YUCCA MOUNTAIN PROJECT

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

Update on Engineered Barrier System Performance: Performance Assessment Insights

Presented to:
Nuclear Waste Technical Review Board

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Outline

- Summary of integrated presentations
- Overview of Engineered Barrier System (EBS) processes
- Key conclusions relevant to localized corrosion on the waste package (WP) surface
- Environment on the WP surface and associated uncertainties
- Implementation of the localized corrosion model for Total System Performance Assessment – License Application (TSPA-LA)
- Example results
- Summary

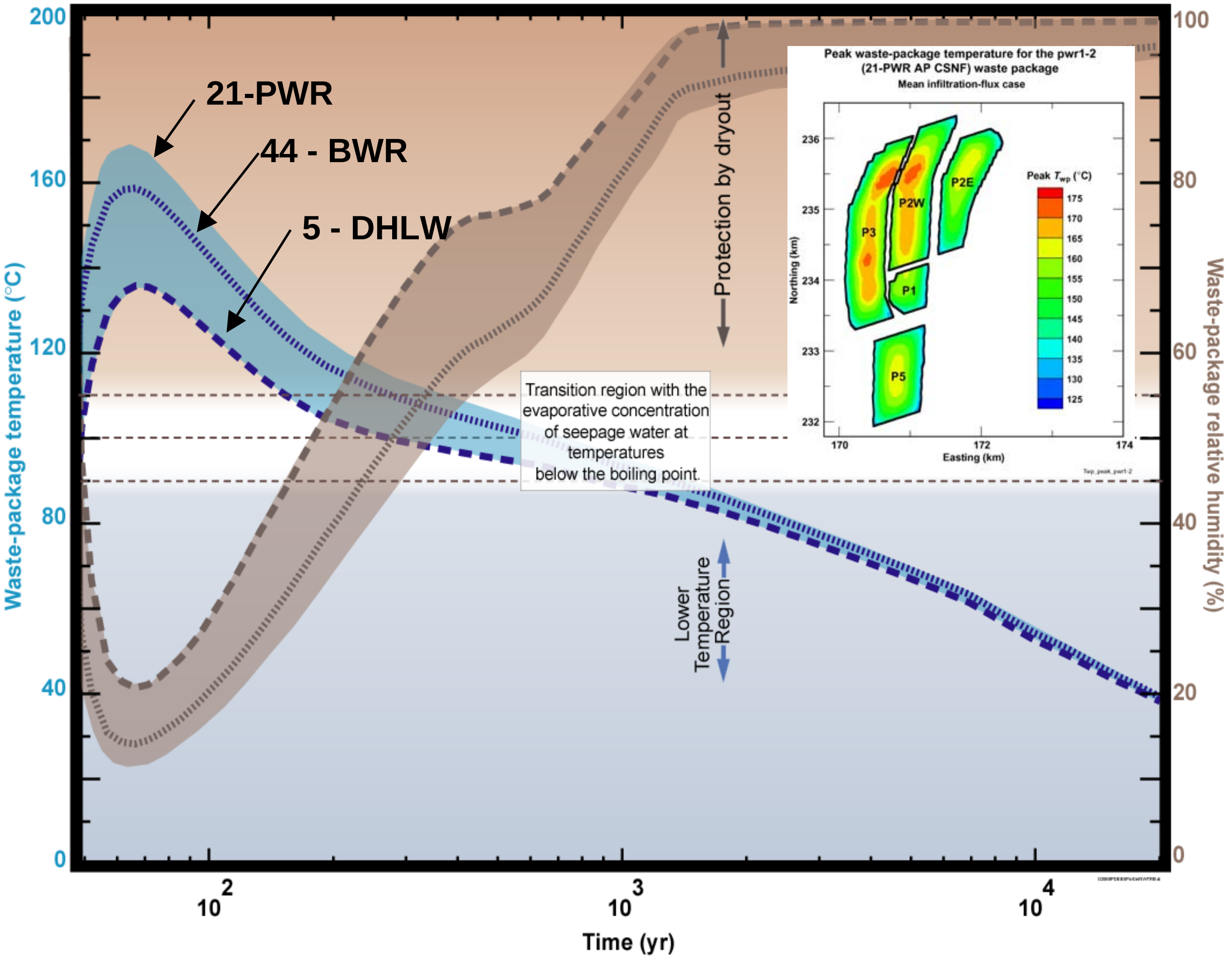
Regulatory/Licensing Considerations

- Conclusions and model results presented herein are preliminary
- Final conclusions and model results will be included in the licensing basis (e.g., analysis/modeling reports)

