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Sandia National Laboratories yucca mountain project
OCRWM Lead Laboratory for Repository Systems

Corrosion Performance of the Engineered Barrier in the Yucca Mountain Repository

Presented at:

Third International Workshop on Long-Term Prediction of Corrosion Damage in Nuclear Waste Systems

State College, PA

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Materials Reliability

Sandia National Laboratories

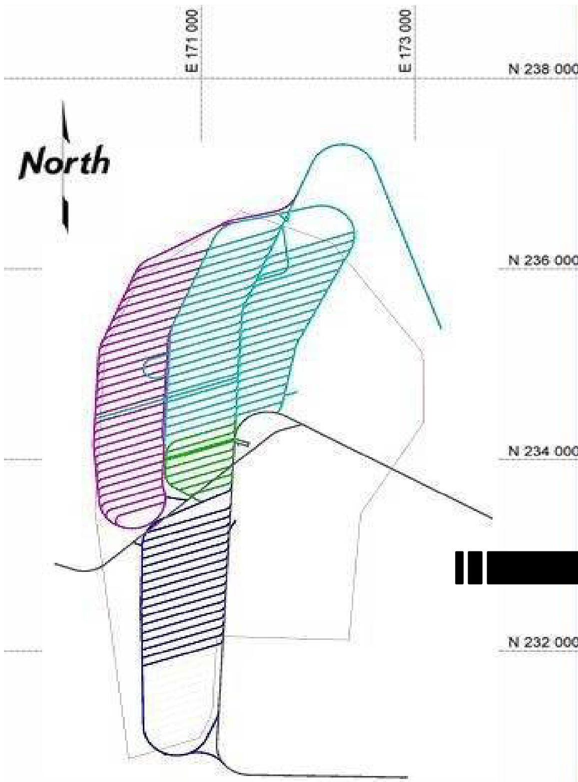
Not LSN Relevant

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Background

- Review the site
- Governing documents/procedures/laws
- FEPs
- TSPA
- Environment
- Corrosion model
- Current efforts

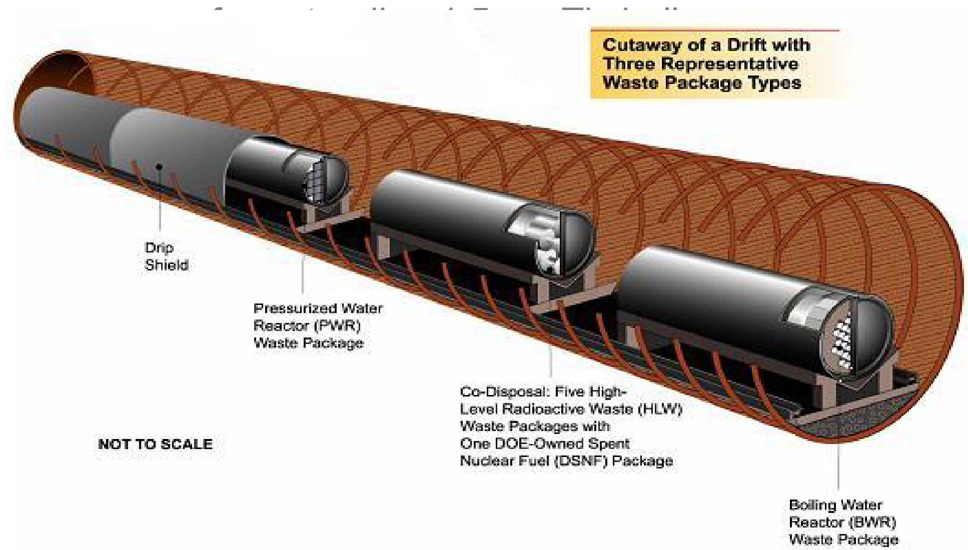
Yucca Mountain Subsurface Design



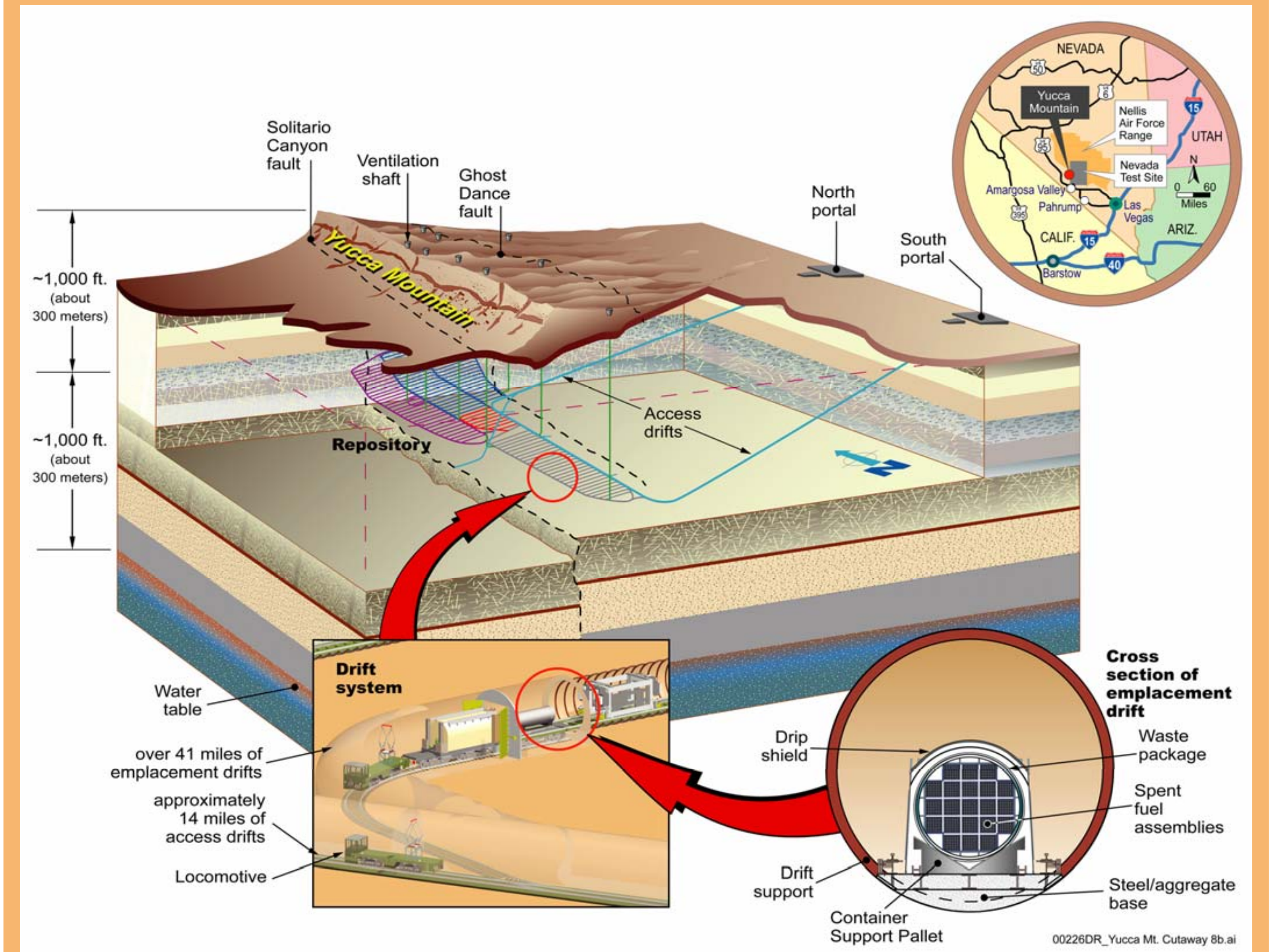
Emplacement drifts
- 5.5 m diameter
- 50-90 drifts, each ~ 1 km long

Waste packages
- ~12,000 packages
- ~ 5 m long, 2 m diameter
- outer layer 2 cm Alloy 22 (Ni-Cr-Mo-V)
- inner layer 5 cm stainless steel

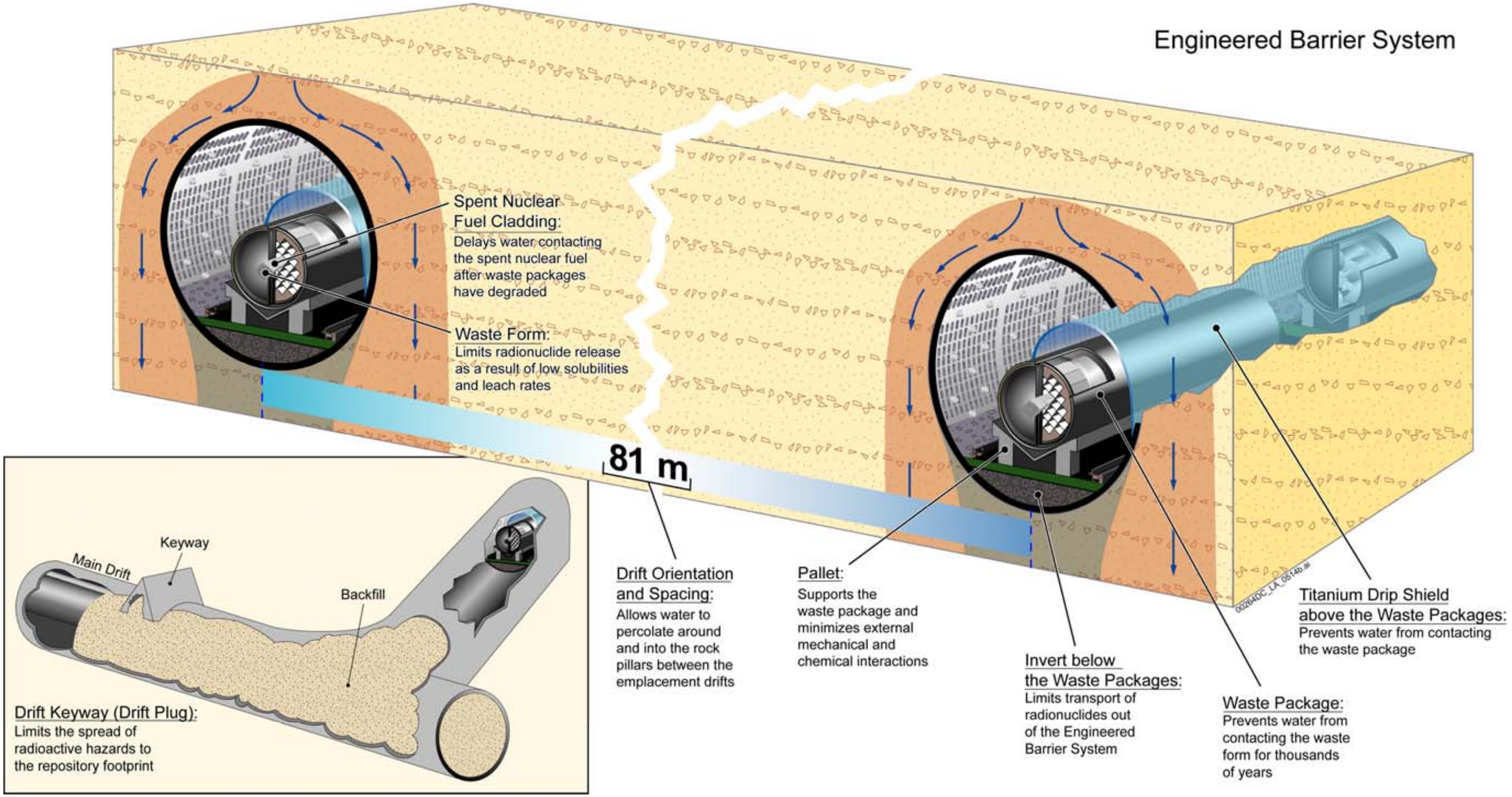
Drip shields



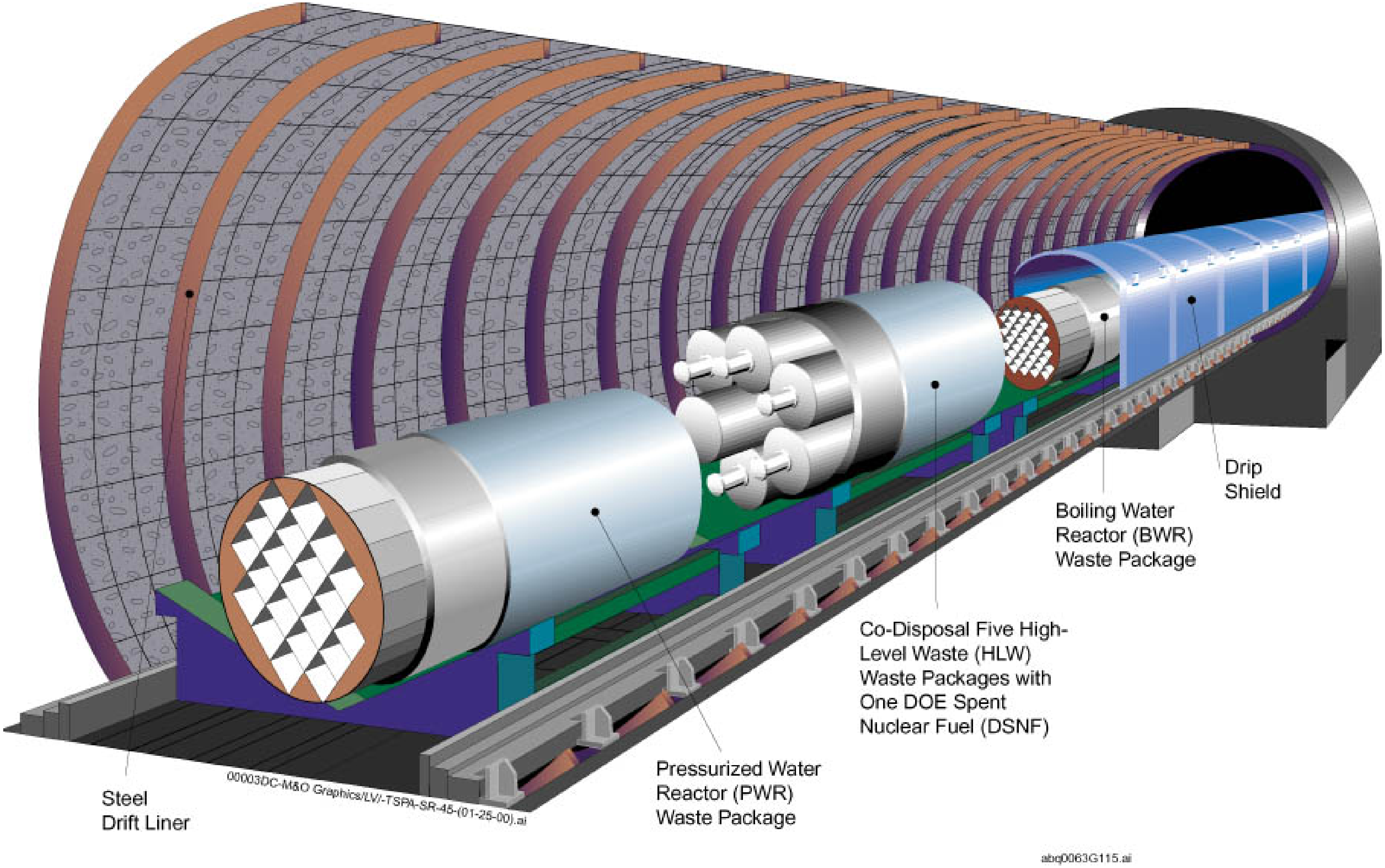
The Natural and Engineered Barrier System



Engineered Barrier System



Waste Packages in a Disposal Drift



Policies and Procedures which Govern YMP

Congress Defines the Rules

- 1982 – Congress established the Nuclear Waste Policy Act (NWPA) for the disposal of high-level radioactive waste and commercial spent nuclear fuel
- 1987 – NWPA amended to select only Yucca Mountain for characterization as a potential repository site
  - Yucca Mountain is limited by law to 70,000 metric tons of spent fuel and high-level waste
  - ~130,000 metric tons of spent fuel and high level waste are projected from currently existing sources

1957	1982	1987	1992	2002
NAS Supported deep geologic disposal	Congress passes Nuclear Waste Policy Act	Congress selects Yucca Mountain for study	Energy Policy Act sets EPA standard process	President recommends, Congress approves Yucca Mountain

10 CFR Part 63—Performance Assessment and Postclosure Requirements

- Postclosure performance objectives
  - 63.113 Performance objectives for the geologic repository after permanent closure
- Postclosure performance assessment
  - 63.114 Requirements for performance assessment
  - 63.115 Requirements for multiple barriers
- Subpart L—Postclosure public health and environmental standards
  - 63.304 Reasonable expectation
  - 63.305 Required characteristics of the reference biosphere

10 CFR Part 63—Performance Assessment and Postclosure Requirements

- Postclosure individual protection standard
  - 63.311 Individual protection standard after permanent closure
  - 63.312 Required characteristics of the reasonably maximally exposed individual (RMEI)
- Human-intrusion standard
  - 63.321 Individual protection standard for human intrusion
  - 63.322 Human intrusion scenario
- Groundwater protection standards
  - 63.331 Separate standards for protection of ground water
  - 63.332 Representative volume
- Uncertainty and sensitivity analyses (10 CFR 63.114, 10 CFR 63.115)

Regulatory Basis for Probabilistic Analyses

- Definition of performance assessment (10 CFR 63.2)
  - "Performance assessment means an analysis that:
    - Identifies the features, events, processes (except human intrusion), and sequences of events and processes (except human intrusion) that might affect the Yucca Mountain disposal system and their probabilities of occurring during 10,000 years after disposal;
    - Examines the effects of those features, events, processes, and sequences of events and processes upon the performance of the Yucca Mountain disposal system; and
    - Estimates the dose incurred by the reasonably maximally exposed individual, including the associated uncertainties, as a result of releases caused by all significant features, events, processes, and sequences of events and processes, weighted by their probability of occurrence."

