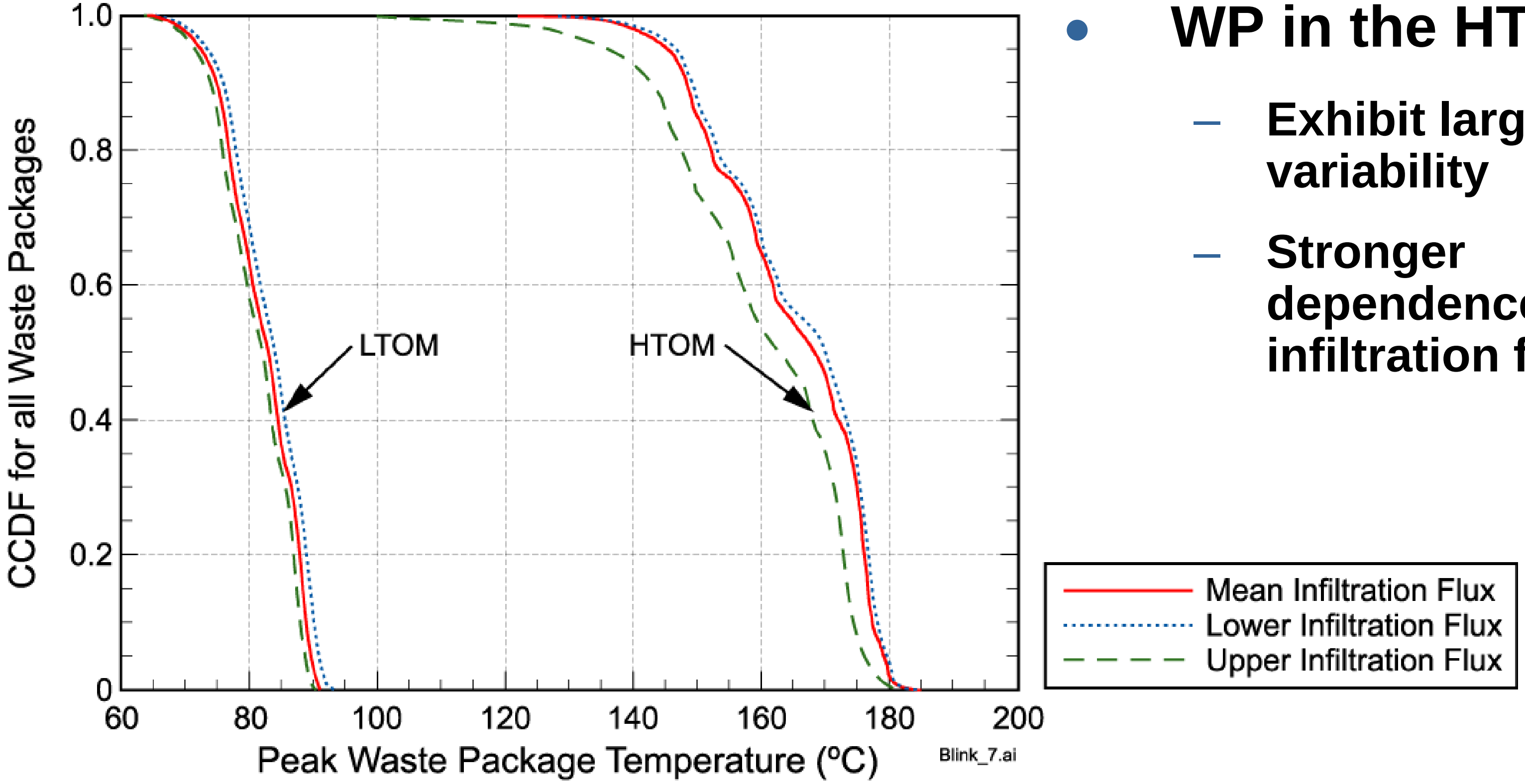
- **LTOM has less effective radiation, increasing ΔT(WP-DW), which decreases RH_{WP}**

Invert Evaporation Sensitivity to Location



Sensitivity of Waste Package Temperature to Infiltration Rate and Operating Mode

(All Waste Package Types and Locations)



- **WP in the HTOM**
  - **Exhibit larger variability**
  - **Stronger dependence on infiltration flux**

Impact of Thermal Operating Mode

- **WP Temperatures**
  - **HTOM peak WP temperatures range from 126 - 185°C vs 65 - 91°C for LTOM (mean infiltration)**
  - **Temperatures sensitive to thermal K, more so for HTOM**
  - **HTOM exhibits larger variability in WP temperatures and stronger dependence on infiltration flux**
- **WP RH tends to be lower in the LTOM with less variability and dependence on infiltration**