Integrated Presentations on Evaluating Engineered Barrier Performance

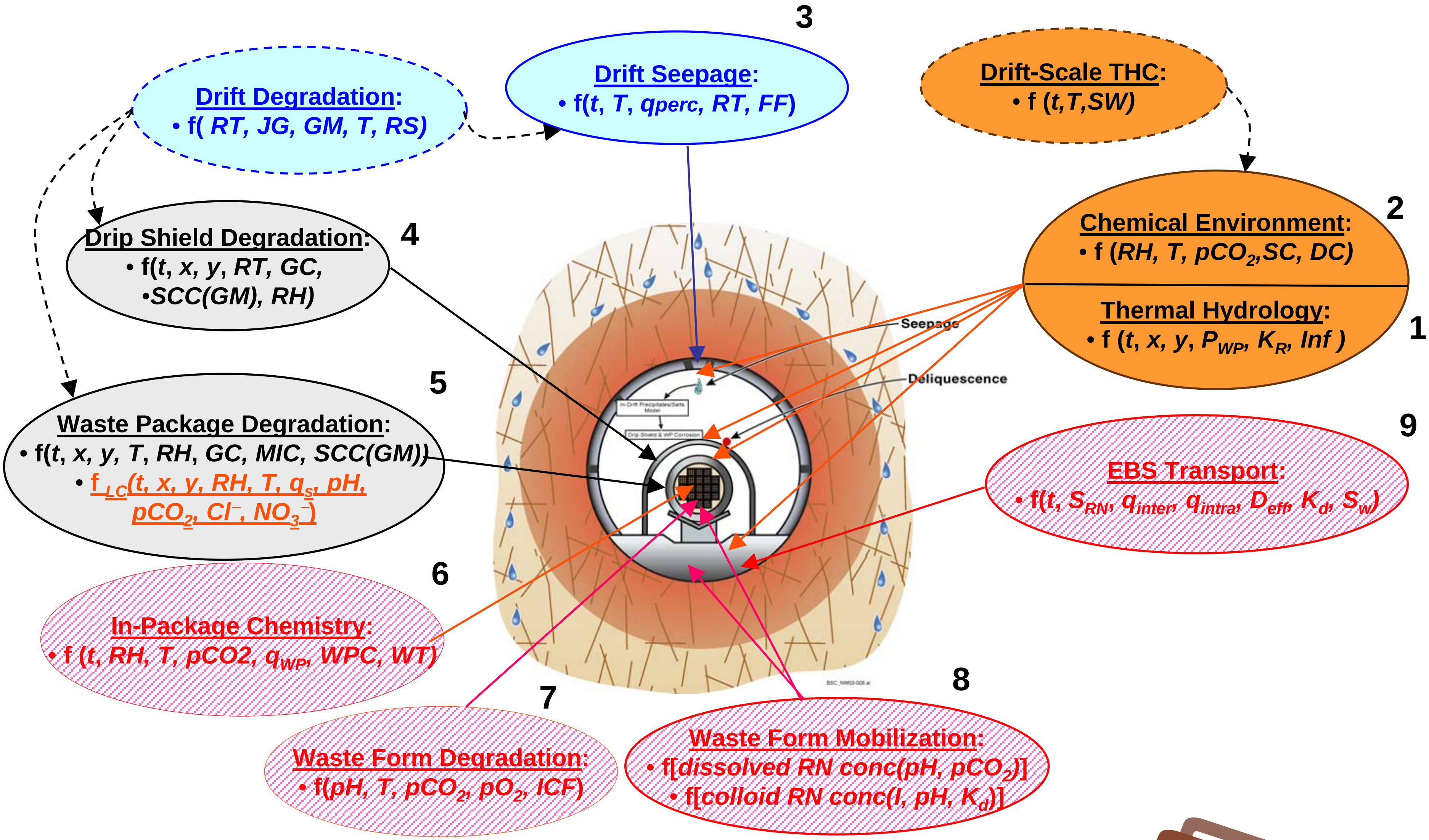
- **Characterization of the Unsaturated Zone: Bo Bodvarsson**
  - **Unsaturated zone coupled processes, evolution of chemistry in the rock**
- **Characterization of the In-drift Environment: Mark Peters**
  - **In-drift processes, evolution of chemistry in the drift**
- **Materials Performance: Joe Farmer**
  - **Effects on corrosion of the WP**

Evolution of In-Drift Environment



Legend
BWR - boiling water reactor
DHLW - defense high-level (radioactive) waste
PWR - pressurized water reactor

Engineered Barrier System Processes Modeled in Total System Performance Assessment



Drift Degradation:
- f(RT, JG, GM, T, RS)

Drift Seepage:
- f(t, T, $qperc$, RT, FF)

Drift-Scale THC:
- f (t,T,SW)

Drip Shield Degradation:
- f(t, x, y, RT, GC,
- $SCC(GM)$, RH)

Chemical Environment:
- f (RH, T, pCO_2,SC, DC)

Thermal Hydrology:
- f (t, x, y, P_{WP}, K_R, Inf)

Waste Package Degradation:
- f(t, x, y, T, RH, GC, MIC, $SCC(GM)$)
- $f_{LC}(t, x, y, RH, T, q_s, pH, pCO_2, Cl^-, NO_3^-)$

EBS Transport:
- f(t, S_{RN}, q_{inter}, q_{intra}, D_{eff}, K_d, S_w)

In-Package Chemistry:
- f (t, RH, T, $pCO2$, q_{WP}, WPC, WT)

Waste Form Degradation:
- f(pH, T, pCO_2, pO_2, ICF)

Waste Form Mobilization:
- f[dissolved RN conc(pH, pCO_2)]
- f[colloid RN conc(I, pH, K_d)]

Key Conclusions Relevant to Localized Corrosion on the Waste Package Surface

- **Drift seepage will not occur for crown temperatures above boiling temperature**
- **Highly unlikely that dust deliquescence on WPs will initiate localized corrosion**
- **If seepage water reaches WPs, conditions suitable for localized corrosion may occur during the thermal period**
- **In the nominal scenario class, drip shield (DS) performance will prevent seepage water from reaching WPs, and the occurrence of localized corrosion is highly unlikely**
- **DS damage in the seismic scenario class allows seepage to reach WPs, and conditions for localized corrosion may exist following early post-closure seismic events**

Environment on Waste Package Surface

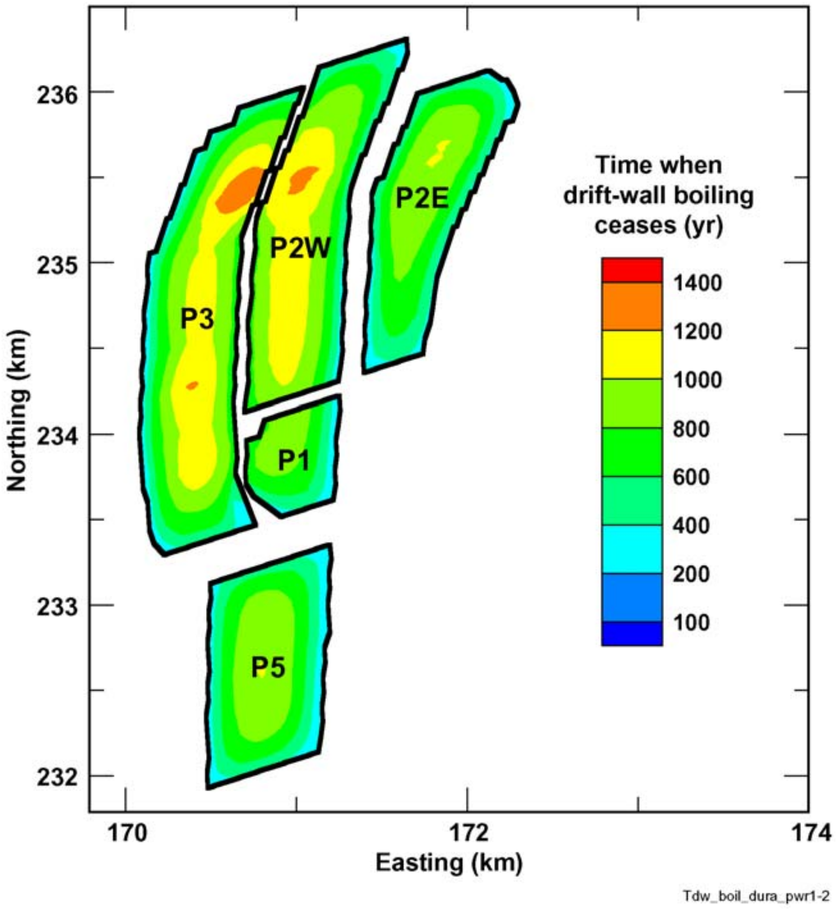
- **Key Parameters contributing to the chemical environment on the WP surface**
  - **Incoming seepage composition and rate (calculated by Drift-Scale Thermal-Hydrological-Chemical (THC) Model and Drift Seepage Model)**
  - **Composition of dust deliquescence on DS/WP surface (calculated by the Chemical Environment Model)**
  - **Temperature (calculated by the Thermal Hydrology (TH) Model)**
  - **Relative Humidity (calculated by the TH Model)**
  - **Evolution of in-drift chemistry (calculated by the EBS Chemical Environment Model)**
- **Thermal and chemical variables important to localized corrosion on WP surface**
  - ***T, RH***
  - ***pH, NO_3^-, Cl^-***
  - ***NO_3^- / Cl^-***