Regulatory Basis (cont.)

- Screening Features, Events, and Processes: 10 CFR 63.114 d,e,f
  - "Any performance assessment used to demonstrate compliance with §63.113 must:
    - ...Consider only events that have at least one chance in 10,000 of occurring over 10,000 years.
    - ...Specific features, events, and processes of the geologic setting must be evaluated in detail if the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission.
    - ...Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting [doses or releases] would be significantly changed by their omission."

Regulatory Basis (cont.)

- *Reasonable Expectation* and regulating on the mean of an uncertainty analysis:
  - 10 CFR 63.303: "DOE must demonstrate that there is a reasonable expectation of compliance with this subpart before a license may be issued. In the case of the specific numerical requirements … compliance is based upon the mean of the distribution of projected doses of DOE's performance assessments which project the performance of the disposal system for 10,000 years after disposal"

Reasonable Expectation (10 CFR 63.304)

- *Reasonable Expectation* means that the Commission is satisfied that compliance will be achieved based upon the full record before it. Characteristics of reasonable expectation include that it:
  1. Requires less than absolute proof because absolute proof is impossible to attain for disposal due to the uncertainty of projecting long-term performance
  2. Accounts for the inherently greater uncertainties in making long-term projections for the performance of the Yucca Mountain disposal system
  3. Does not exclude important parameters from assessments analyses simply because they are difficult to precisely quantify to a high degree of confidence; and
  4. Focuses performance assessments and analyses on the full range of defensible and reasonable parameter distributions rather than only upon extreme physical situations and parameter values

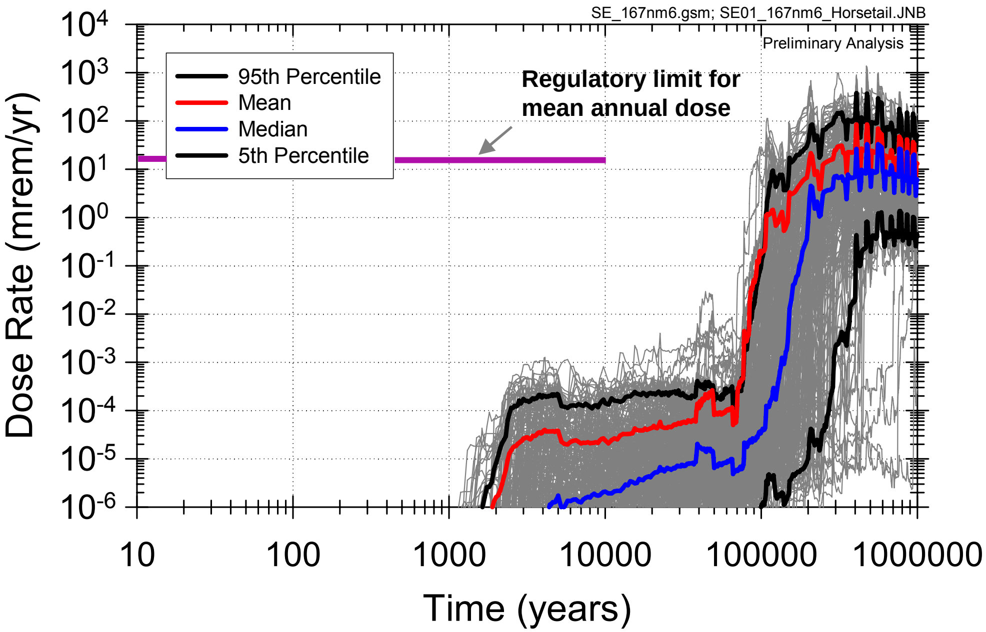
Implementing Reasonable Expectation

- Intent is to encourage objective treatment of uncertainty while avoiding to the extent practicable extreme conservatisms and eliminating potential non-conservatisms
- Project's goal is to create analyses that provide an unbiased treatment of uncertainty
  - Full realism is neither expected nor achievable
- Conservatism remains appropriate and acceptable for the compliance analyses in some circumstances
  - FEP screening justifications may be conservative
  - Conservative assumptions may be used where alternative information is unavailable or not suitable for use in licensing, or where conservatisms save significant resources, or where they allow simplifications that can be shown to have little or not impact
  - Assertions of conservatism must be demonstrated at the system level
- Parallel analyses (the "Performance Margin Analyses" or PMA) will consider alternatives that relax conservative assumptions to evaluate margin in the compliance analyses

Individual Protection Requirements 10,000-year Standards

Representative Dose History

Nominal Performance from 2002 TSPA-FEIS Model



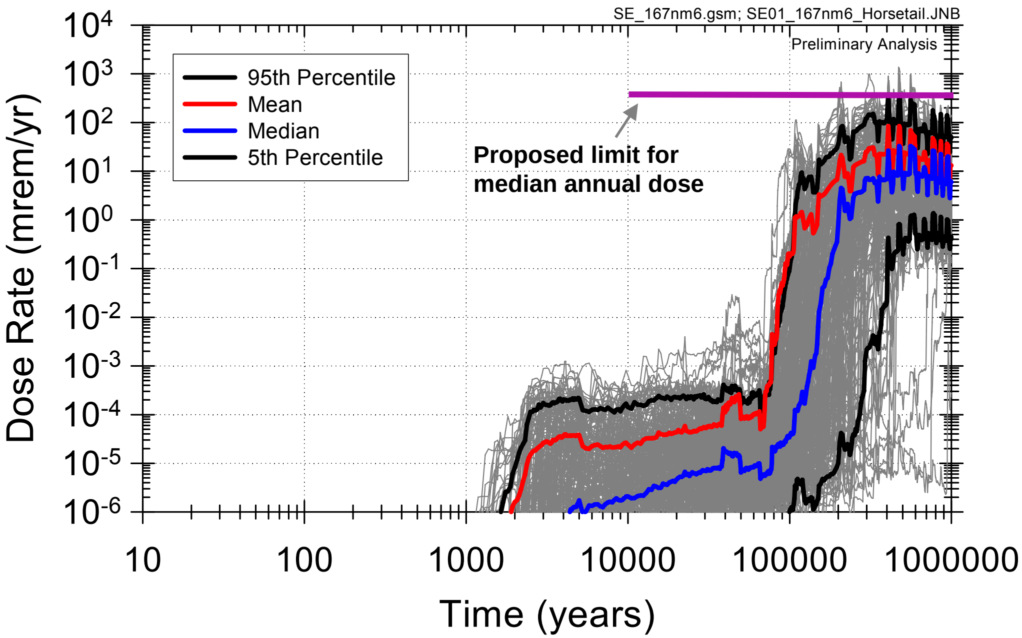
10 CFR 63.311

"DOE must demonstrate, using performance assessment, that there is a reasonable expectation that, for 10,000 years following disposal, the reasonably maximally exposed individual receives no more than an annual dose of 0.15 mSv (15 mrem) from releases from the undisturbed Yucca Mountain disposal system. DOE's analysis must include all potential pathways of radionuclide transport and exposure"

Individual Protection Requirements
Proposed Million-year Standards

Representative Dose History

Nominal Performance from 2002 TSPA-FEIS Model



Proposed 10 CFR 63.303(b)

"Compliance is based upon the median of the projected doses from DOE's performance assessments for the period after 10,000 years of disposal and through the period of geologic stability…"

Proposed 10 CFR 63.311(a)(2)

"DOE must demonstrate…a reasonable expectation… [of an annual dose no more than] … 3.5 mSV (350 mrem) after 10,000 years but within the period of geologic stability."

Other Postclosure Regulatory Standards

- Groundwater Protection Standard 10 CFR 63.331
  - Sets limits on concentrations of radionuclides in groundwater
  - Applies to undisturbed performance only (no disruptive events with annual probabilities less than 10^{-5})
- Human Intrusion Standard 10 CFR 63.321
  - Applies Individual Protection Standards to the conditional consequences of a single, stylized borehole intrusion
  - Applies to undisturbed performance only (no disruptive events with annual probabilities less than 10^{-5})
  - Does not include direct releases to the surface
- Multiple Barrier Requirement 10 CFR 63.115
  - DOE must identify barriers and describe capabilities to limit water flow, radionuclide release, or radionuclide transport
  - No quantitative subsystem requirements; this is a descriptive requirement rather than a performance standard

Regulatory Specifications

- Reasonably maximally exposed individual
  - Lives in the accessible environment above the point of highest concentration in the contaminated plume
  - Has diet and lifestyle of today's inhabitants of Amargosa Valley
  - Drinks 2 liters of contaminated groundwater per day with concentrations based on annual water use of 3000 acre-feet
  - Is an adult
- DOE should not project changes in society, biosphere (other than climate), human biology, or increases in human knowledge
- DOE must vary factors related to the geology, hydrology, and climate based on cautious, but reasonable assumptions consistent with present knowledge

Features, Events, and Processes

FEP Analysis and Scenario Development

- Purpose: … *focus the representation of the system on those features, events, and processes that most affect compliance with the overall performance objective*
  (Yucca Mountain Review Plan [YMRP], NUREG-1804, Section 2.2.1.2)
- Four-part process described by NRC (YMRP Section 2.2.1.2)
  - Identification of an initial list of FEPs
  - Screening of the initial list of FEPs
  - Formation of scenario classes using the reduced set of FEPs
  - Screening of scenario classes
- Overall methodology based on Cranwell et al., 1990 (NUREG/CR-1667)

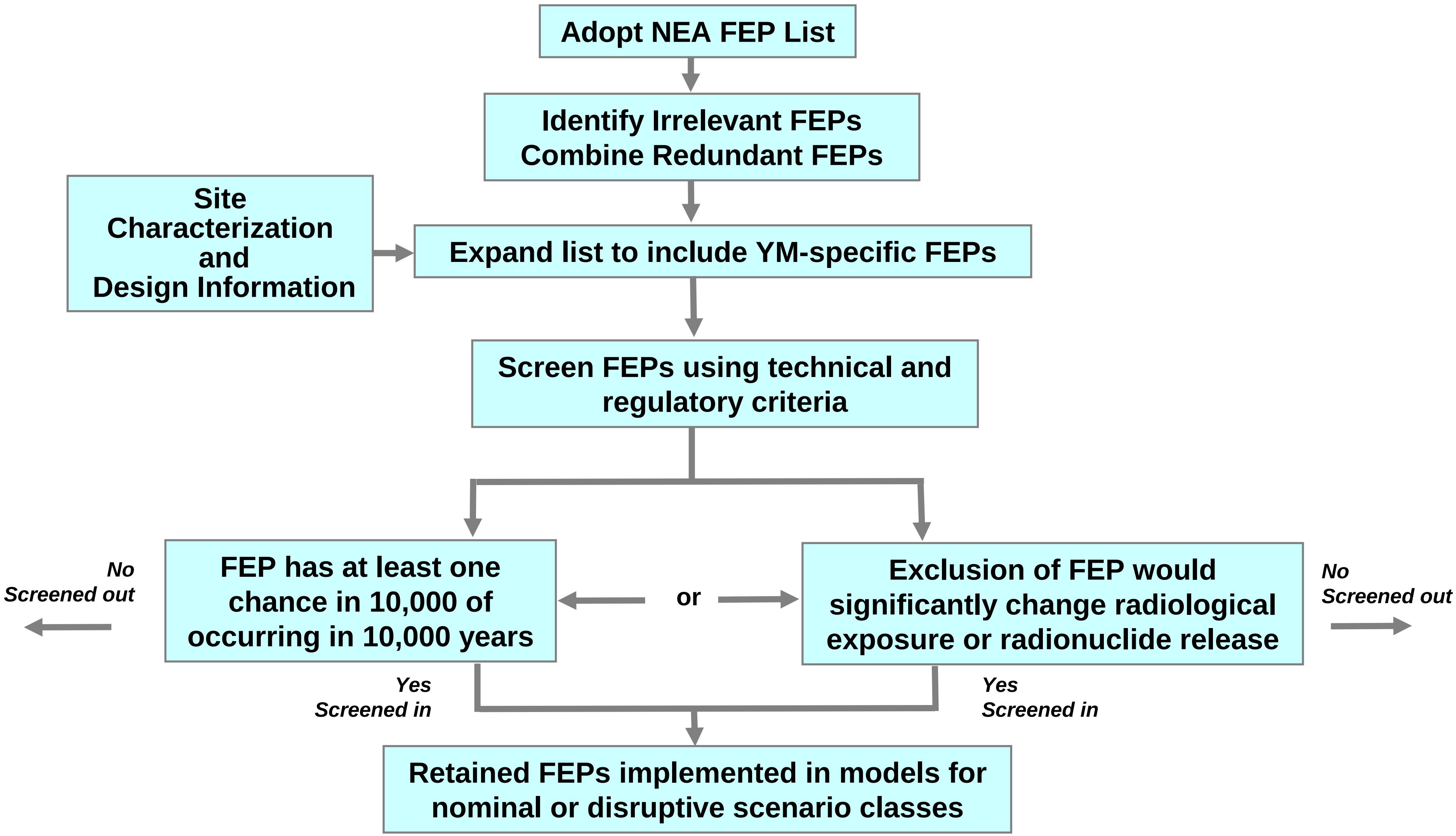
Identification of Initial YMP FEP List

- Initial FEP list for the 2001 SR
  - 1261 FEPs from NEA international database
    - Canada, Sweden, Switzerland, U.K., WIPP
  - 292 site-specific FEPs from Yucca Mountain Project (YMP) literature
  - 95 additional FEPs from internal technical review
  - 8 additional FEPs from external review
    - NRC audits, Key Technical Issue meetings
- Grouped for SR into 328 “primary” FEPs
- Reorganized into 375 FEPs for the license application (LA)

Identification of YMP PA FEPs

- Builds on TSPA-SR FEP list
- 375 YMP FEPs for PA
  - Each FEP encompasses a single process or event, or a few closely related or coupled processes
  - Each FEP is aggregated to the coarsest level at which a technically sound screening decision can be made while still maintaining adequate detail for analysis
  - YMP FEPs are a comprehensive list that address all issues identified from:
    - NEA international FEP database
    - Site-specific FEPs from YMP literature
    - Iterative reviews of earlier YMP FEP lists
    - Evaluation of multiple classification structures
    - Independent analysis using interaction diagrams
  - FEP configuration management process to identify and track the effect of ongoing work and design changes on FEPs

Evaluating Features, Events, and Processes



Documentation of FEPs

- FEPs have been documented to date in 10 topical analysis/model reports (AMRs)
  - Each FEP discussion includes
    - FEP description
    - FEP screening decision with justification
    - Reference to description of implementation of included FEPs
- Final FEP documentation will be provided in a single report
- Preliminary FEP documentation to date is available in a searchable Microsoft Access database
  - FEP Database content provided for background information only; newer updates to two AMRs (UZ and SZ) are available on the OCRWM website
  - Some FEPs discussions are changing significantly as a result of current work, and users should confirm information with project staff

Scenario Classes for Yucca Mountain

- Definition and division of scenario classes is based on the type of screened-in initiating events
- Representations of possible future states of the repository
  - Igneous scenario class
    - Contains included features, events, and processes (FEPs) associated with igneous disruption
  - Seismic scenario class
    - Contains included FEPs associated with seismic disruption
  - Early failure scenario class
    - Contains included FEPs associated with early failures of waste package (WP) and drip shield (DS) failures
  - Nominal scenario class
    - Contains all included FEPs anticipated to occur in the absence of disruption, intrusion, and early failures of WP and DS
  - Human intrusion scenario/assessment (a special regulatory case)
    - Contains included FEPs associated with drilling intrusion

Features, Events, and Processes Considered for Corrosion Model

- Error in waste emplacement
- General corrosion of the waste package
- General corrosion of the drip shields
- SCC of waste packages
- SCC of drip shields
- LC of waste packages
- LC of drip shields
- Hydride cracking of waste packages
- Hydride cracking of drip shields
- MIC of waste packages
- MIC of drip shields
- Internal corrosion of waste packages prior to breach
- Mechanical impact on waste package
- Mechanical impact on drip shields
- Early failure of waste packages
- Early failure of drip shields
- Copper corrosion in EBS
- LC on WPOB due to dust deliquescence
- Physical form of waste package and drip shield
- Oxygen embrittlement of the drip shields
- Mechanical effects at EBS component interfaces
- Rockfall
- Creep of metallic materials in the waste package
- Creep of metallic materials in the drip shield
- Volume increase of corrosion products impacts waste package
- Electrochemical effects in EBS
- Thermal sensitization of waste packages
- Thermal sensitization of drip shields
- Thermal expansion/Stress of in-drift EBS components
- Gas generation (H_2) from waste package corrosion
- Radiolysis
- Radiation damage in EBS