Impact of Thermal Operating Mode

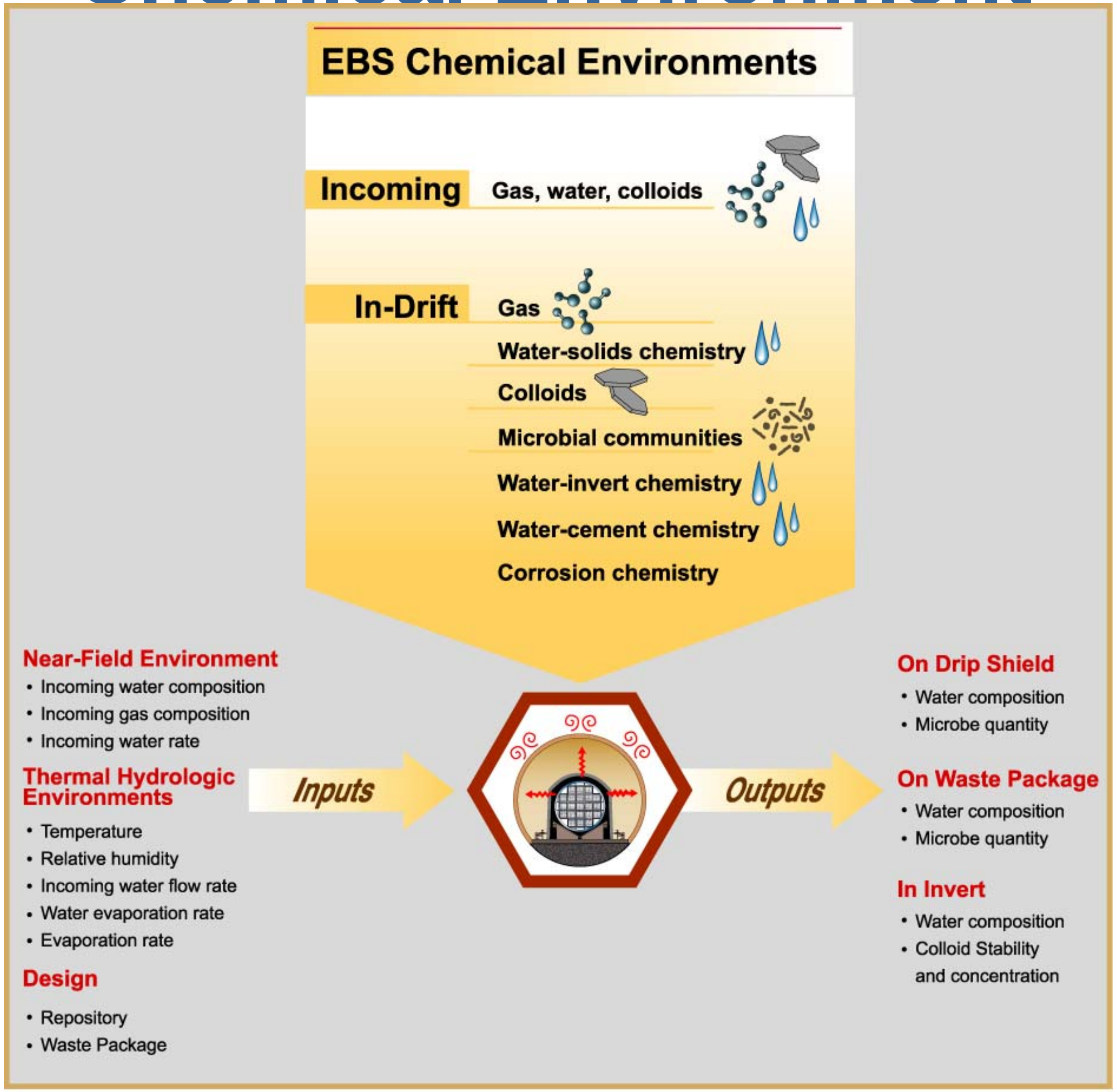
(Continued)

- **Invert saturation**
  - **Invert dry up to 1000 yrs depending on location in HTOM**
  - **Saturation trends similar in both operating modes after 1000 yrs**
- **Invert evaporation rate**
  - **Tends to be more variable and higher in HTOM after 1000 yrs**

Multiple Lines of Evidence

- **Fully 3-dimensional NUFT simulations**
- **Single Heater Test**
- **Drift-scale test**
- **Large-block test**
- **Thermal-properties from laboratory and field tests**
- **1/4-scale DS condensation test**
- **1/4-scale ventilation and natural convection tests**
- **Thermal hydrological chemical laboratory tests**