Engineered Barrier System Thermal Hydrology Model and Total System Performance Assessment Abstraction

- The EBS TH model represents repository footprint shape and location with respect to stratigraphy
- Includes repository-scale and temporal variability in percolation flux
- Includes uncertainty in percolation flux and thermal conductivity (K)
- 5 cases are simulated for TSPA-LA
  - 3 infiltration fields, each with mean K
  - Low infiltration with low K
  - High infiltration with high K
- Results are abstracted from the EBS TH model for all WPs in the repository

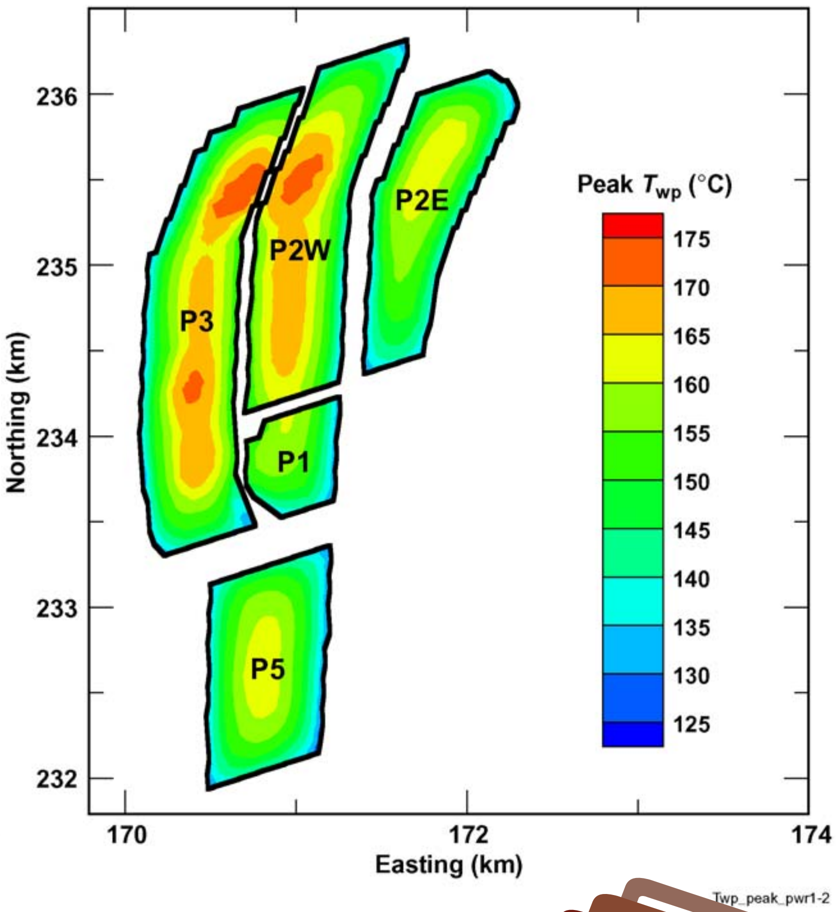
Engineered Barrier System Multiscale Thermal Hydrology Model

Representative Results



Time when drift-wall boiling ceases for the pwr1-2 (21-PWR AP CSNF) waste package