From ANL-EBS-PA-000002, Rev. 5

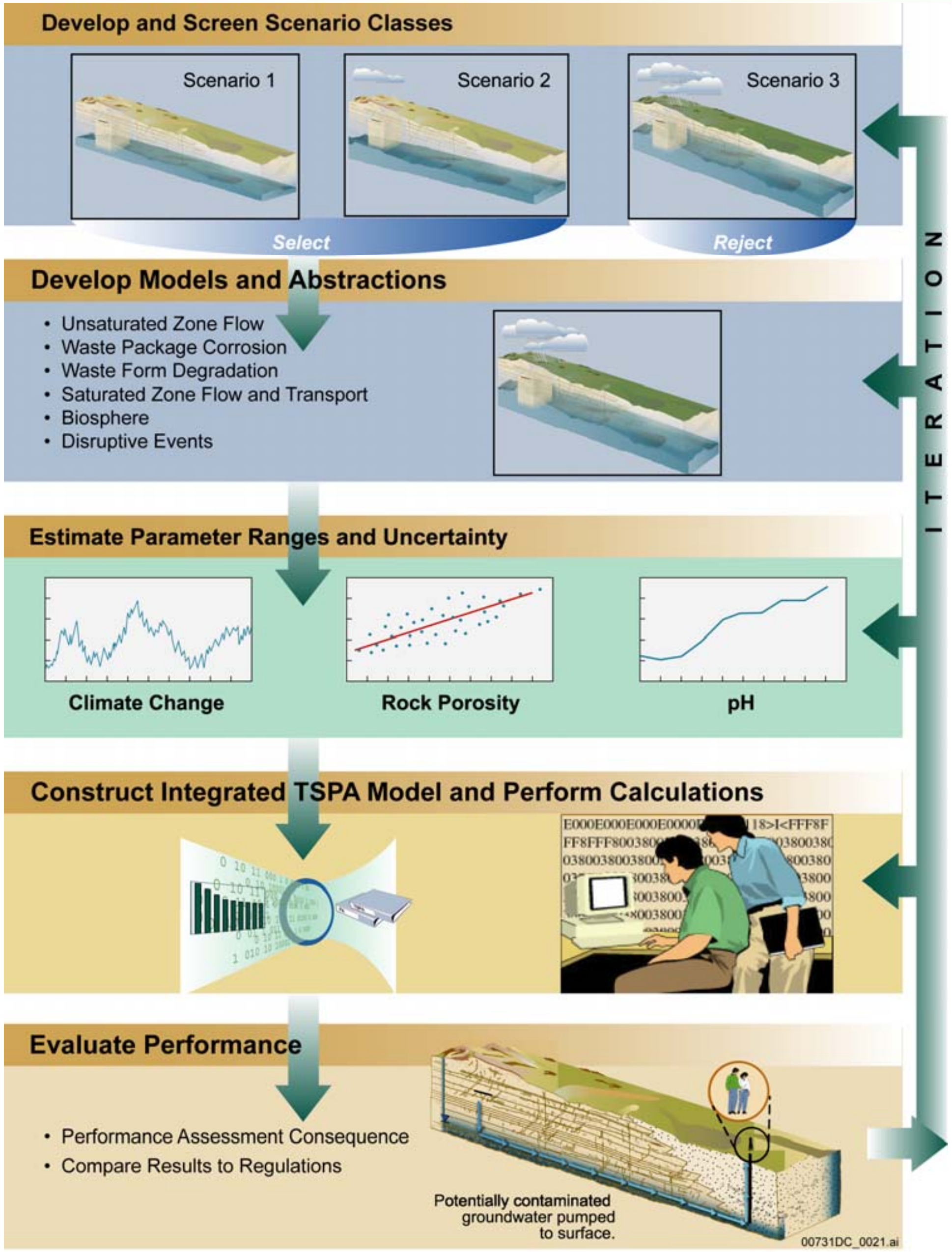
Total System Performance Assessment

Key Requirements for TSPA

- Provide a clearly traceable and transparent roadmap for the inclusion of specific features, events, and processes (FEPs) in the TSPA Model
- Compute dose to the reasonably maximally exposed individual for the various standards (individual protection, human intrusion)
  - Include the effect of parameter and model uncertainty on the results (Monte-Carlo-based analysis)
  - Answer the risk triplet in clear, systematic fashion
- Demonstrate capability of multiple barriers
- Compute groundwater concentrations at the accessible environment
- Be transparent, traceable, and controlled under the applicable QA procedures
- Be designed in such a way that model validation and confidence (i.e., technical bases) can be transparently demonstrated

Major Steps in the Iterative TSPA

- Screen FEPs and develop scenario classes
- Develop models and abstractions, along with their scientific basis, for logical groupings of FEPs within scenario classes
- Evaluate uncertainty in models and parameters
- Construct integrated TSPA model using all retained FEPs and perform calculations for the scenario classes and "modeling cases" within scenario classes
- Evaluate total-system performance; incorporating uncertainty through Monte Carlo simulation



Treatment of Uncertainty in TSPA

- Q1: What can happen?
- Q2: How likely is it to happen?
- Q3: What are the consequences if it does happen?
- Guidance from NRC's YMRP
  - *Risk-Informed Review Process for Performance Assessment*—***The performance assessment quantifies repository performance, as a means of demonstrating compliance with the postclosure performance objectives at 10 CFR 63.113. The U.S. Department of Energy performance assessment is a systematic analysis that answers the triplet risk questions: what can happen; how likely is it to happen; and what are the consequences.***
    (NUREG-1804, p. 2.2-1)
- Q4: What is the uncertainty in the answers to the first three questions?

Uncertainty in TSPA

- *Aleatory* uncertainty = inherent randomness in events that could occur in the future
  - Alternative descriptors: irreducible, stochastic, intrinsic, type A
  - Examples:
    - Time and size of an igneous event
    - Time and size of a seismic event
- *Epistemic* uncertainty = lack of knowledge about appropriate value to use for a quantity assumed to have a fixed value
  - Alternative descriptors: reducible, subjective, state of knowledge, type B
  - Examples:
    - Permeabilities, porosities, sorption coefficients, …
    - Rates defining Poisson processes
- Monte Carlo techniques used to incorporate uncertainty in modeling, particularly the epistemic uncertainty

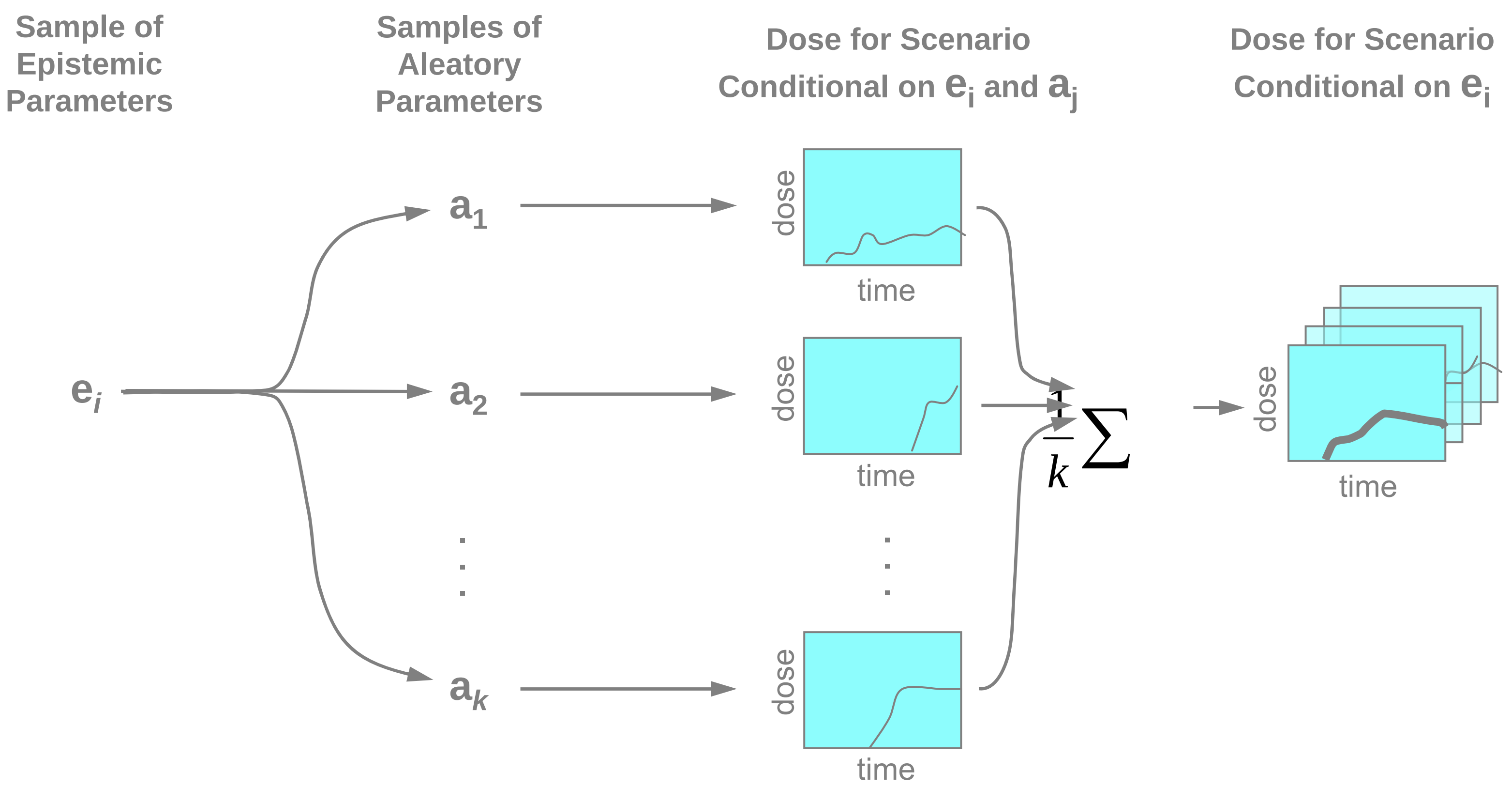
Basic Concepts Underlying TSPA

- Probabilistic characterization of what can happen in the future
  - Answers first two questions in the “risk-triplet”
  - Provides formal characterization of aleatory uncertainty
  - *E.g., assumption that igneous event occurrence is a Poisson process*
- Mathematical models for predicting consequences
  - Answers third question in the “risk-triplet”
  - *E.g., models implemented in GoldSim*
- Probabilistic characterization of uncertainty in TSPA inputs
  - Basis for answering fourth question
  - Provides formal characterization of epistemic uncertainty
  - *E.g., distribution assigned to λ (annual frequency) in Poisson process for igneous event*

Construction of Mean Annual Dose to the RMEI

- Probability-weighted sum of the four major scenario classes:
  - Nominal scenario class
  - Seismic scenario class
  - Igneous scenario class
  - Early-failure scenario class

Calculating the Annual Dose By Scenario Average over Aleatory Uncertainty

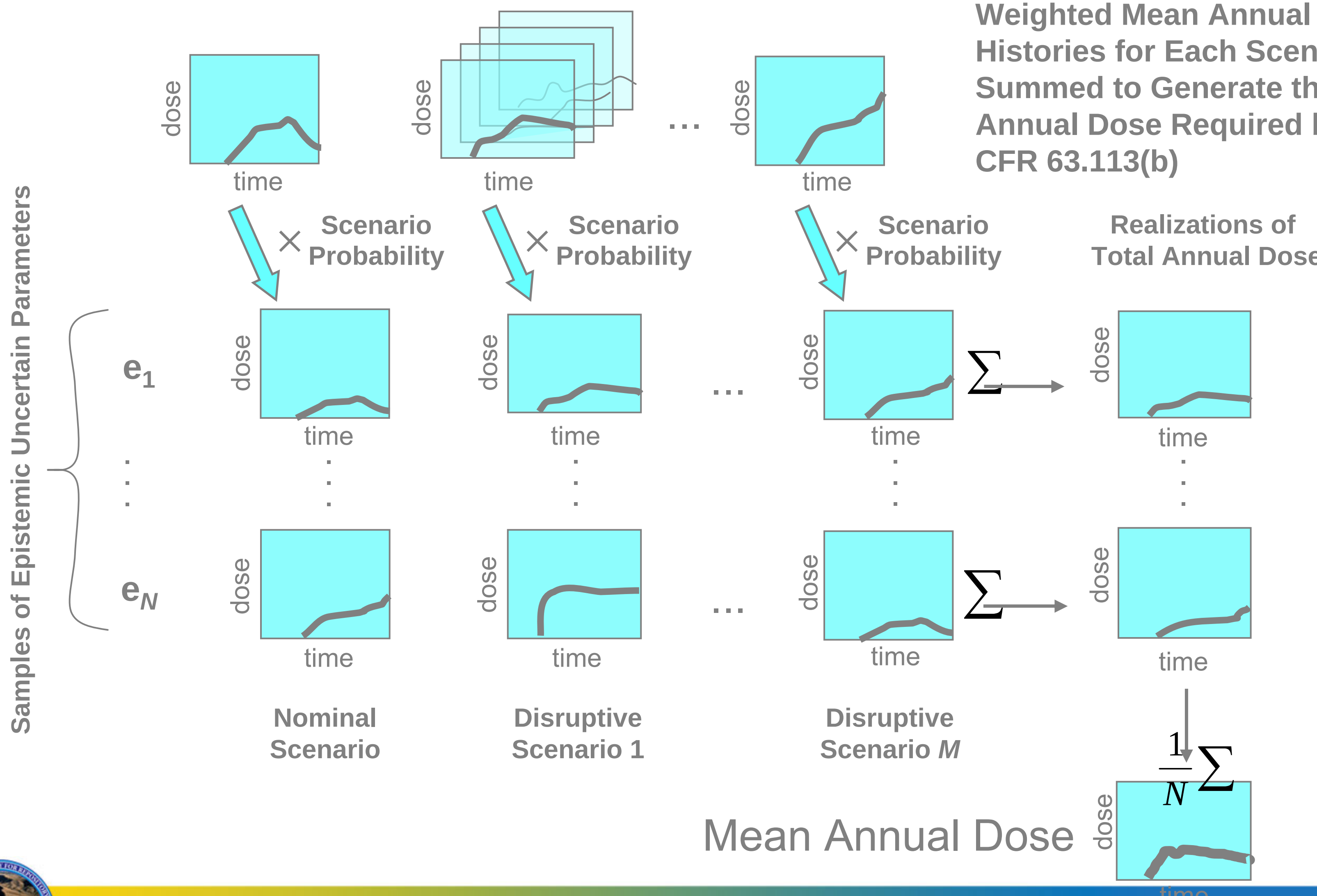


- rate for disruptive event
- permeabilities
- porosities

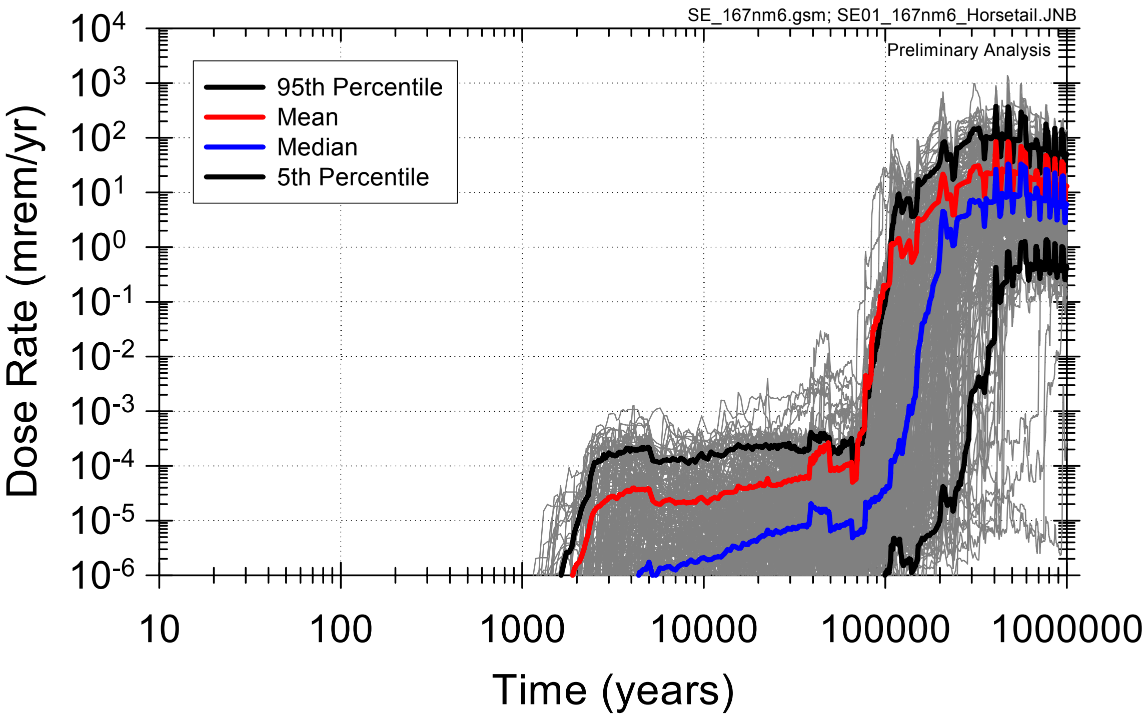
- time of disruptive event
- magnitude of event
- fraction of WP affected

Calculating the Mean Annual Dose
Average over Epistemic Uncertainty

Weighted Mean Annual Dose Histories for Each Scenario are Summed to Generate the Mean Annual Dose Required by 10 CFR 63.113(b)