Engineered Barrier System Chemical Environment



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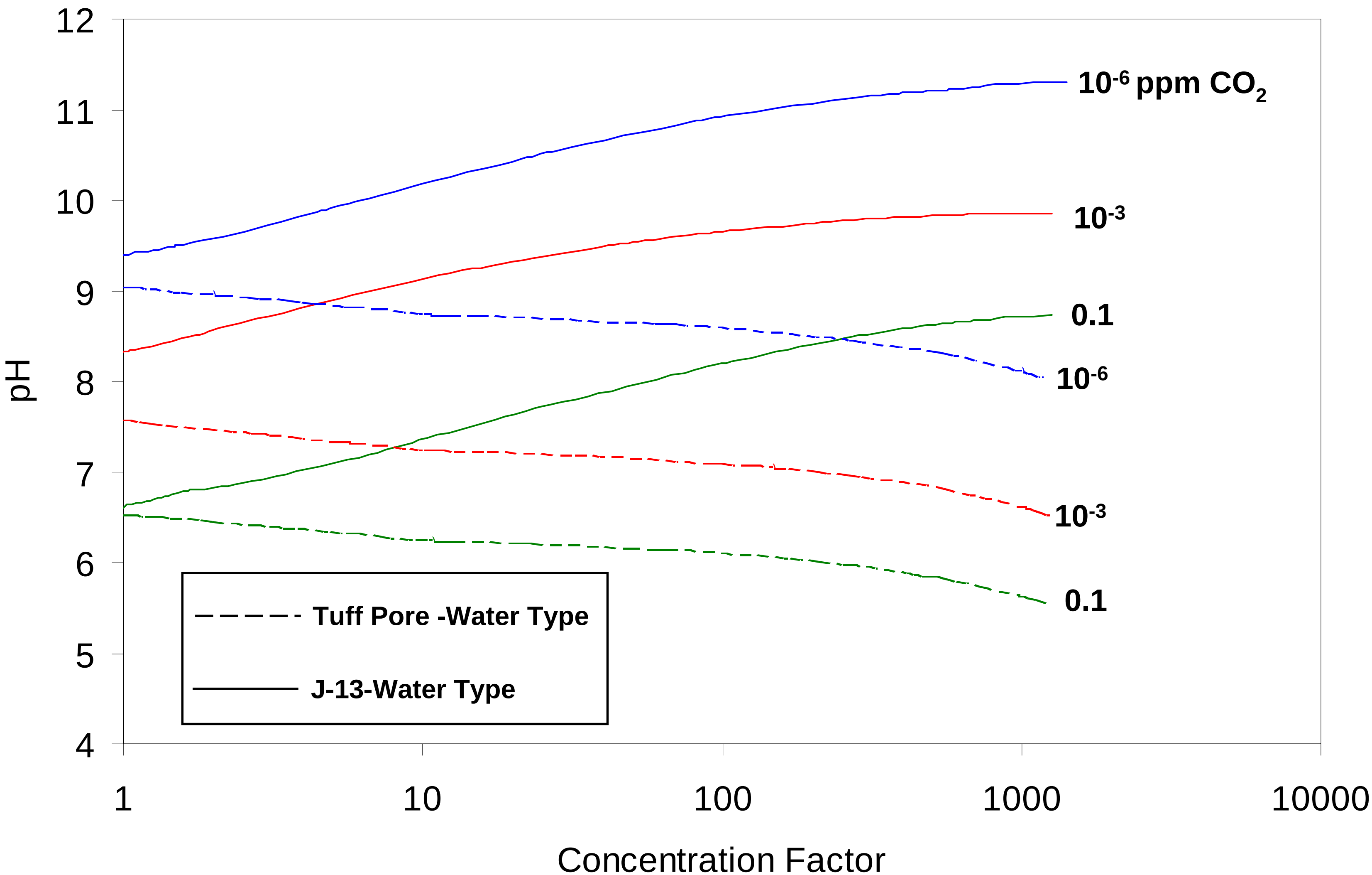
Supplemental Engineered Barrier System Chemical Environment Model

- **Main improvement for the TSPA-SR supplemental chemical environment model is the propagation of uncertainty associated with the composition of water and gas entering the emplacement drifts**
  - **Different PCO_2 soil horizon starting conditions (high PCO_2 and low PCO_2 cases)**
  - **HTOM versus LTOM**