Mean infiltration-flux case



Peak waste-package temperature for the pwr1-2 (21-PWR AP CSNF) waste package

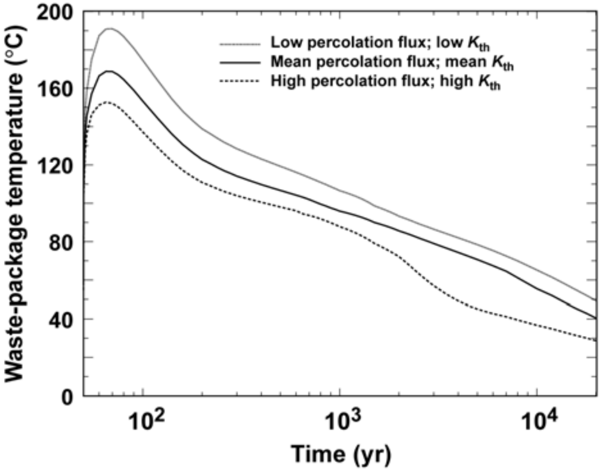
Mean infiltration-flux case

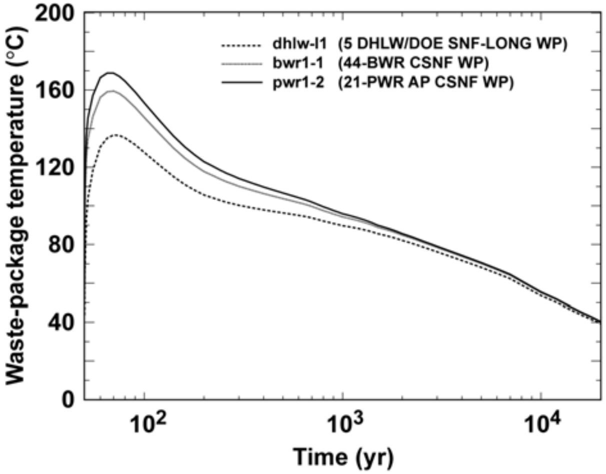
PRELIMINARY

Engineered Barrier System Multiscale Thermal Hydrology Model

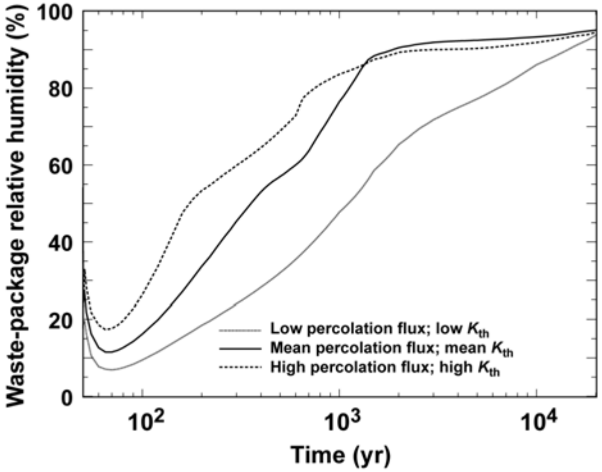
Representative Results

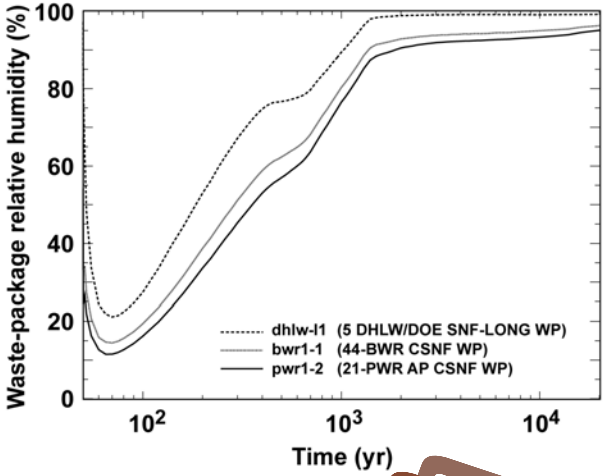
(Continued)





PRELIMINARY



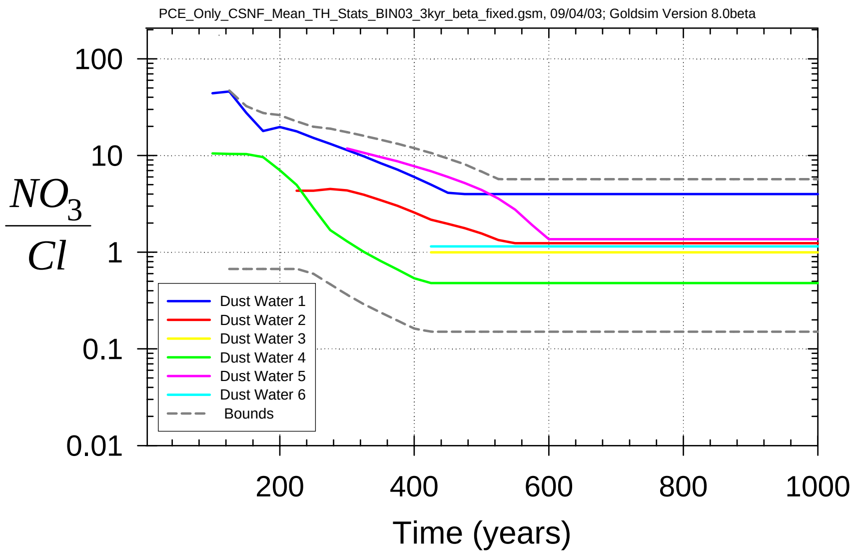


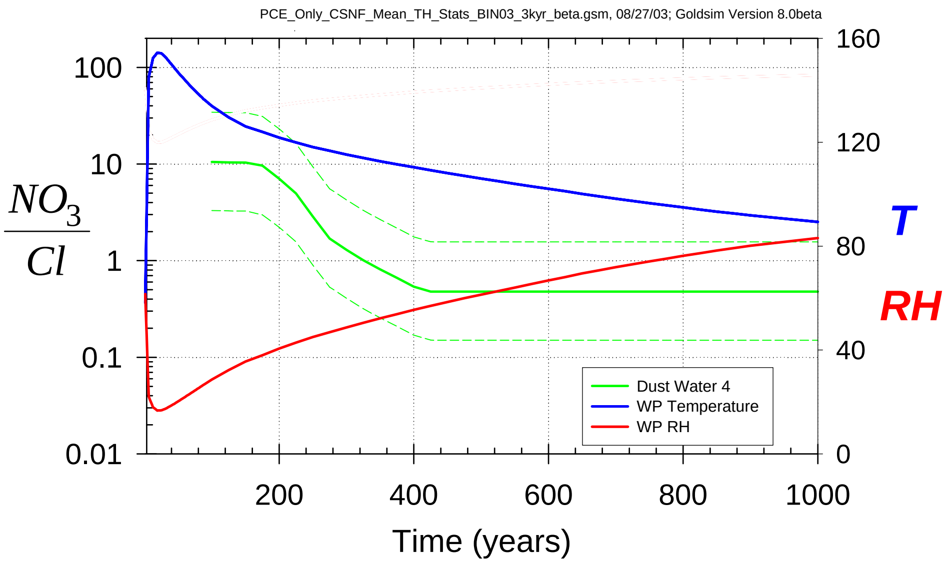
Engineered Barrier System Chemical Environment Model

- **Abstracts seepage water composition output from the drift-scale THC model into 11 bins with common chemical characteristics**
- **Abstracts dust deliquescence compositions into 6 bins with common chemical characteristics**
- **Models evaporative concentration of seepage waters and resultant brines and the formation of deliquescent brines; develops chemistry look-up tables for these brines at multiple levels of pCO_2, T, and RH**
- **Tables used in the TSPA-LA localized corrosion and system models to predict a range of chemical environments**
- **Represents uncertainty associated with**
  - **Composition of incoming seepage**
  - **In-drift pCO_2**
  - **Composition of dust deliquescence that forms on WP/DS surfaces**
  - **Evolution of seepage water evaporation and brine formation**