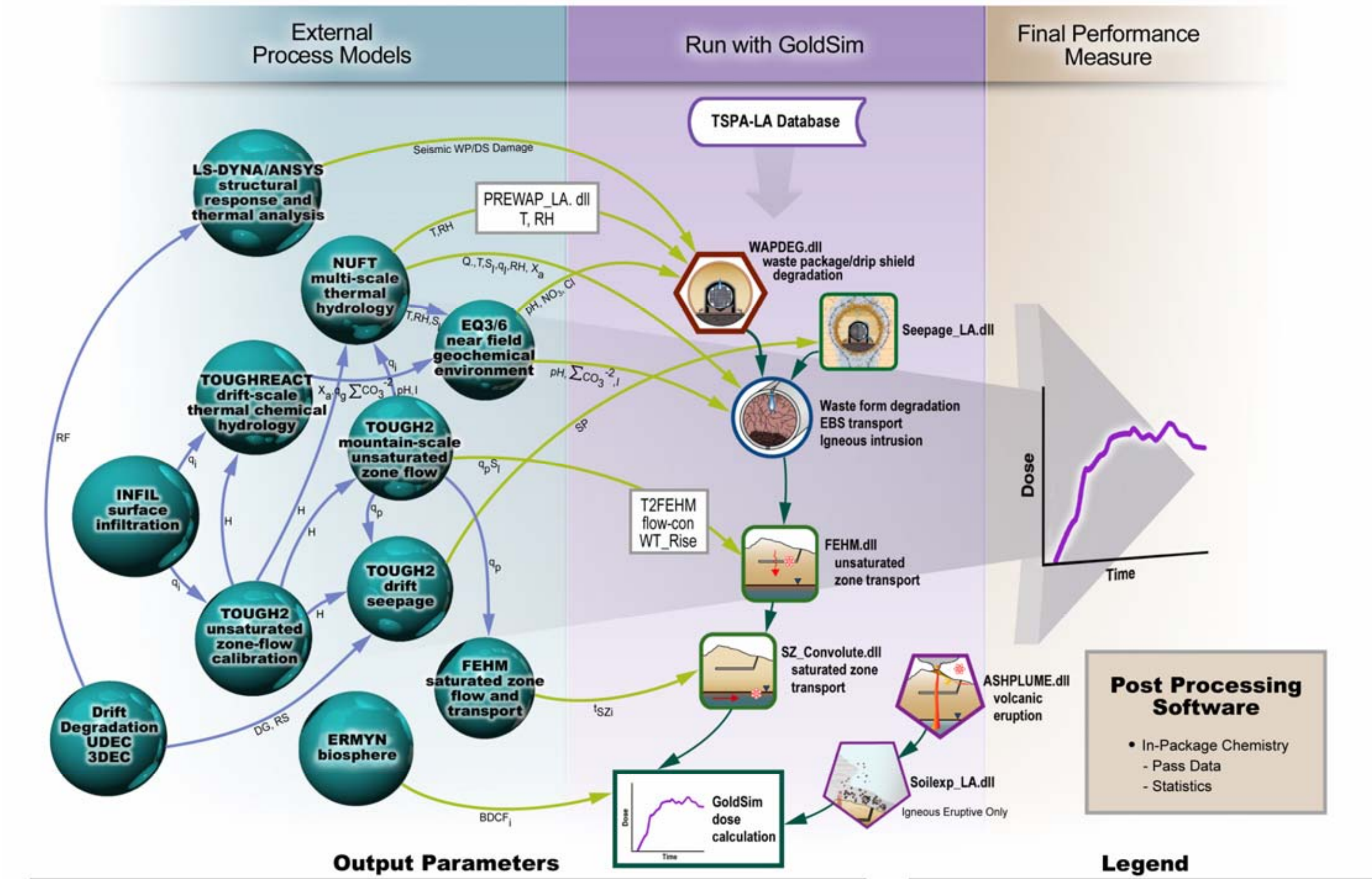
"Horsetail" Plot – 300 Realizations of Epistemic Uncertainty 2002 Example, Nominal Performance Only



Mean annual dose based on 300 realizations of high-temperature operating mode nominal performance. Models and input values are preliminary. Results are for information only, and are not suitable for comparison to regulatory standards. ANL-WIS-PA-000004 Rev. 00 ICN 01 (2002 "one-on analysis" case 12).

- Each curve is a dose history calculated using a single set of sampled input parameter values
- Summary statistical measures are derived from the distribution of model outcomes
- Stability of the mean (or other summary measure) is related to sample size
- Distribution of model results allows detailed sensitivity and uncertainty analysis of intermediate performance measures

TSPA Architecture



Output Parameters

f_S	Fraction of WPs with Seeps	T	Temperature	I	Ionic Strength
EBS	Engineered Barrier System	RH	Relative Humidity	t_{SZi}	Saturated Zone Transport Time
Q_S	Seep Flow Rate	S_l	Liquid Saturation	$BDCF_i$	Biosphere Dose Conversion Factor
Q.	Evaporation Rate	X_a	Air Mass Fraction	q_g	Gas Flux
pH	pH	q_l	Liquid Flux	H	Hydrologic Properties
ΣCO_3^{-2}	Carbonate Concentration	q_i	Infiltration Flux	SP	Seepage Parameters
q_p	Percolation Flux	DG	Drift Geometry	RS	Rock Strength
NO_3	Nitrate Concentration	Cl	Chloride Concentration	RF	Rock Fall Size and Number

Legend

- Response Surface Between Process Models
- Response Surface from Process Model to GoldSim
- Connection in GoldSim
- Preprocessor

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Confidence in Component and System Models

- Multiple approaches to building confidence in component and system models
  - Corroboration with direct observation
  - Corroboration with analog information
  - Corroboration with independent evaluations
  - Corroboration with auxiliary analyses and by comparison of system and subsystem analyses
  - Peer review
- Component models are evaluated individually and in the context of the system model

Acknowledging Uncertainty

- Sources of Uncertainty
  - Incomplete data
    - E.g., hydrologic material properties can never be obtained for all locations
  - Spatial variability and scaling issues
    - E.g., data may be available from small volumes or discrete locations but may be used in models to represent large volumes
  - Measurement error
    - Usually only a minor contributor to total uncertainty
  - Lack of knowledge about the future state of the system
    - E.g., uncertainty about the occurrence of disruptive events
  - Alternative conceptual models
- Monte Carlo techniques used to incorporate uncertainty in modeling

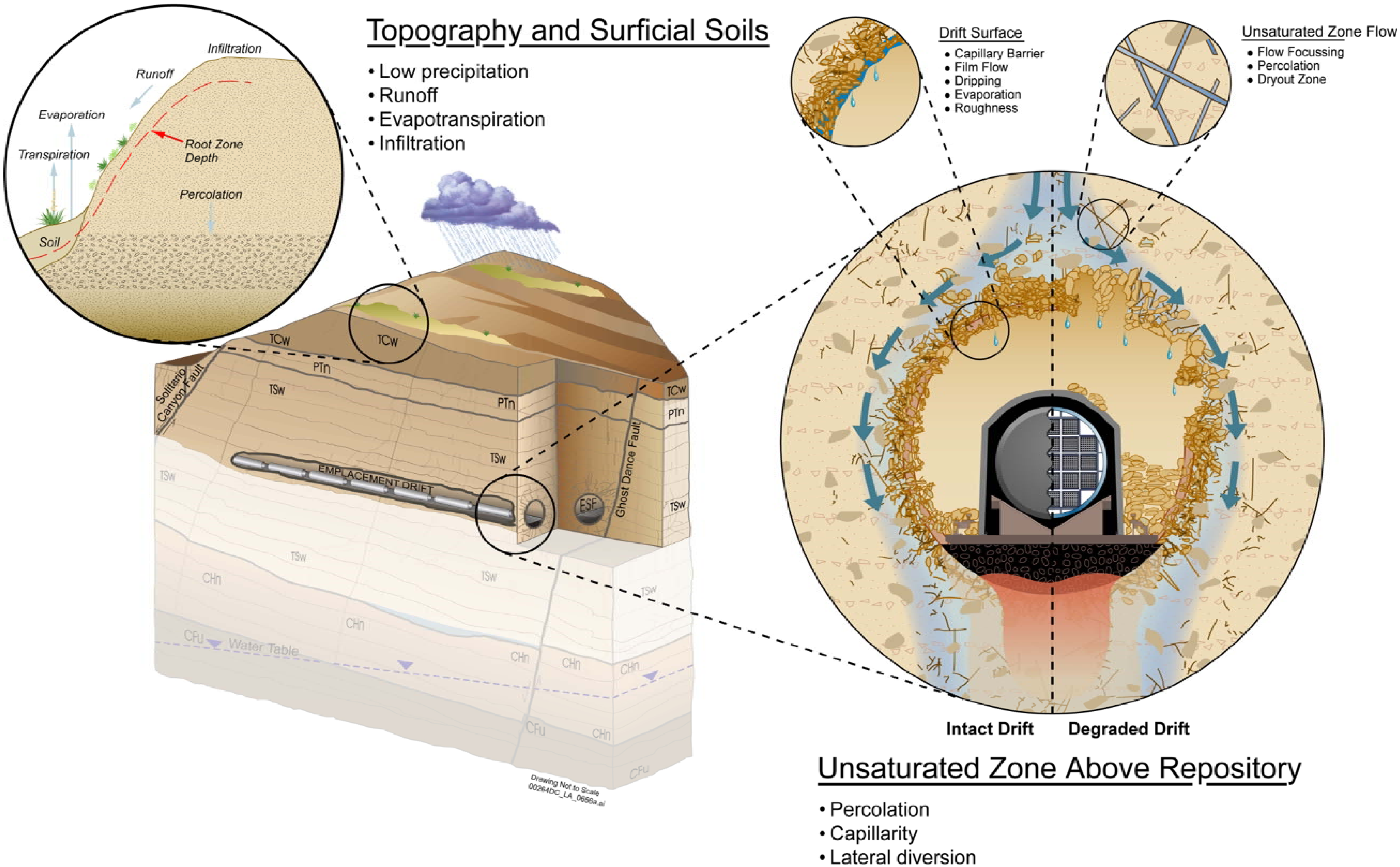
Representative Quantitative Estimates of Barrier Capability and System Performance

All quantitative model results shown in this presentation are for illustration purposes, and are not intended for comparison to regulatory standards

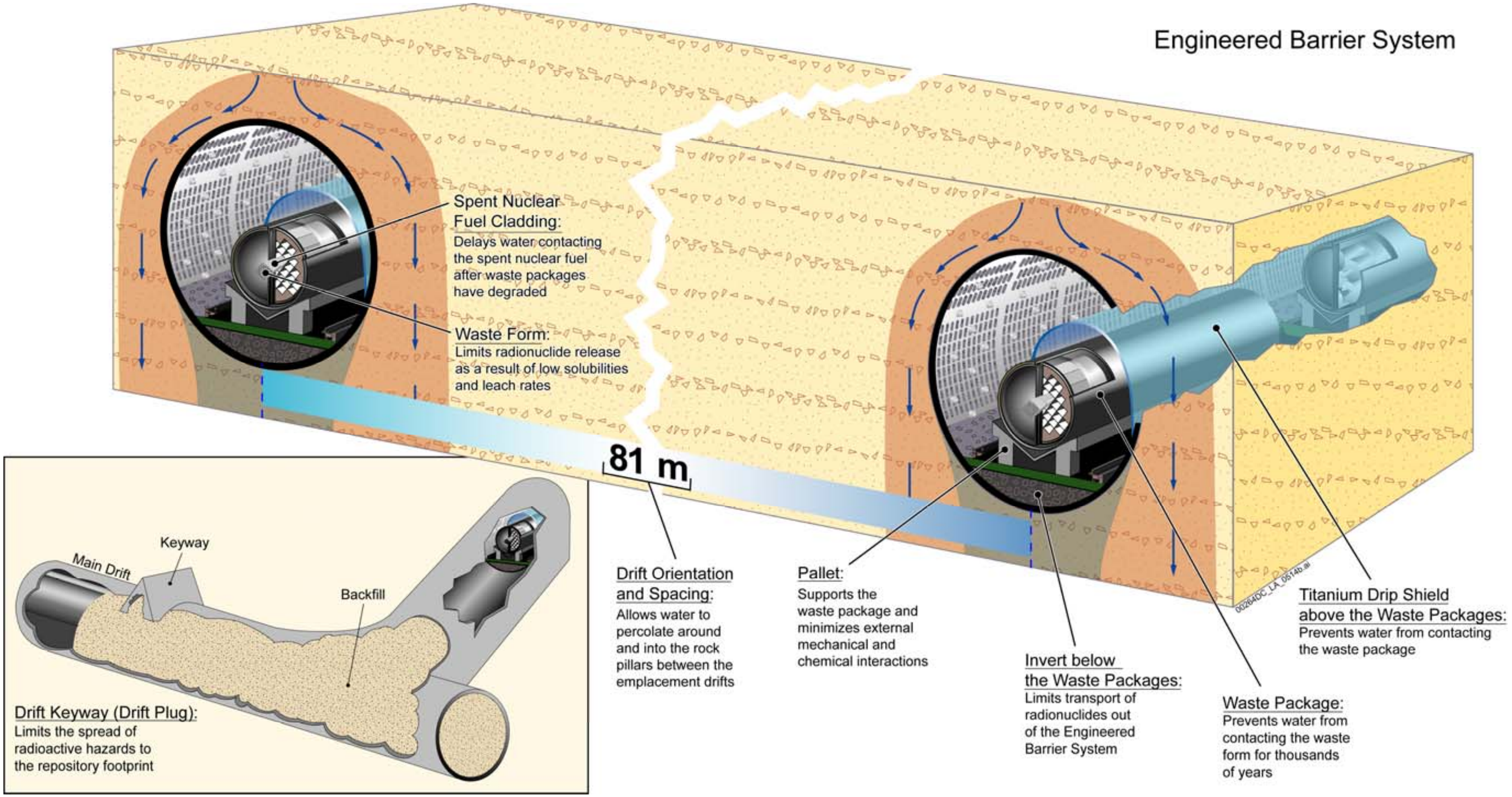
Barrier Capability

- Barriers may
  - Limit water reaching the waste
  - Limit the release of radionuclides from the waste form
  - Limit the transport of radionuclides from the waste form to the human environment
- Barrier performance may be evaluated separately or as part of a system
  - Separately, barrier components have potential capabilities that may not be fully realized within the full system
  - The full system relies on complementary and overlapping capabilities of multiple barriers to ensure performance

Upper Natural Barrier



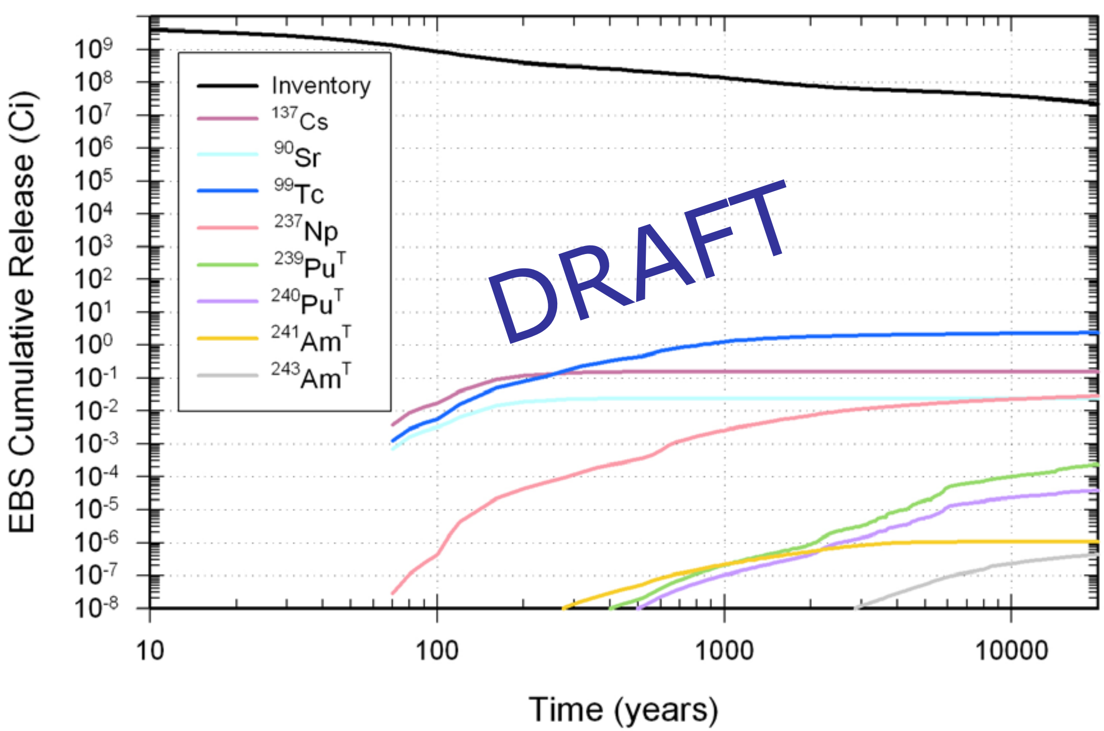
Engineered Barrier System



Example Barrier Capability

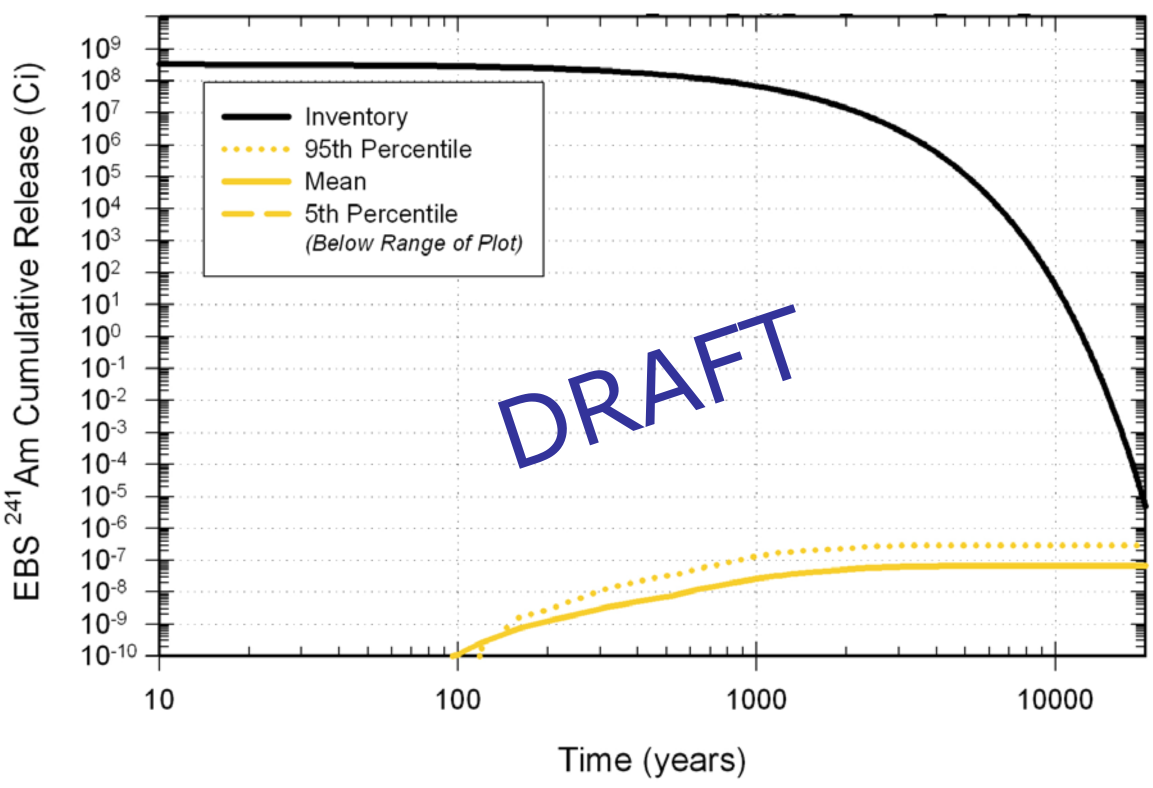
Engineered Barrier System

- Draft cumulative releases from the engineered barrier system
  - Results shown for preliminary analyses of nominal performance with early waste package failures and intact drip shields
  - Total radionuclide inventory (curies) shown for comparison
- The engineered barrier system has the potential to retain the overwhelming majority of the total radioactivity for 10,000 years and beyond