Key Chemical Environment Uncertainties

Key Uncertainty Not Included in S&ER Models	Model Improvements Discussed in SSPA Vol. 1	Included in Supplemental TSPA Model
Composition of liquid and gas entering drifts	Yes	Yes
Seepage/Invert mixing and interactions	Yes	No
Trace elemental compositions and effects on chemistry	Yes	No
Radionuclide sorption onto corrosion products	Yes	Yes
Cement leachate effects on in-drift chemistry	Yes	No
Generation of colloids from corrosion products	Yes	No

Effects of Evaporation and CO_2 Fugacity on pH

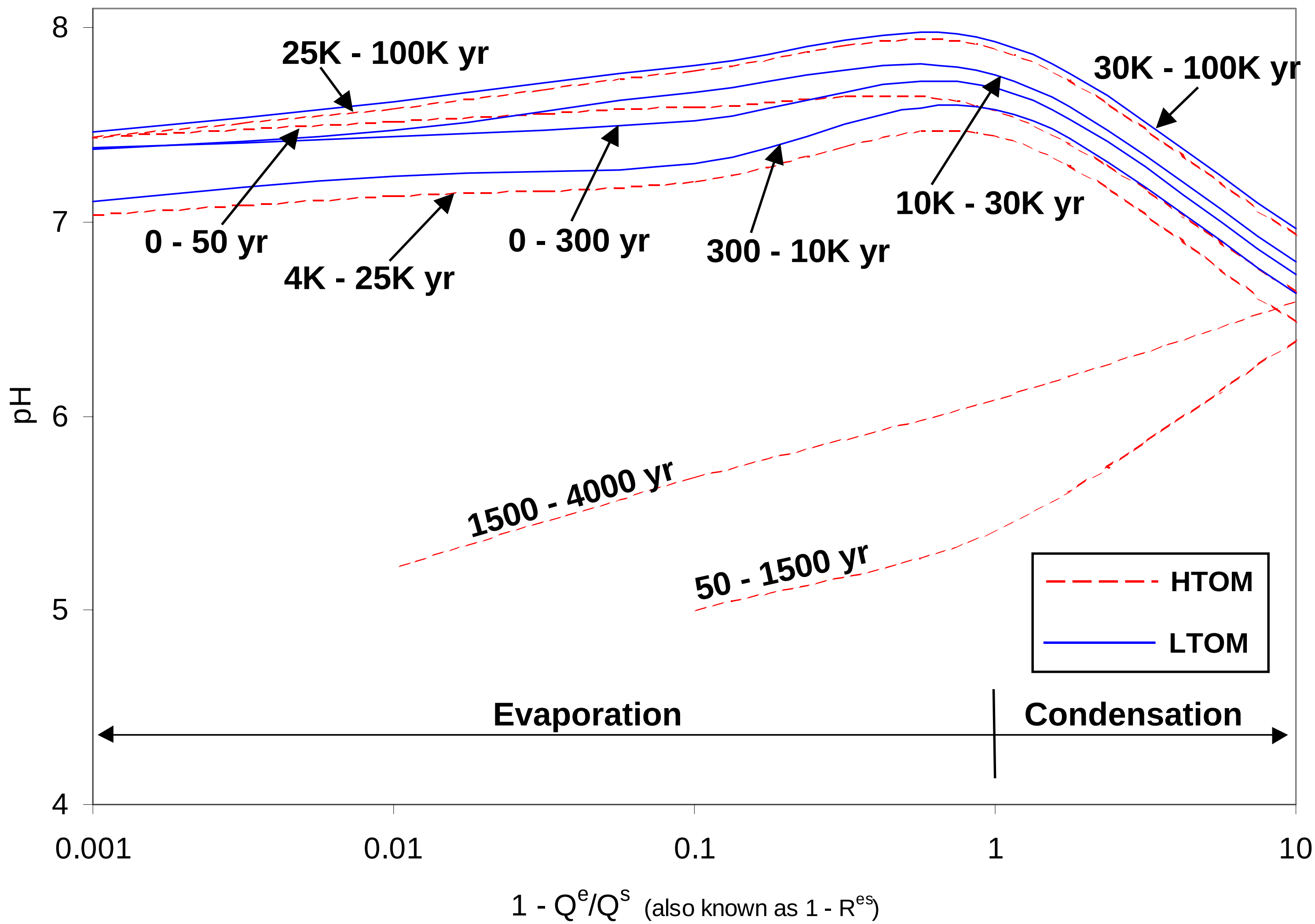


Abstraction Results for High Temperature and High Carbon Dioxide Partial Pressure in the Tptpll Lithology for Matrix Imbibition