Engineered Barrier System Chemistry Abstraction Model

Evolution of Chemistry in Dust Deliquescence and Associated Uncertainty


PCE_Only_CSNF_Mean_TH_Stats_BIN03_3kyr_beta_fixed.gsm, 09/04/03; Goldsim Version 8.0beta

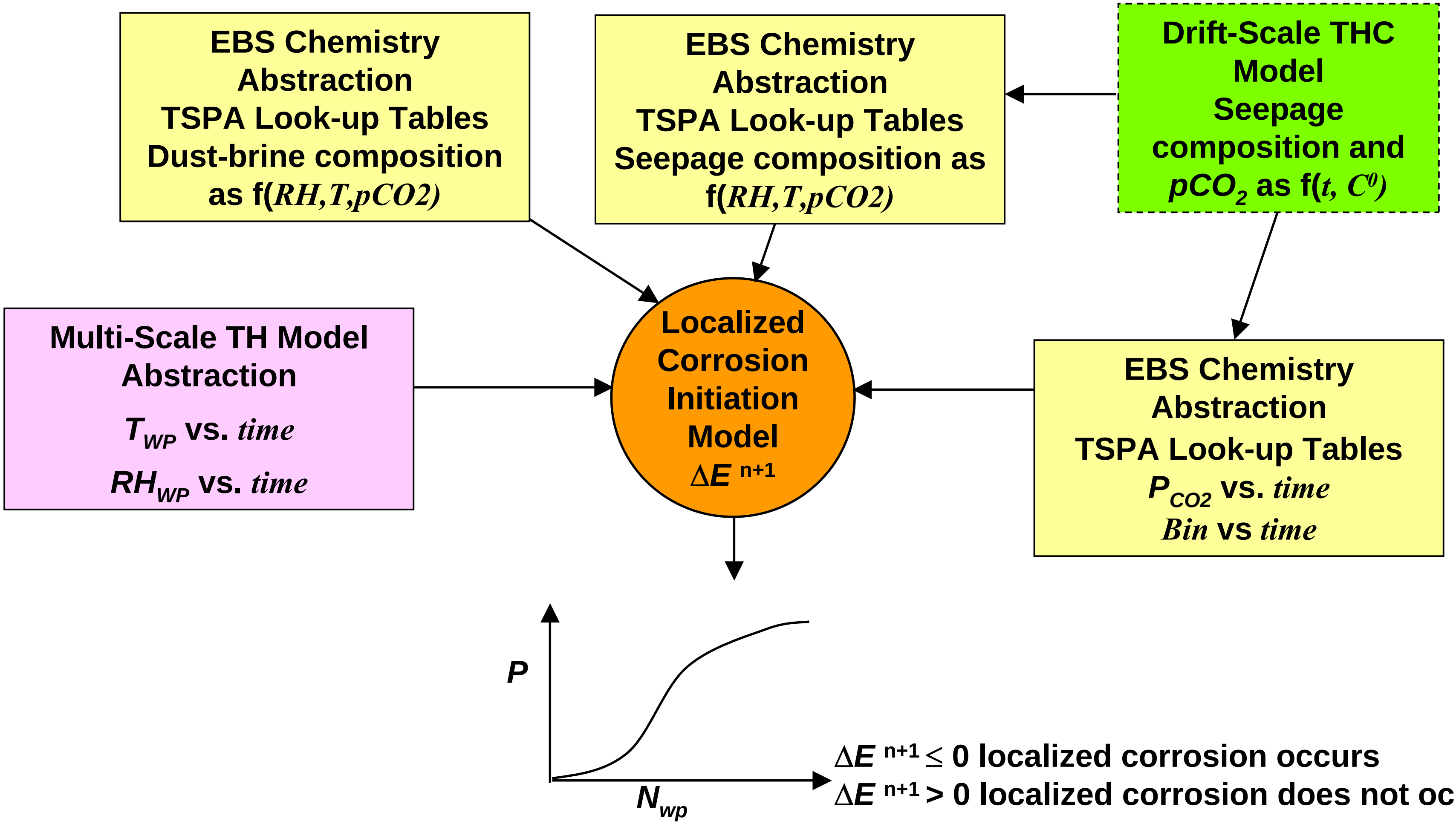

PCE_Only_CSNF_Mean_TH_Stats_BIN03_3kyr_beta.gsm, 08/27/03; Goldsim Version 8.0beta

Preliminary

Implementation of Localized Corrosion Model

- **Implemented using GoldSim software, which is the primary simulation engine that links and runs the TPSA model and its component models**
- **A GoldSim module couples in-drift TH and chemistry with the localized corrosion model**
- **Uncertainties will be sampled and multiple realizations will be computed to exercise the localized corrosion initiation model over the range of potential postclosure environments**
- **Output will include one or more uncertainty distributions (CDFs) for the fraction of packages that experience localized corrosion**
- **CDFs will be incorporated and sampled in the main TSPA-LA model at run time**

GoldSim Localized Corrosion Initiation Model



EBS Chemistry Abstraction
TSPA Look-up Tables
Dust-brine composition as f($RH, T, pCO2$)

EBS Chemistry Abstraction
TSPA Look-up Tables
Seepage composition as f($RH, T, pCO2$)

Drift-Scale THC Model
Seepage composition and pCO_2 as f(t, C^0)

Multi-Scale TH Model Abstraction
T_{WP} vs. $time$
RH_{WP} vs. $time$

Localized Corrosion Initiation Model
ΔE^{n+1}

EBS Chemistry Abstraction
TSPA Look-up Tables
P_{CO2} vs. $time$
Bin vs $time$

$\Delta E^{n+1} \leq 0$ localized corrosion occurs
$\Delta E^{n+1} > 0$ localized corrosion does not occur

Localized Corrosion Initiation Model

- Localized corrosion initiation model uses empirical regression equations for corrosion potential (E_{corr}) and crevice repassivation potential (E_{rcrev})
- Regression equations were developed using Yucca Mountain Project and Center for Nuclear Waste Regulatory Analysis crevice repassivation potential data from cyclic potentiodynamic polarization tests on Alloy 22
- Combined test data represent a wide range of exposure environments
- Regression equations include dependence on temperature, pH, chloride concentration, and nitrate concentration