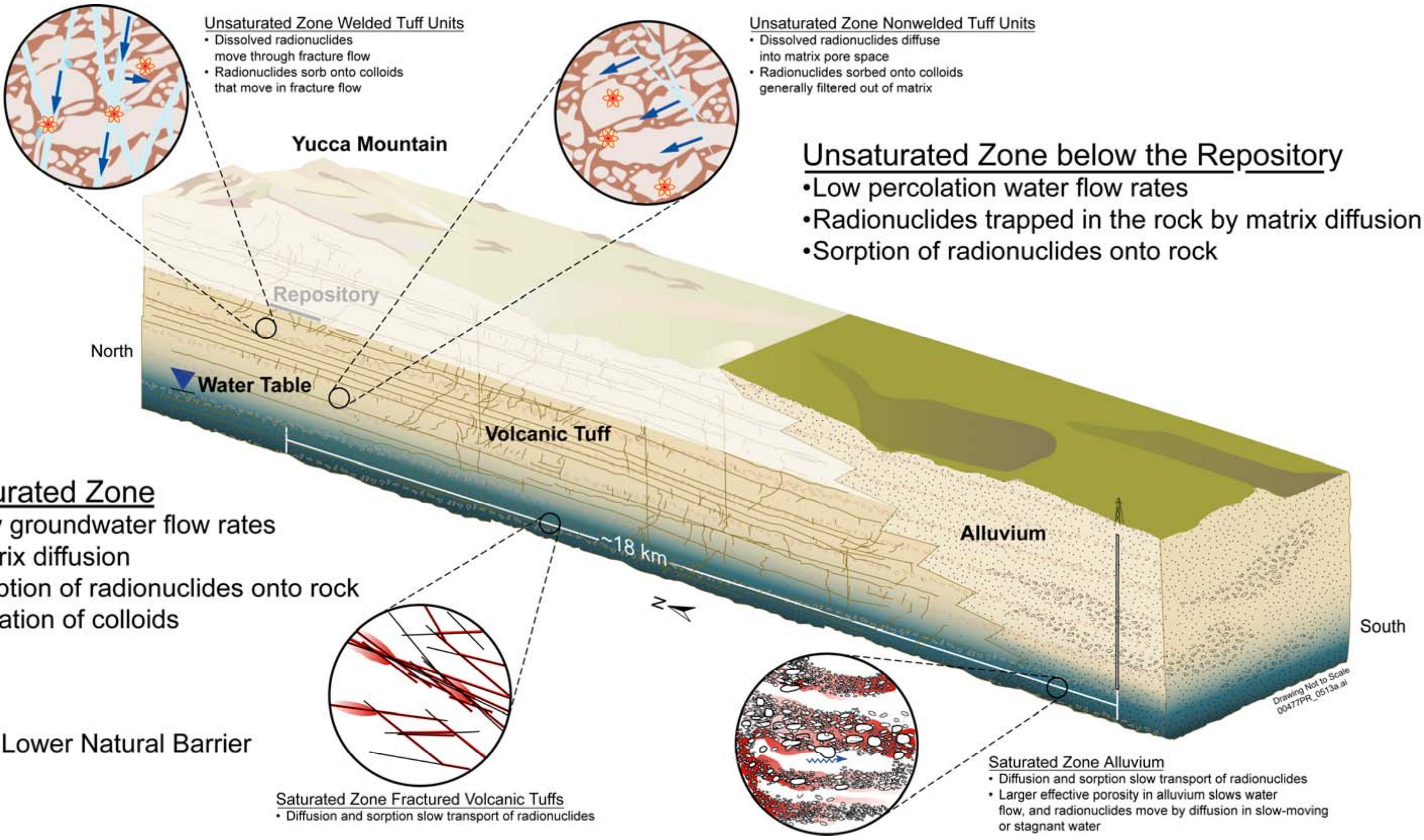


Example Barrier Capability
Engineered Barrier System (cont.)

- Draft cumulative releases of a single species (^{241}Am) from the engineered barrier system
  - Results shown for preliminary analyses of nominal performance with early waste package failures and intact drip shields
  - Total ^{241}Am inventory (curies) shown for comparison



Lower Natural Barrier



Unsaturated Zone below the Repository

- Low percolation water flow rates
- Radionuclides trapped in the rock by matrix diffusion
- Sorption of radionuclides onto rock

Saturated Zone

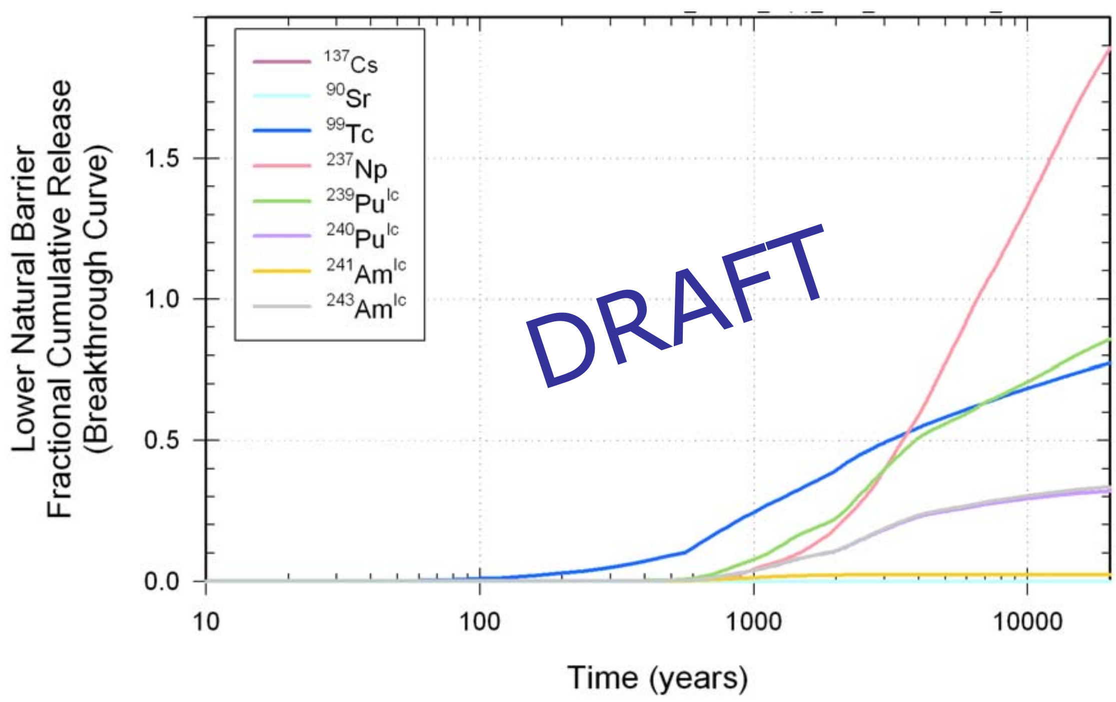
- Low groundwater flow rates
- Matrix diffusion
- Sorption of radionuclides onto rock
- Filtration of colloids

Lower Natural Barrier

Example Barrier Capability

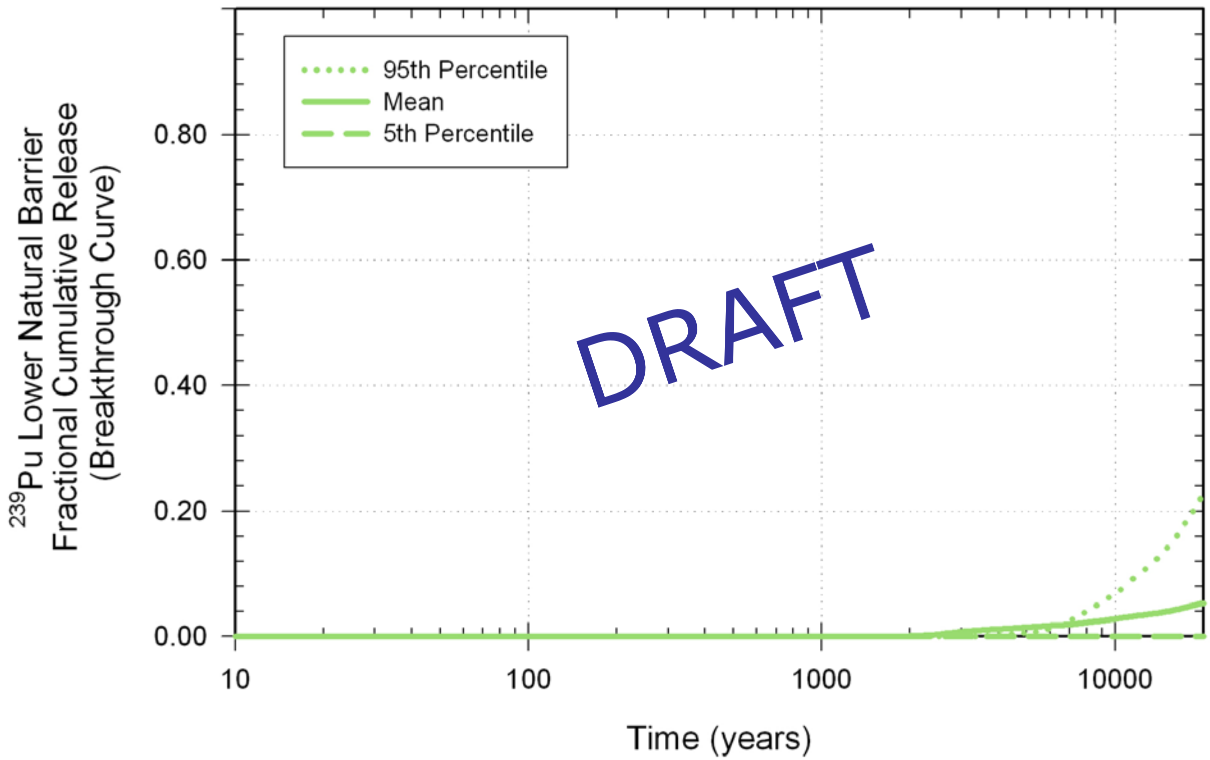
Lower Natural Barrier System (cont.)

- Draft releases from the lower natural barrier system
  - Mean cumulative fractional releases from a hypothetical unit pulse at time zero
  - Radioactive decay and ingrowth are included
- The lower natural barrier has the potential to retain most radiouclides many thousands of years; some species much longer



Example Barrier Capability
Lower Natural Barrier System (cont.)

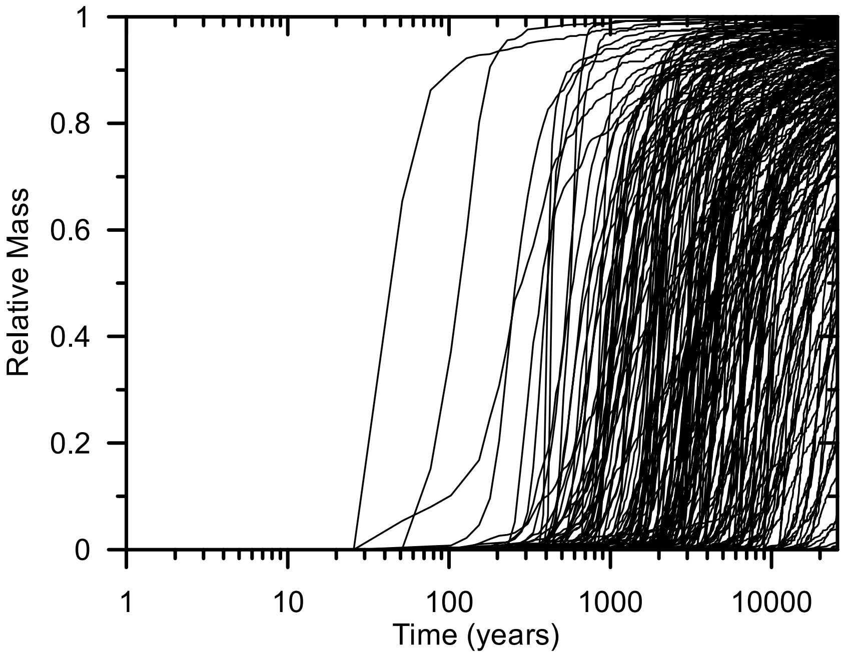
- Draft releases of ^{239}Pu from the lower natural barrier system: example for a strongly-sorbing species
  - Mean cumulative fractional releases of dissolved ^{239}Pu from a hypothetical unit pulse at time zero
  - Radioactive decay and ingrowth are included

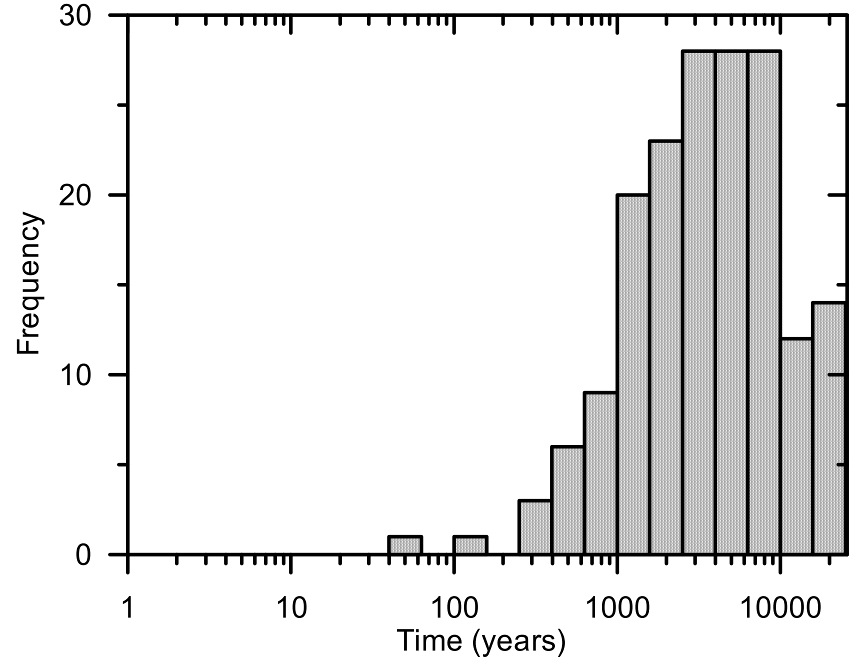


Example Barrier Component Capability

Saturated Zone Transport

Np: A Moderately-Sorbing Species





Mass breakthrough fraction (left) and distribution of median transport times (right)

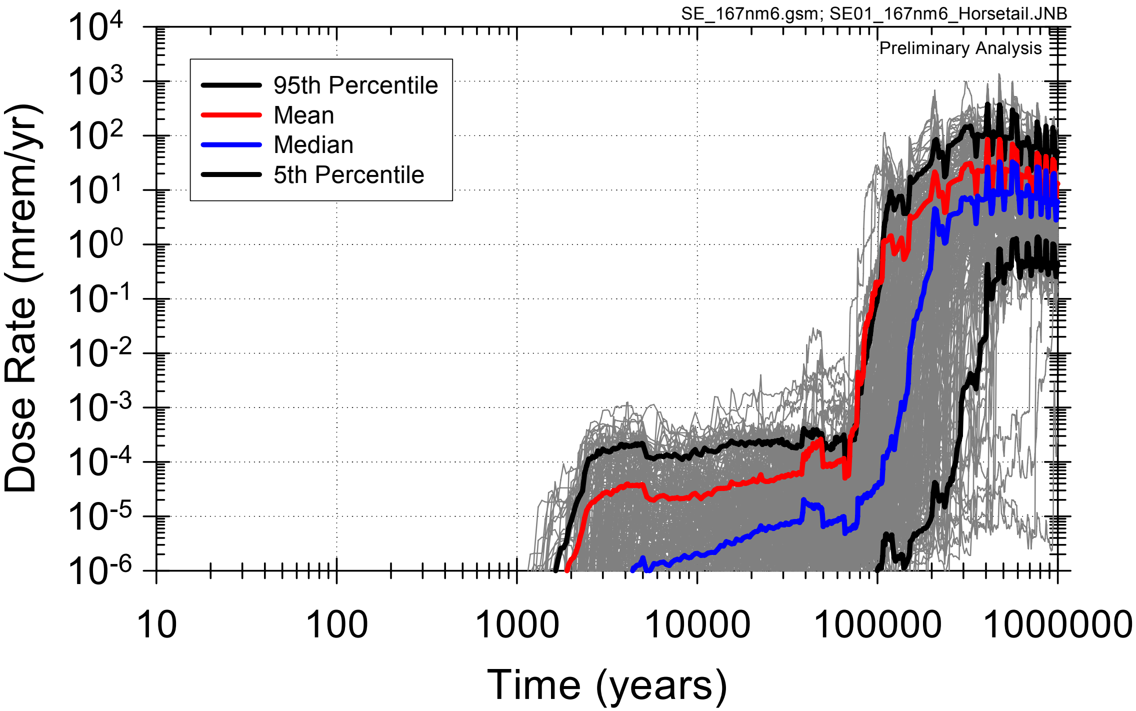
Multiple realizations showing uncertainty in material properties

Radioactive decay and ingrowth not included

MDL-NBS-HS-000021 Rev. 02, Figure 6-42. Preliminary results for illustration purposes only. Glacial transition climate.