	Preclosure	**Boiling**	**Cool Down**	**Extended Cool Down**	**Transition to Ambient**	**Ambient**
	(0-50 yr)	**(51-1,500 yr)**	**(1,501-4,000 yr)**	**(4,001-25,000 yr)**	**(25,001-100,000 yr)**	**(100,001-1,000,000 yr)**
Actual THC Model Run Time (yr)	5.00	250.01	2,000.00	10,000.00	50,001.50	Averaged
Temperature (°C)	75.02	120.68	93.89	53.96	27.44	23.26
PCO_2 (v.frac)	1.56E-03	2.15E-05	4.60E-05	3.40E-03	9.44E-04	7.13E-04
pH	7.86	8.27	8.04	7.70	8.33	8.43
Ca (mol/L)	8.75E-04	2.30E-02	1.37E-02	1.97E-03	2.01E-03	2.13E-03
Mg (mol/L)	3.54E-04	2.87E-02	2.45E-03	1.50E-05	1.35E-04	1.53E-04
Na (mol/L)	4.40E-03	2.24E-01	3.96E-03	3.71E-03	5.02E-03	4.82E-03
Cl (mol/L)	3.26E-03	2.24E-01	1.60E-02	3.27E-03	3.31E-03	3.31E-03
SiO_2(aq) (mol/L)	3.78E-03	7.10E-02	6.32E-03	3.40E-03	1.52E-03	1.46E-03
HCO_3 (mol/L)	8.30E-04	2.35E-05	4.13E-05	1.73E-03	3.15E-03	3.19E-03
SO_4 (mol/L)	1.17E-03	5.35E-02	9.67E-03	1.19E-03	1.20E-03	1.21E-03
K (mol/L)	4.39E-04	4.20E-02	6.11E-04	2.12E-04	1.24E-04	1.03E-04
AlO_2 (mol/L)	1.24E-08	3.93E-12	2.59E-08	2.05E-09	7.25E-10	5.06E-10
F (mol/L)	5.53E-04	4.18E-04	2.15E-04	3.66E-04	3.24E-04	3.04E-04
$HFeO_2$ (mol/L)	5.47E-11	2.81E-09	8.49E-10	4.36E-11	4.53E-12	1.86E-12

Source: Data derived from THC simulations thc6_ht1 (Table 6.3.1.5-1) and thc6_16_25_g4_amb (DTN: LB0011DSTTHCR1.001 [DIRS 154759]) as archived in Jolley (2001 [DIRS 154762]).

pH for Higher CO_2 Case
Pore Water - Type Seepage



Impact of Thermal Operating Mode

- Two general types of waters
  - Matrix water (pH goes down with evaporative concentration)
  - Fracture water (pH goes up with evaporative concentration)
- Matrix water used in supplemental TSPA
- HTOM will tend to have a lower pH and higher ionic strength because of higher evaporation rates

Multiple Lines of Evidence

- Formation of natural brines and evaporites
- Laboratory evaporation studies
- Handbook solubility values of soluble salts
- Waters mixing in oceans, estuaries, and lakes
- Thermal-hydrological-chemical laboratory column experiments

Supplemental Engineered Barrier System Flow and Transport Model

- Main improvements for the TSPA-SR supplemental EBS flow and transport model are
  - Seepage evaporation at the DS
  - DS and WP flux models
  - In-package diffusion
  - Radionuclide sorption

Key Flow and Transport Uncertainties

Key Uncertainty Not Included in S&ER Models	Model Improvements Discussed in SSPA Volume 1	Included in Supplemental TSPA Model
Seepage Evaporation	Yes	Yes
Drip shield and waste package fluxes	Yes	Yes
Drip shield condensation	Yes	No
Bath-tub flow	Yes	No
Diffusion in waste package	Yes	Yes
Diffusion from waste package to invert	Yes	No
Diffusion through invert	Yes	Yes
Microbial sorption and transport	Yes	No

Impact of Thermal Operating Mode on Engineered Barrier System Transport

- **EBS Flow**
  - Evaporation rates are a function of thermal response
- **EBS transport**
  - Diffusion coefficient is a direct function of temperature
  - Diffusion coefficient is a function of the time-dependent saturation
  - Adsorption of water vapor is a function of RH

Multiple Lines of Evidence

- **EBS 1/4-scale tests**
  - **Condensation beneath DS**
  - **Flux through DS**
- **Laboratory data for diffusivity of unsaturated crushed tuff**
- **Laboratory column transport and sorption tests**
- **Published investigations of colloid characteristics, behavior, and transport properties**
- **Field data on colloid facilitated transport at Nevada Test Site and Los Alamos National Laboratory**

Summary

- Improved understanding of uncertainties associated with EBS environments and processes
- Improved understanding will help plan future work
- Conclusions regarding the impact of thermal operating modes on performance will be discussed in Mike Wilson's and Jim Blink's talks