Localized Corrosion Initiation Model

- **Crevice repassivation potential**

$$E_{rcrev} = E_{rcrev}(T, pH, Cl^-, NO_3^-, \frac{NO_3^-}{Cl^-})$$

- **Long-term corrosion potential**

$$E_{corr} = E_{corr}(T, pH, Cl^-, \frac{NO_3^-}{Cl^-})$$

- **Localized corrosion initiates when**

$$\Delta E = (E_{rcrev} - E_{corr}) \leq \mathbf{0}$$

- **Uncertainty in the parameter coefficients is represented**

Summary of Independent Variables and Uncertainties

- **In-drift TH**

$$\left.\begin{aligned} T_{WP} &= T(x_{WP}, y_{WP}, t, K_r, Inf) \\ RH_{WP} &= RH(x_{WP}, y_{WP}, t, K_r, Inf) \end{aligned}\right\} \text{5 TH Cases}$$

- **Dust deliquescence, crown seepage, and gas compositions**

$$\left.\begin{aligned} C_{Si} &= C_{Si}(x_c, y_c, t, SW_i) \\ pCO_{2i} &= pCO_{2i}(x_c, y_c, t, SW_i) \\ C_{Di} &= C_{Di}(x_{WP}, y_{WP}, t, SD_i) \end{aligned}\right\}$$

5 seepage and *pCO$_2$* histories
6 dust deliquescence waters

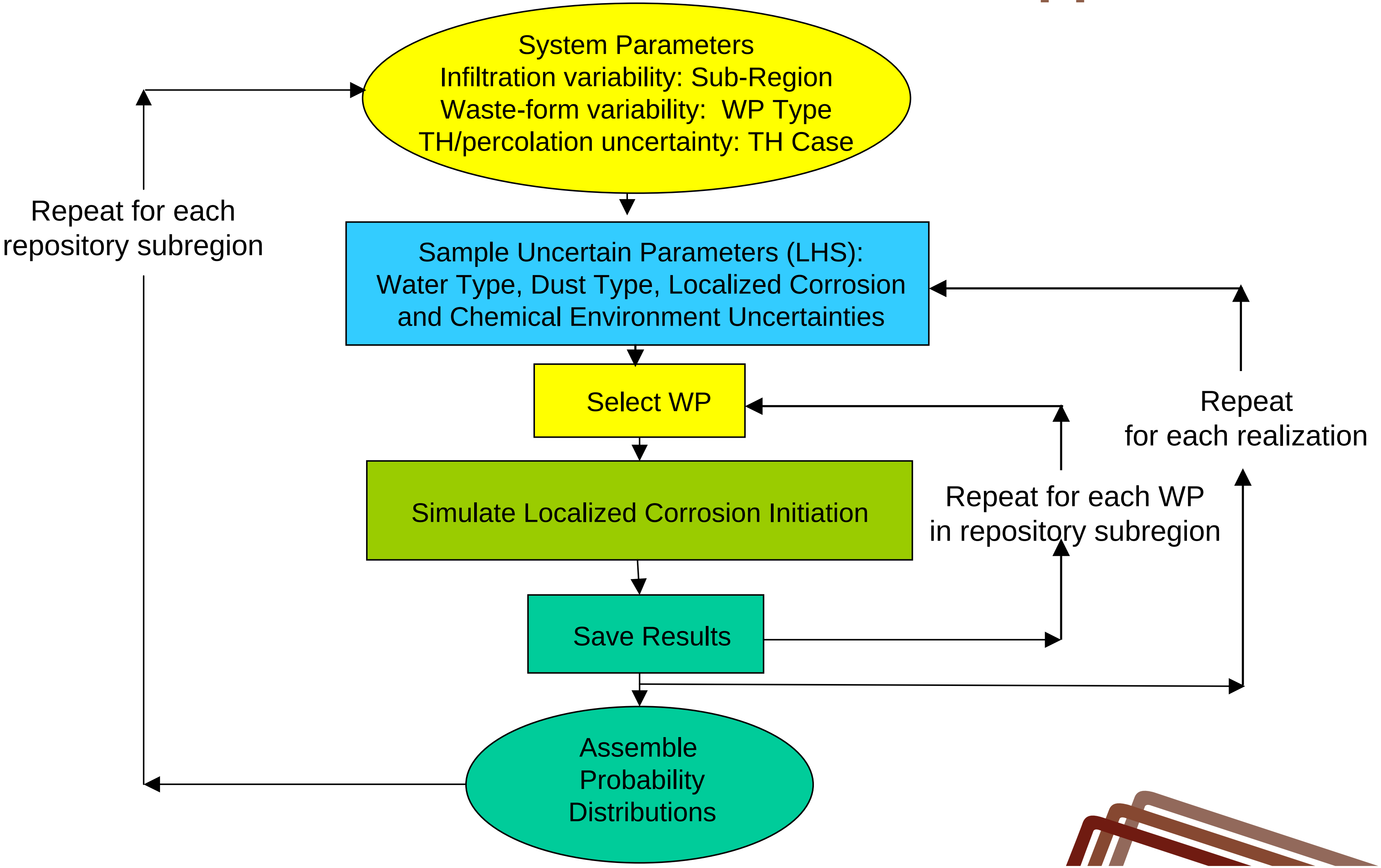
- **Evolution of in-drift chemistry**

$$pH_{WP} = pH(x_{WP}, y_{WP}, T_{WP}, RH_{WP}, pCO_{2i}, C_{ji}) + U_{pH}$$

$$NO^-_{3\,WP} = NO^-_3(x_{WP}, y_{WP}, T_{WP}, RH_{WP}, PCO_{2i}, C_{ji}) + U_{NO_3^-} \qquad j = D, S$$

$$Cl^-_{WP} = Cl^-(x_{WP}, y_{WP}, T_{WP}, RH_{WP}, PCO_{2i}, C_{ji}) + U_{Cl^-}$$

Implementation of Localized Corrosion Initiation Model and Uncertainties in Total System Performance Assessment-License Application



System Parameters
Infiltration variability: Sub-Region
Waste-form variability: WP Type
TH/percolation uncertainty: TH Case

Sample Uncertain Parameters (LHS):
Water Type, Dust Type, Localized Corrosion and Chemical Environment Uncertainties