System Performance

2002 Example, Nominal Performance Only



Mean annual dose based on 300 realizations of high-temperature operating mode nominal performance. Models and input values are preliminary. Results are for information only, and are not suitable for comparison to regulatory standards. ANL-WIS-PA-000004 Rev. 00 ICN 01 (2002 "one-on analysis" case 12).

Each curve is a dose history calculated using a single set of sampled input parameter values

Each curve is a possible "realization" of the model; each is an equally likely outcome of the model

Summary statistical measures are derived from the distribution of model outcomes

Stability of the mean (or median) is related to sample size

Distribution of model results allows detailed sensitivity and uncertainty analysis of intermediate performance measures

In-Drift Environmental Conditions

Two Types of Chemical Environments

Deliquescence

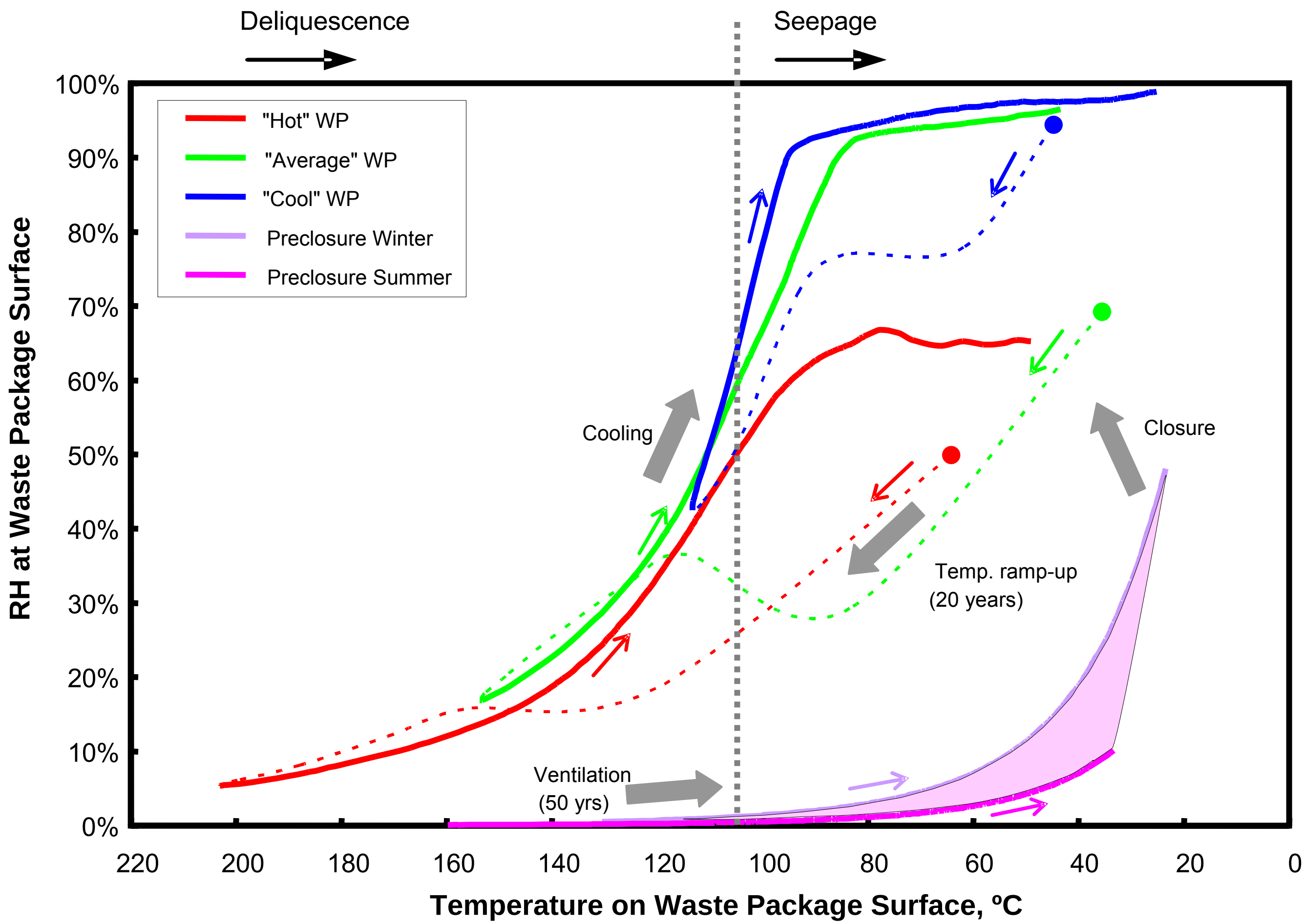
- Soluble salts deposited on the WP during pre-closure
- Drip shields control post-closure dust accumulation
- Multi-salt assemblages control deliquescence at higher temperatures
- Brine compositions become dilute as T decreases and RH increases
- Amount of brine contacting metal surfaces is limited
- Chemistry is moderated by contact with rock-forming minerals in dust
- Brines change with time due to degassing, deliquescence

Seepage

- Seepage may occur after cooldown (T_{WP} < 105°C)
- WP outer barrier is protected by the drip shields
- Residence time (equilibrium with T, RH at WP surface) controls the corrosion environment
- Chemical conditions (pH, Cl^-, NO_3^-, NO_3^-/Cl^-) are potentially corrosive early during cooldown
- Chemical fractionation may occur during transport

Evolution of Temperature/RH on the Waste Package Surface

Deliquescence can occur immediately after closure. Seepage can occur only after the drift wall drops below 100ºC (max waste package temperature ~105ºC).



DTN: SN0508T0502205.015

Relevant Dust Sources and Composition

Current model is based on two sources of dust:

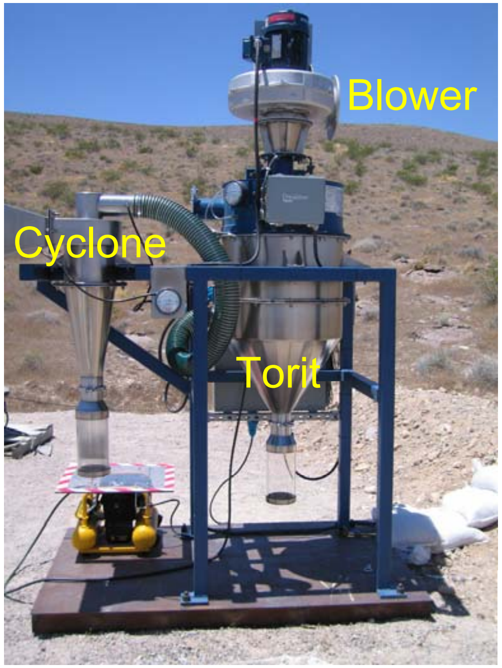
- Yucca Mountain tunnel dusts
  - Dominantly rock powder, <1% highly soluble salts (Peterman et al., 2003, *IHLRWM Conf. Proceedings*)
  - Important deliquescent mineral assemblages:
    - $NaCl-KNO_3$
    - $NaCl-KNO_3-NaNO_3$
    - $NaCl-KNO_3-NaNO_3-Ca(NO_3)_2$
- Atmospheric dust
  - Site-specific data, 6 locations near YM (Reheis and Kihl, *JGR*, 1995)
    - Highly soluble salt load—10.5% (avg)
    - Carbonate content—9.5% (avg)
  - Solubles—NADP regional precipitation (rain-out) data

Sample #	Ca mg/L	Mg mg/L	K mg/L	Na mg/L	NH_4^+ mg/L	NO_3^- mg/L	Cl^- mg/L	SO_4^{2-} mg/L	NO_3^-/Cl^-
NV00-2002	0.48	0.044	0.013	0.059	0.26	1.14	0.09	0.46	7.3
NV00-2001	0.66	0.068	0.042	0.113	0.69	2.15	0.16	1.01	7.7
NV00-2000	1.21	0.137	0.055	0.263	1.01	3.24	0.36	1.35	5.2

NADP/NTN 2000, Part 2.; NADP/NTN 2001, Part 2.; NADP/NTN 2002, Part 2.

Site-specific Dust Samples for Planned Update

- South Pad cyclonic collector (300 cfm):
  - Began operating on 6/29/2005
  - A moisture sensor and controller stop the blower during rainstorms
  - Two collectors
    - Cyclone separator for large particles (>5 μm)
    - Torit filtration separator for smaller particles (to <0.5 μm)



Analyses (averages of duplicated analyses)

Collection Date Ending:	Ca mg/L	Mg mg/L	K mg/L	Na mg/L	NH_4^+ mg/L	NO_3^- mg/L	Cl^- mg/L	SO_4^{2-} mg/L	NO_3^-/Cl^-	HCO_3^- mg/L	TDS %
03-Aug-05	2260	525	852	950	59.8	6690	548	1580	7.0	2820	1.68
08-Sep-05	1190	301	664	644	97.6	3100	389	725	4.6	291	0.79
10-Jan-06	598	1290	1640	12500	112	29000	2600	15600	6.4	449.5	6.97
18-May-06	4370	1040	1580	4510	232	16500	1840	6150	5.1	4310	4.12
07-Jun-06	3240	758	1530	2940	446	11400	1510	4080	4.3	4930	3.14

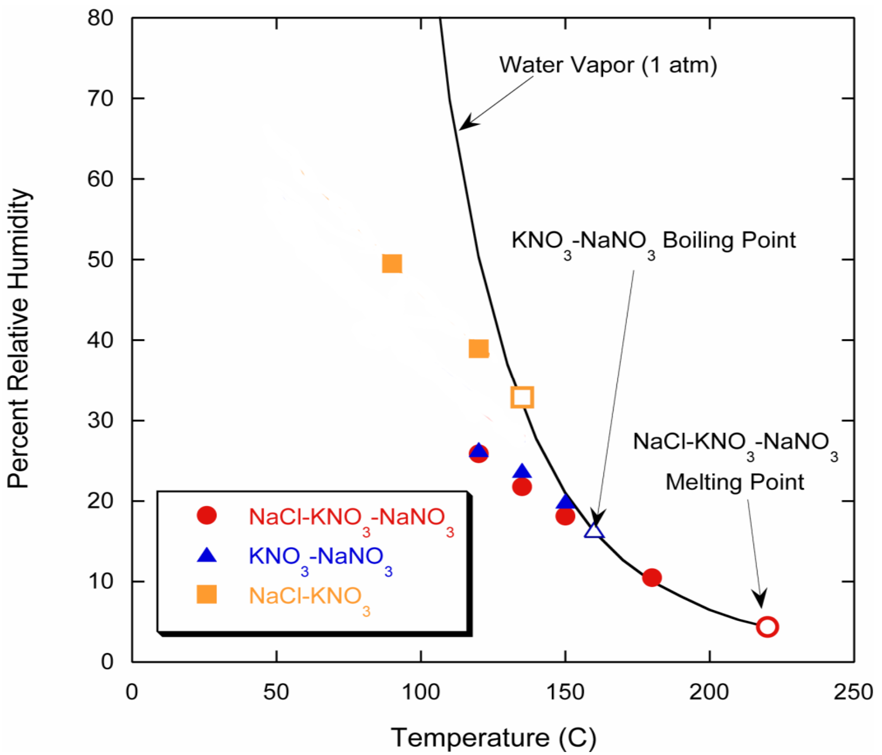
Preliminary Data – DTN TBD

Conditions of Deliquescence

Experimental data:

- Ammonium salts thermally decompose and won't contribute to the deliquescent mineral assemblages
- NaCl - KNO_3 → 134ºC
- NaCl - KNO_3 - $NaNO_3$ → transition to hydrous melt at 220ºC, Dryout at ~300ºC
- NaCl - KNO_3 - $NaNO_3$ - $Ca(NO_3)_2$ → boiling point >400ºC
- Maximum temperature at the waste package surface: 203ºC

(ANL-EBS-MD-000049 Rev. 03)



DTNs: LL050903412251.150
LL050901931032.009
LL050800623121.053

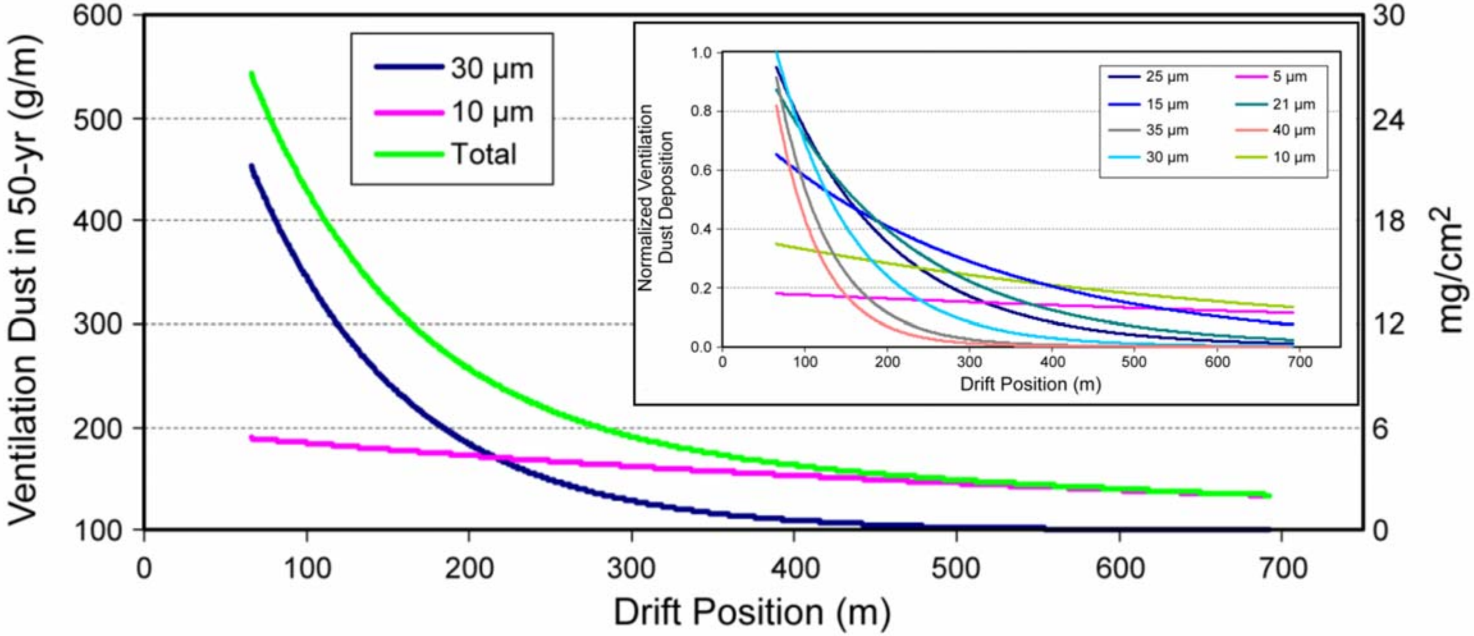
Processes Affecting Brine on the Waste Package Surface

- Acid degassing — $H^+_{(aq)} + Cl^-_{(aq)} \leftrightarrow HCl_{(aq)} \leftrightarrow HCl_{(g)}$
  - Ca-chloride brines degas and dry out (TGA experiments)
  - Multiple-salt assemblages can deliquesce at higher temp:
    - Acid-degassing may occur initially, but less as pH increases
    - Brines may not degas sufficiently to dry out
    - NO_3/Cl minimum ratio is controlled by temperature
- Reactions with silicate minerals in dust
  - Silicate dissolution buffers pH
  - Ca, Mg removed from brine as silicate phases
  - Deliquescence RH generally increases (brines may dry out)
  - Possible consumption of chloride by silicates
    - Scapolite-, cancrinite-, sodalite-, prehnite-group minerals
    - Clays (exchange for hydroxides)
- Dilution with decreasing temperature, increasing humidity

Salt Amount and Brine Volumes

- Estimate the amount and composition of dust deposited
  - Atmospheric dust load (site-specific data) : 22 μg/m^3 (typical)
  - Drift and ventilation design parameters
  - Upper-bound particle size (10 and 30 μm)
  - Deposition on first waste package in drift
  - Ventilation period: 50 years
  - Dry particle deposition model (Sehmel, 1980)
- Estimate brine volumes
  - Dust soluble salt content (site-specific): 10.5%
  - Ammonium minerals volatilize (~1/2 of total salts)
  - Thermodynamic modeling with Pitzer database