Select WP

Simulate Localized Corrosion Initiation

Save Results

Assemble Probability Distributions

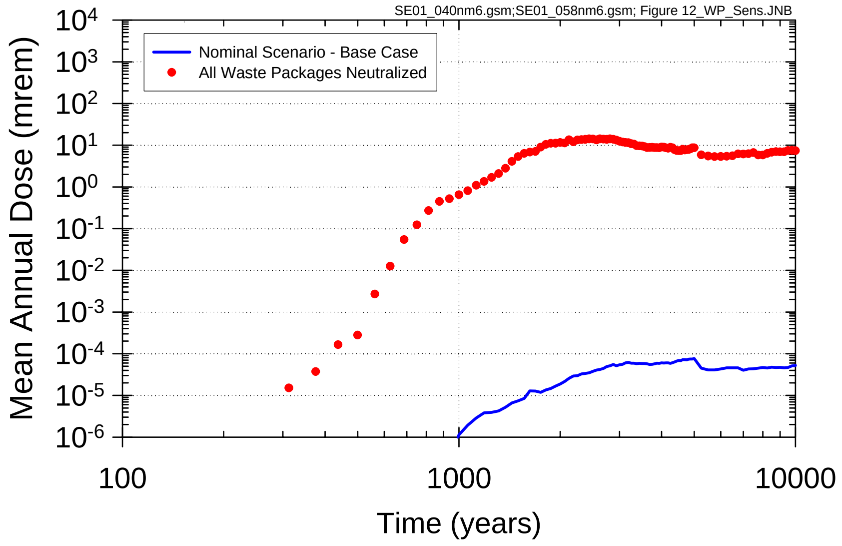
Repeat for each repository subregion

Repeat for each realization

Repeat for each WP in repository subregion

Example 1: Impact of Assumed Waste Package Failure

- **Simulations based on the following assumptions***
  - **WP neutralization**
    - **No DS failure**
    - **The surface area on all WPs is assumed to be 100% failed at beginning of simulation**
  - **Nominal scenario**
    - **1 early WP failure in each realization in nominal scenario; ~4% surface area failed**
  - **This example**
    - **Peak mean annual dose rate of ~20 mrem/yr scales linearly with number of failed WPs**
    - **Assume 1% of WPs fail due to dust deliquescence initiated localized corrosion**
      - **Result ~ 0.2 mrem/yr**

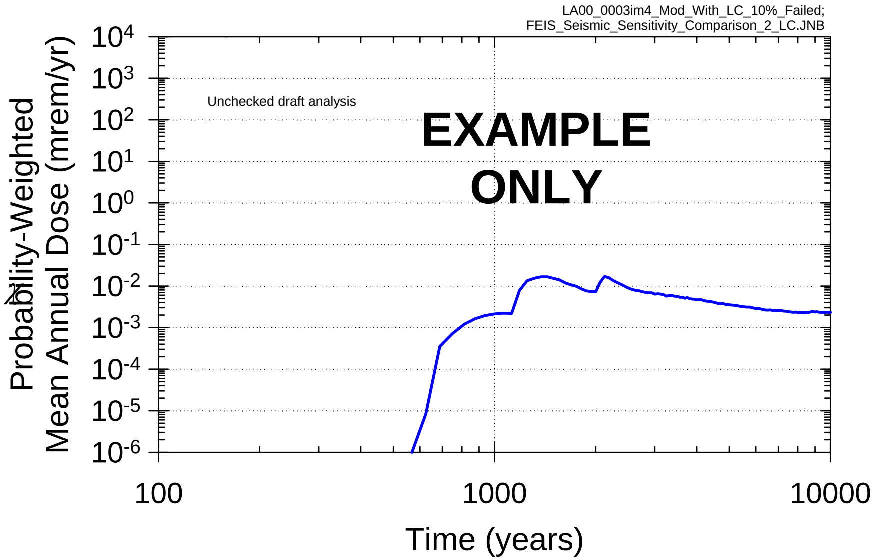


***Example results shown in plot taken from *Risk Information to Support Prioritization of Performance Assessment Models*, TDR-WIS-PA-000009 REV 01, ICN 01, BSC 2002**

Note: If localized corrosion did occur due to dust deliquescence, WP failure area would likely be much less than 100% of WP surface

Example 2: Impact of Assumed Drip Shield Damage and Seepage-Initiated Localized Corrosion

- **Assumptions**
  - **Assume DS damage event annual frequency is 1 × 10^{-6} per year**
  - **WP degradation due to localized corrosion only**
  - **Initiating event must occur within the 1500 yrs after closure**
    - **Seepage will not contact WPs unless a disruptive event damages the DSs**
    - **Unlikely that localized corrosion will occur after 1500 years**
  - **3 percent of surface area on all DSs is failed**
  - **10 percent of WPs contacted by seepage within 1500 years after closure experience localized corrosion**
  - **10 percent of the surface area on WPs that experience localized corrosion is failed**



Summary

- Variability and uncertainty in in-drift THC processes are accounted for in the modeling approach for EBS degradation processes
- Key Performance Assessment (PA) insights into EBS performance include:
  - Drift seepage will not occur for crown temperatures above boiling temperature
  - Highly unlikely that dust deliquescence on WP will initiate localized corrosion
  - If seepage water reaches the WPs, conditions suitable for localized corrosion may occur during the thermal period
  - In the nominal scenario class, DS performance will prevent seepage water from reaching WPs, and the occurrence of localized corrosion is highly unlikely
  - DS damage in the seismic scenario class allows seepage to reach WPs, and conditions for localized corrosion may exist following early post-closure seismic events

Summary

(Continued)

- Two examples estimate the impact of localized corrosion
  - Example 1 assumes 1 percent of all WPs completely fail by dust deliquescence initiated localized corrosion and no DS failure
    - Mean annual dose rate is ~ 0.2 mrem/yr
  - Example 2 assumes seepage-initiated localized corrosion is caused by a DS damage event prior to 1500 yrs having an annual frequency of 1×10^{-6} per year
    - Probability-weighted mean annual dose rate is ~ 0.02 mrem/yr