Salt Amount and Brine Volume

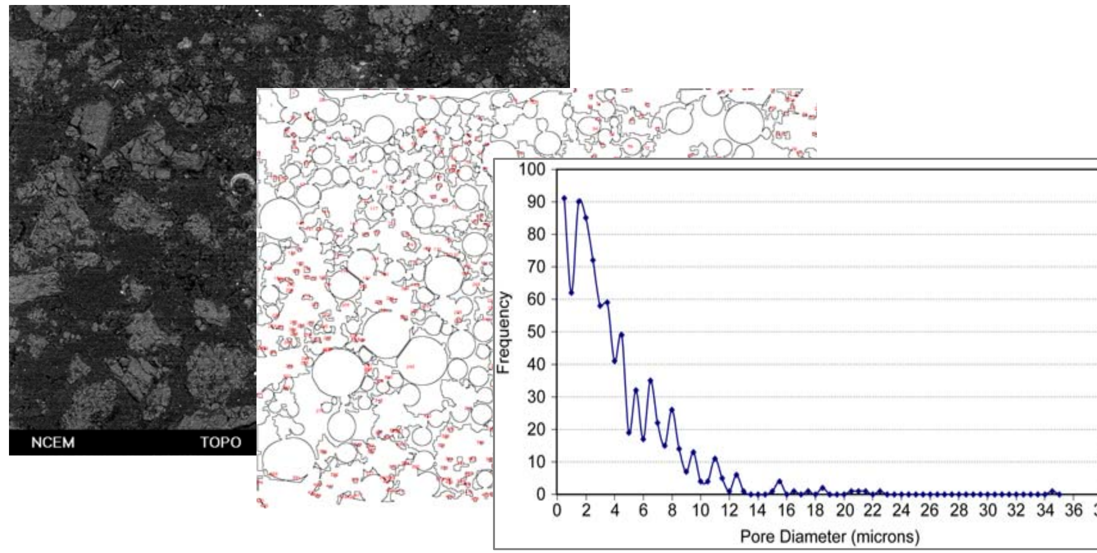


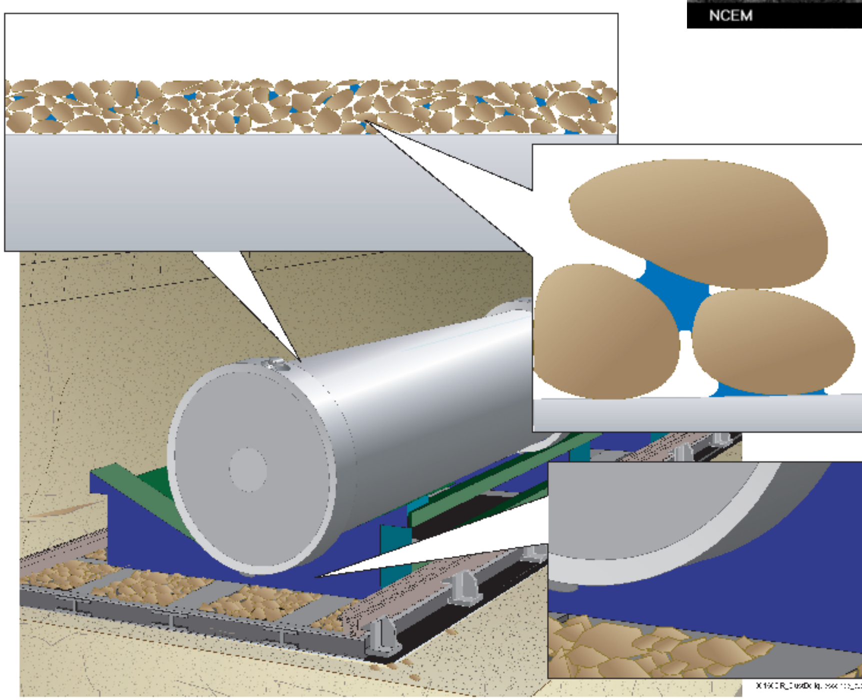
DTN: SN0508T0502205.016

- Upper bound for dust deposited: 26 mg/cm^2
  - 260 µm thick layer for bulk density 1 g/cm^3
  - Rock dust may add mass, not soluble salts
- Upper bound brine volume: 1.8µL/cm^2 (18 µm thick layer)
  - At 120°C; less volume at higher temperatures
  - Assumes all salts are internally mixed (no geometric isolation)
  - Average liquid saturation for dust layer ~11% for porosity of 60%
- Lower bound approx. 1 order of magnitude less at 200°C

Impact of Small Predicted Brine Volumes

- **Dust capillary response: ~ 1μm**
- **Capillary retention in dust limits contact with metal surface**





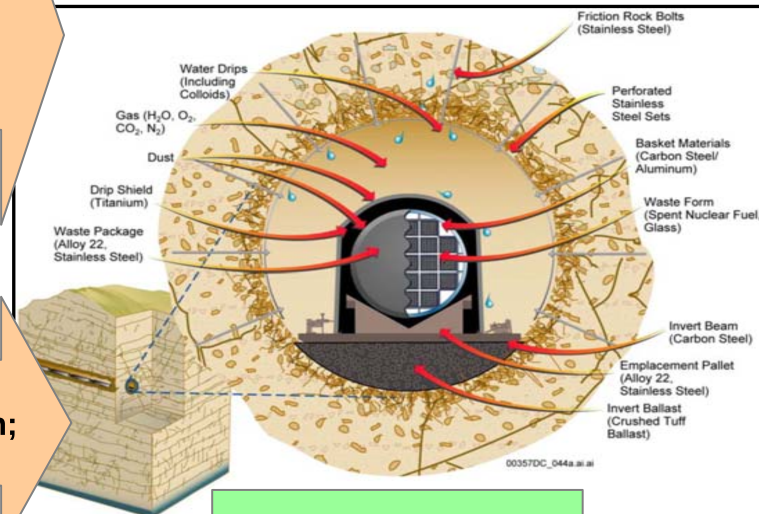
- **Dust layer is unsaturated—rapid gas diffusion into/out of the dust.**
- **Scale limitations on development of compositional gradients (e.g., O_2)**
- **Capillary hold-up in dust layer**

Conceptual Model

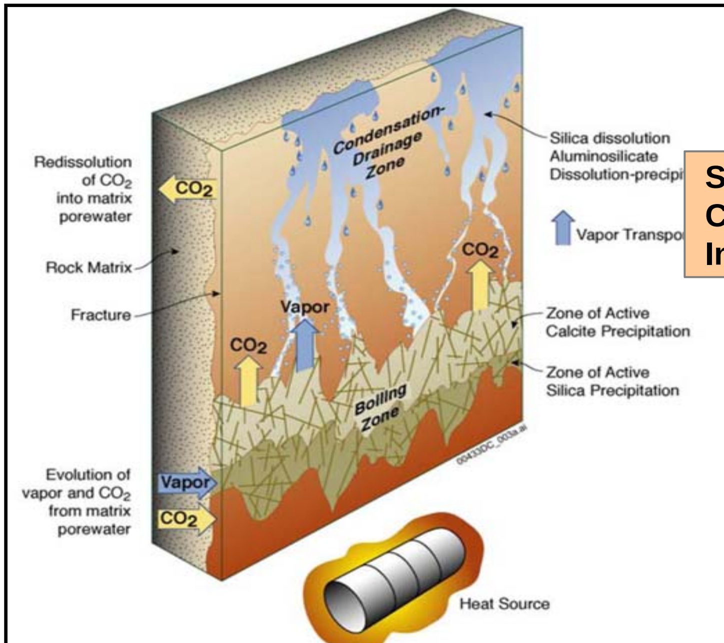
Near-Field / In-Drift Chemistry

Equilibrium Thermodynamic (Pitzer) Model for Evaporative Evolution

Physical & Chemical Environment Model



THC Seepage Model



Seepage Composition; In-Drift P_{CO2}

To TSPA:

Composition of Evaporated Seepage Water $f(T, P_{CO2}, RH)$

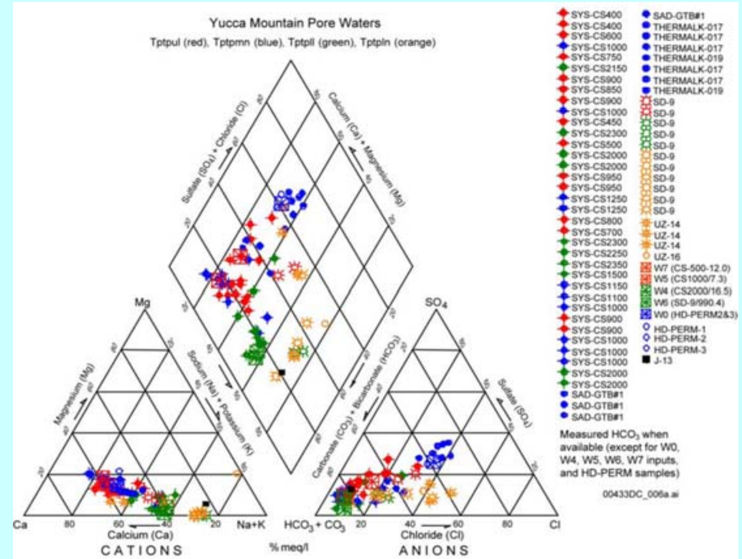
pH, I, [Cl], (NO_3^-/Cl^-)

MDL-NBS-HS-000001 REV 04 Figure 6.2-2 and ANL-EBS-MD-000033 REV 05 Figure 6.4-1

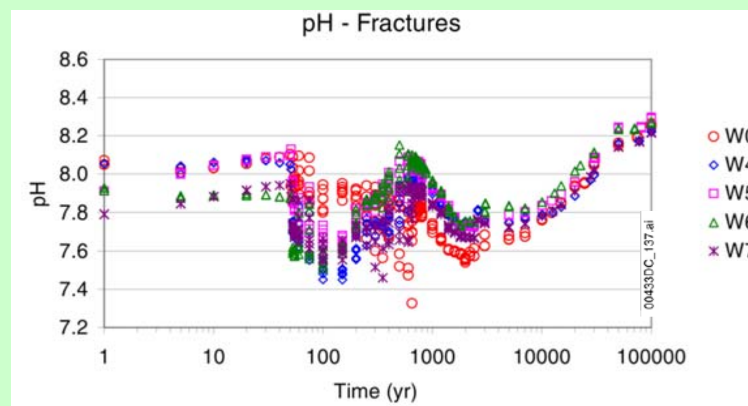
THC Seepage Model

Model Approach

- Initial/boundary conditions selected from available porewater analyses
  - Approx. 100 porewaters analyzed
  - NO_3^-/Cl^- ratios typically > 0.5
  - Group in 2-3 clusters based on chemical divides and statistics
- Thermal-hydrologic-chemical model
  - Repository center and edge conditions
  - Identify potential seepage waters, compositions
  - Validation using drift scale test results
- Abstracted output:
  - Compositions for potential seepage waters
  - CO_2 fugacity vs. time



Source DTNs: GS030408312272.002, GS020408312272.003, GS020808312272.004, GS031008312272.008, MO0005PORWATER.000.



Source DTN: LB0302DSCPTHCS.002, LB0307DSTTHCR2.002

Physical and Chemical Environment (P&CE) Model

- Corrosion environment
  - Evaporative equilibrium
  - Salt separation effect
- Binning approach
  - Bins based on chemical divides and other similar characteristics
  - Statistical median water for each bin
  - Create “bin history tables” by mapping bins to THC runs
- Preliminary results -11 bins
  - Lookup tables wrt T, PCO2, RH
  - Outputs NO3-, Cl-, pH, ionic strength
  - Uncertainty propagated

W0		W4		W5	
Time	Crown	Time	Crown	Time	Crown
10	4	10	10	10	7
51	5	51	11	51	11
53	5	53	11	53	11
55	6	55	11	55	11
60	6	60	11	60	11
75	5	75	11	75	11
100	5	100	11	100	11
150	4	150	11	150	11
200	4	200	11	200	11
250	3	250	11	250	11
300	3	300	11	300	11
350	3	350	11	350	11
400	3	400	11	400	11
500	4	500	5	500	9
600	4	600	5	600	11
650	5	650	11	650	11
700	11	700	11	700	11
751	11	751	11	751	11
790	11	801	11	785	11
801	11	804	11	801	11
1001	11	1001	11	1001	11
1201	11	1201	11	1201	11
1401	11	1401	11	1401	11
1601	11	1601	11	1601	11
1801	11	1801	5	1801	5
2001	4	2001	4	2001	4
2202	11	2202	11	2202	11
2402	11	2402	11	2392	11
3002	11	2597	11	2402	11
5003	11	3002	11	3002	11
7005	6	5003	11	5003	11
10007	6	7005	9	7005	9
12310	7	10007	7	10007	10
15010	7	12598	7	12304	7
20013	8	15010	8	15010	7
50035	8	20013	8	20013	8
		50035	8	50035	8

Bin History Tables From P&CE Model
(DTN: MO0312SPAPCESA.002)

Summary: Seepage Environment

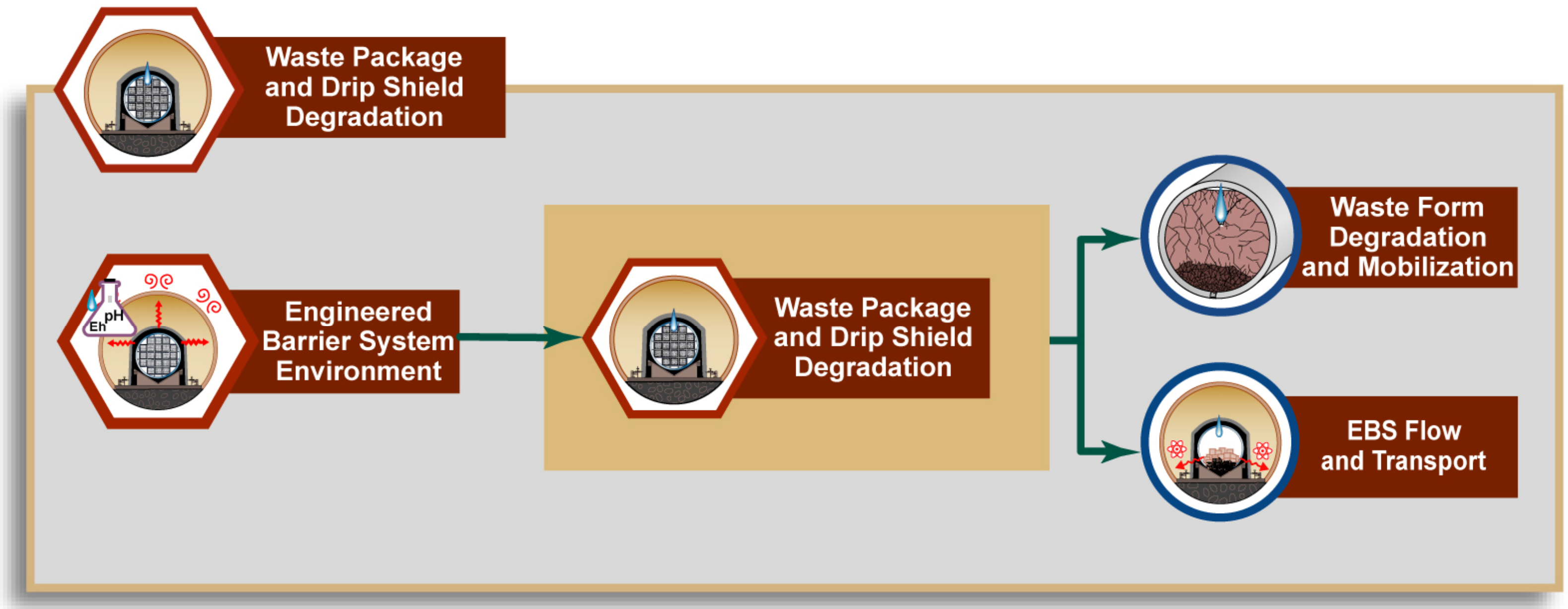
- **Waste package temperature <105ºC**
- **RH varies from approx. 40% to 99+%**
- **Salt separation effect implemented for RH < 77%**
- **NO3-/Cl-controlled by ambient water composition**
- **Ca-Cl brines predicted during peak thermal period**
- **Wide range of pH (4.5 to 10.5 plus uncertainty)**
  - **Higher pH after cooldown (T_{dw}< 100ºC)**
  - **Increasing pH as repository cools**
- **Greatest potential for corrosive seepage chemistry occurs early during cooldown**
- **Open system with respect to gases (background acid gas concentrations low)**

Summary: Deliquescence Environment

- **Brines can form only in small amounts at elevated T**
- **Physical environment**
  - **Unsaturated**
    - **Open system with respect to gases**
  - **Capillary and adsorptive retention in the dust layer further decreases available brine volume**
- **Chemical environment**
  - **NaCl – KNO_3 (–$NaNO_3$) (–$Ca(NO_3)_2$) salt systems**
    - **Deliquescence at higher temp. requires multiple-salt assemblages**
  - **Nitrate-rich; NO3-/Cl-increases with higher temperature**
  - **Acid degassing**
    - **May occur initially; less as pH increases; unlikely to dry out**
    - **Background acid-gas pressures are very low**
    - **NO_3^-/Cl^- minimum ratio is controlled by temperature**
  - **Reaction with silicates buffers pH, removes divalent cations**