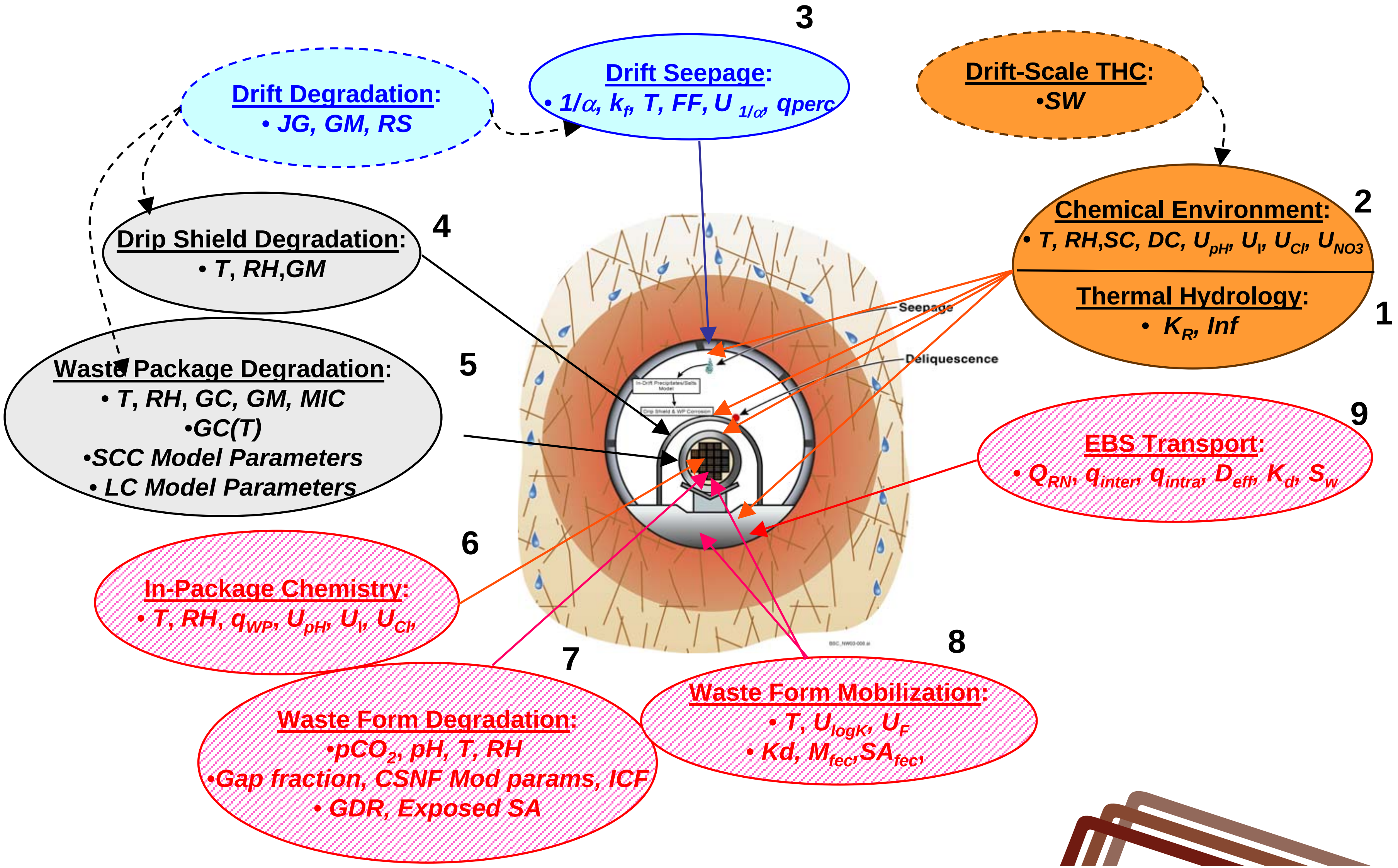
Backup

Nomenclature

_GM_ – ground motion
_RT_ – rock type
_JG_ – joint geometry
_RS_ – rock strength
WPC – WP components
_WT_ – waste type
_SC_ – seepage composition
_DC_ – dust composition
_GC_ – general corrosion rate
_FF_ – flow focusing factor
Inf – infiltration
_SW_ – starting water
P_{WP} – WP power output
U_j – model uncertainty for parameter _j_
q_{intra}, q_{inter} – inter- and intragranular fluxes through invert

SCC – stress corrosion cracking
ICF – initial clad failure fraction
pCO_2 – partial pressure of carbon dioxide
_RH_ – relative humidity
MIC – microbial induced corrosion
q_{perc} – percolation flux
_T_ – temperature
_t_ – time
K_R – host rock thermal conductivity
S_{RN} – radionuclide mass release rate from WF

Engineered Barrier System Parameter and Model Uncertainties Represented in Total System Performance Assessment



Drift Degradation:
- JG, GM, RS

3
Drift Seepage:
- $1/\alpha$, k_f, T, FF, $U_{1/\alpha}$, qperc

Drift-Scale THC:
- SW

2
Chemical Environment:
- T, RH,SC, DC, U_{pH}, U_I, U_{Cl}, U_{NO3}

1
Thermal Hydrology:
- K_R, Inf

4
Drip Shield Degradation:
- T, RH,GM

5
Waste Package Degradation:
- T, RH, GC, GM, MIC
- GC(T)
- SCC Model Parameters
- LC Model Parameters

9
EBS Transport:
- Q_{RN}, q_{inter}, q_{intra}, D_{eff}, K_d, S_w

6
In-Package Chemistry:
- T, RH, q_{WP}, U_{pH}, U_I, U_{Cl}

7
Waste Form Degradation:
- pCO_2, pH, T, RH
- Gap fraction, CSNF Mod params, ICF
- GDR, Exposed SA

8
Waste Form Mobilization:
- T, U_{logK}, U_F
- Kd, M_{fec}, SA_{fec}

Thermal-Hydrological Seepage Model Demonstrates that Vaporization Barrier is Effective

(from Bodvarsson 05/13/2003, Slide 23)

- **Water cannot penetrate through the vaporization barrier as long as the local temperature at the drift wall is above boiling**
- **Temperature drops below boiling typically after 1000 years of waste emplacement**
  - **The "percolation" flux may be slightly enhanced above ambient from thermal perturbation**
  - **Seepage percentage is always smaller than the respective ambient reference values**
- **Long term ambient seepage defines an upper limit for the potential magnitude of seepage during the thermal period**

Post-Closure Drip Shield Failure Mechanisms

Failure Mechanism	Drip Shield Post-Closure Assessment (Nominal)		Drip Shield Post-Closure Assessment (Seismic)	
	Included in TSPA	Screened Out*	Included in TSPA	Screened Out*
General Corrosion	X		X	
Localized Corrosion		X		X
Aging and Phase Stability		X		X
Fabrication Defects		X		X
Microbial Influenced Corrosion		X		X
Gamma Radiolysis		X		X
Stress Corrosion Cracking		X	X	
Hydrogen Induced Cracking		X		X
Rock Fall		X	X	

*Screened out on basis of low consequence or low probability of occurrence