Modeling the Corrosion Process

Identification and Linkages of Abstractions



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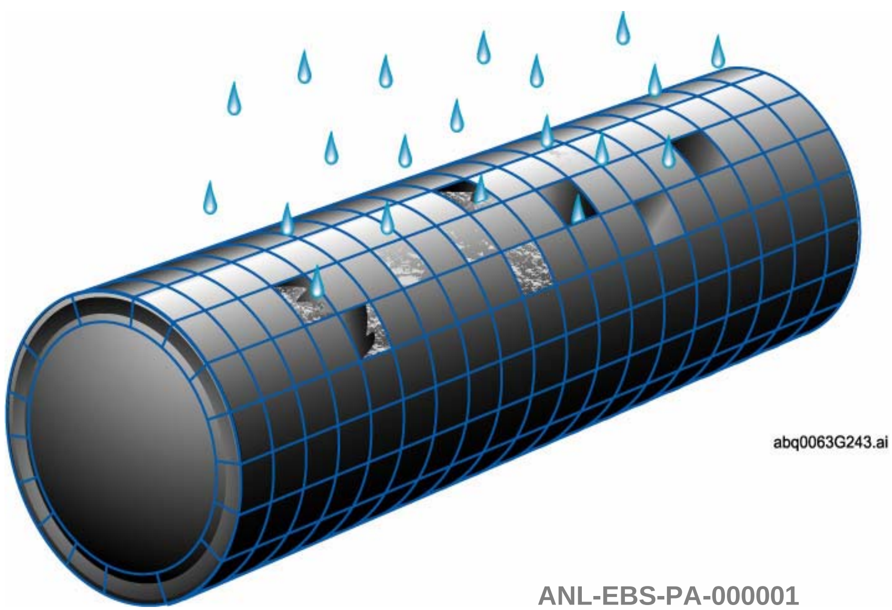
EBS = Engineered Barrier System

Objectives of Waste Package and Drip Shield Degradation Abstraction

- Provide EBS flow and transport model and waste form degradation and mobilization model the
  - Number of patch and crack breaches per failed waste package (WP)
  - Number of patch breaches per failed drip shield (DS)
  - Number of early failed WPs and DSs



ANL-EBS-PA-000001

Inputs, Outputs, Basis for Model Confidence

Waste Package and Drip Shield Degradation

- *Alloy 22 Degradation*
  - *General Corrosion (GC) and MIC*
  - *Stress Corrosion Cracking (SCC)*
  - *WP Early Failure*
  - *Localized Corrosion*
- *Titanium Grade 7 Degradation*
  - *General Corrosion*

Inputs

EBS Chemical Environment
- pH, Cl, NO_3

EBS Thermal-Hydrologic Environment Submodel
- Temperature
- Relative Humidity

Alloy 22 General Corrosion Rate

Alloy 22 Stress Profiles

Alloy 22 Stress Intensity Factor Profiles

Alloy 22 Closure Weld Defects Data

Titanium Grade 7 General Corrosion Rate
- Topside of Drip Shield
- Underside of Drip Shield

Outputs

EBS Flow Submodel
- Number of Patch Breaches/Failed WP
- Number of SCC Breaches/Failed WP
- Number of Patch Breaches/Failed DS

Waste Form Degradation and Mobilization
- WP and DS Breach Ratio
- Fraction of Failed WPs

EBS Transport Submodel
- Number of Patch Breaches/Failed WP
- Number of SCC Breaches/Failed WP
- Number of Early Failed WPs
- Fraction of GC and SCC Failed WPs

Model Confidence Foundation
- Short- and Long-Term Corrosion Testing
- Standard Approaches to Corrosion Modeling
- Nuclear Industry Experience
- Materials Science Literature
- Field Data

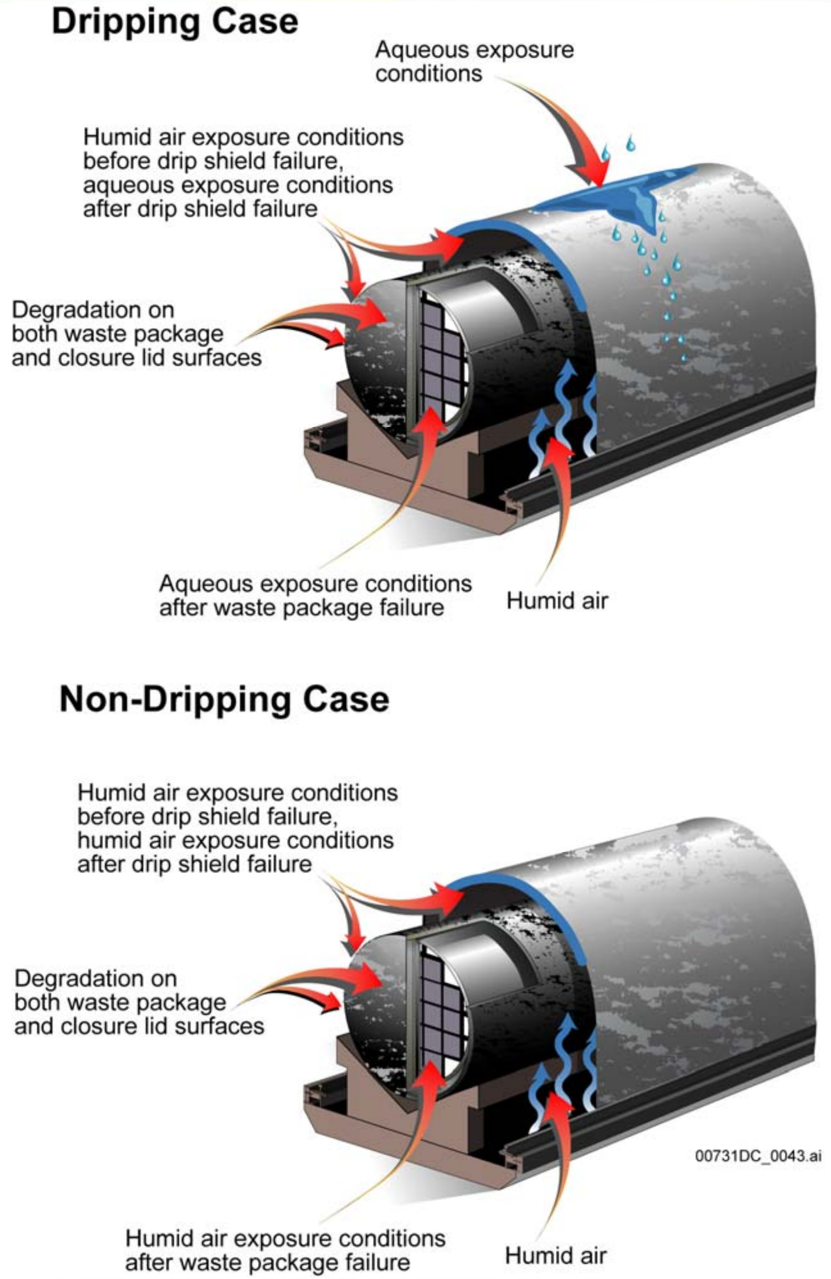
00731DC_0026.ai

Model Assumptions

- Alloy 22 WP outer barrier
  - GC occurs at all times
  - GC rates time independent
  - LC is represented by crevice corrosion
  - LC rates time independent
  - SCC occurs regardless of exposure environment
  - MIC treated as GC rate multiplier
- Titanium grade 7 DS plates
  - GC occurs at all times
  - GC rates time independent

WP and DS Degradation Conceptual Model

- DS degradation (GC) not dependent on seepage contact
- WP GC and SCC not dependent on seepage water contact
- WP LC can initiate only if seepage contacts the WP surface
  - After DS failure



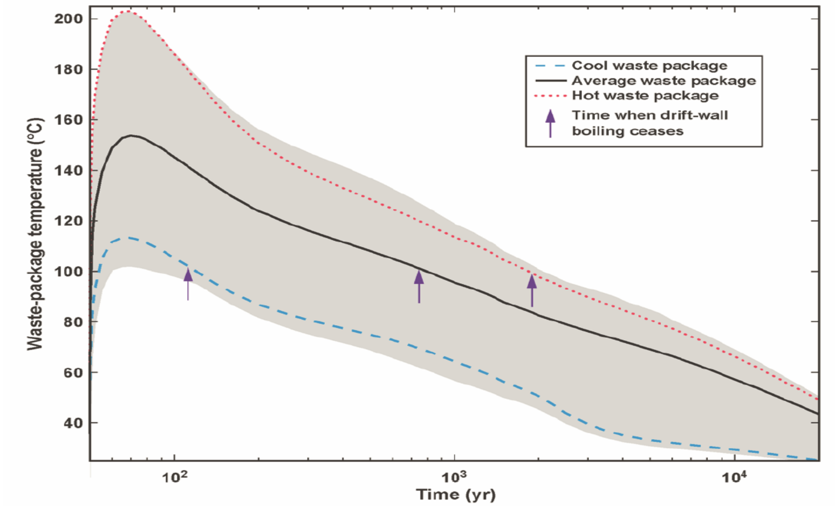
Treatment of Uncertainty and Variability

- Treatment of uncertainty
  - WP GC temperature dependence
  - WP LC initiation model parameters
  - WP SCC stress and stress intensity factor profiles
  - WP SCC growth model parameters
  - WP MIC GC rate multiplier
  - DS GC rate
- Treatment of variability
  - WP GC/LC temperature/chemical inputs
  - WP GC pre-exponent term
  - WP SCC stress and stress intensity factor profiles
  - WP SCC closure weld flaw size/number

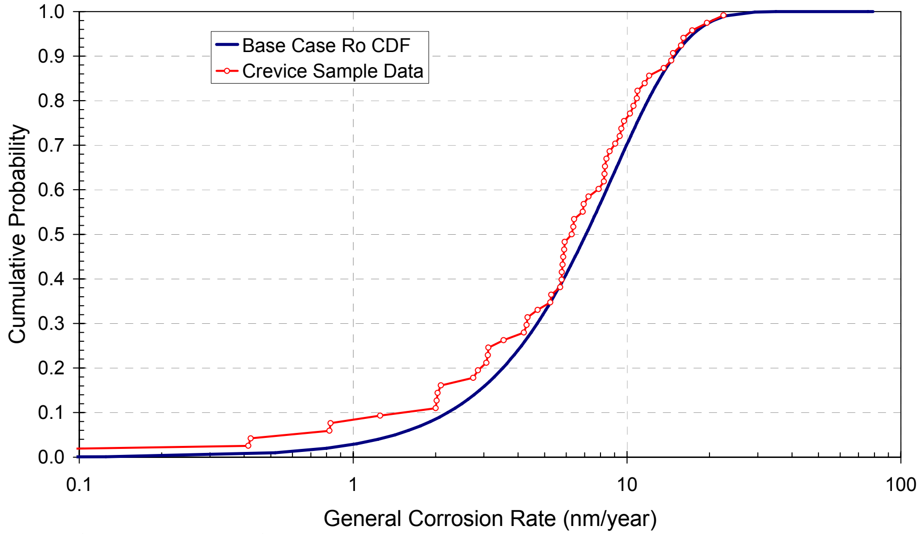
Technical Basis for Abstraction

- Short and Long-term experimental data
  - Up to 5-year weight-loss measurements
  - Up to 3-year corrosion potential (E_{corr}) measurements
  - WP mock-ups
- Validation / confidence evaluation
  - Comparison to literature data
  - Alternative conceptual models
- References
  - General Corrosion and Localized Corrosion of Waste Package Outer Barrier, ANL-EBS-MD-000003 Rev 02, ICN 00
  - General Corrosion and Localized Corrosion of the Drip Shield, ANL-EBS-MD-000004 Rev 02, ICN 00
  - Stress Corrosion Cracking of the Drip Shield and Waste Package Outer Barrier, ANL-EBS-MD-000005 Rev 02, ICN 00
  - Analysis of Mechanisms for Early Waste Package/Drip Shield Failure, CAL-EBS-MD-000030 REV00C, ECN 02

Implementation—WP GC



ANL-EBS-MD-000049



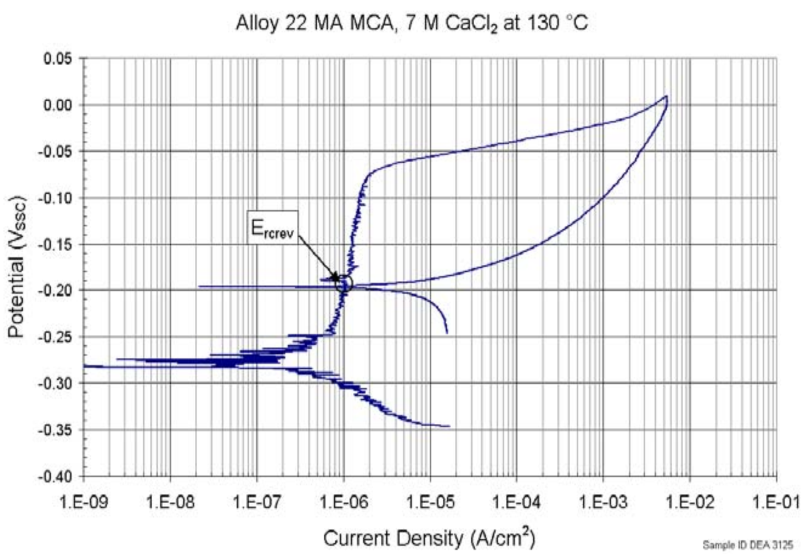
ANL-EBS-MD-000003

$$\text{Rate} = f_{MIC} \exp\left(C_o - \frac{C_1}{T} \right)$$

- Temperature profiles
  - Spatial variability (WP-to-WP)
- C_o, pre-exponent, based on Weibull distribution fit to weight-loss data
  - Spatial variability (patch-to-patch)
- **C_1, temperature dependence, based on normal distribution from polarization data**
  - **Epistemic uncertainty**
- **f_{MIC}, MIC multiplier**
  - **Epistemic uncertainty**

Implementation—WP LC

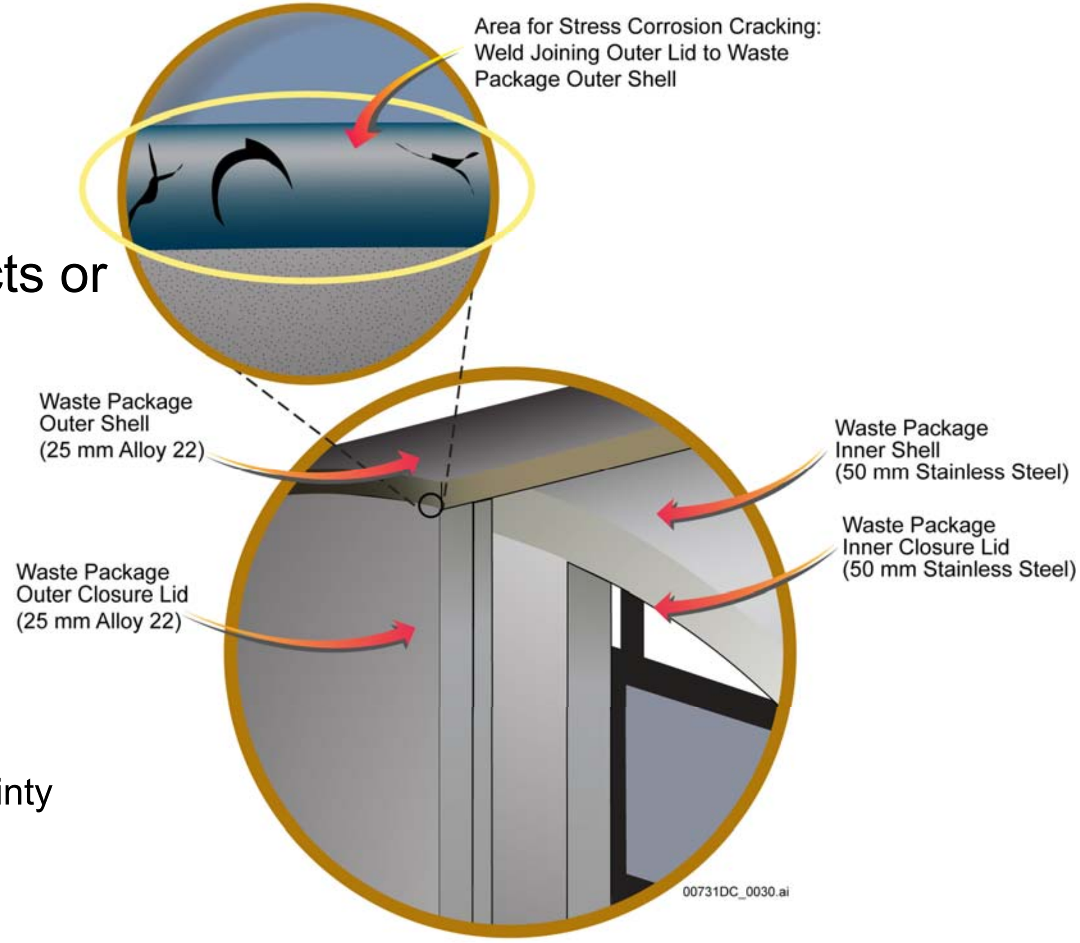
- Waste package areas contacted by seepage may be subject to LC
- If seepage occurs at RH < ~70% then model initiates LC
  - Potential for salt separation
- If seepage occurs at RH > ~70%
  - Compare
    - E_{corr}, long-term corrosion potential, to
    - E_{rcrev}, crevice repassivation potential
  - If $E_{corr} \geq E_{rcrev}$ model initiates LC
    - E_{corr} and E_{rcrev} are functions of T, pH, [Cl $^-$], and [NO_3^-]
      - Epistemic uncertainty in fitting parameters
      - Spatial variability from thermal and chemical variations



ANL-EBS-MD-000003

Implementation—WP SCC

- Only in closure weld regions (in absence of seismicity)
  - Weld region plasticity burnished
  - Initiates at incipient defects or weld flaws
- Growth by Slip Dissolution Model
  - Rate of crack growth a function of
    - Stress intensity factor
      - Mainly epistemic uncertainty
    - Repassivation rate
      - Epistemic uncertainty

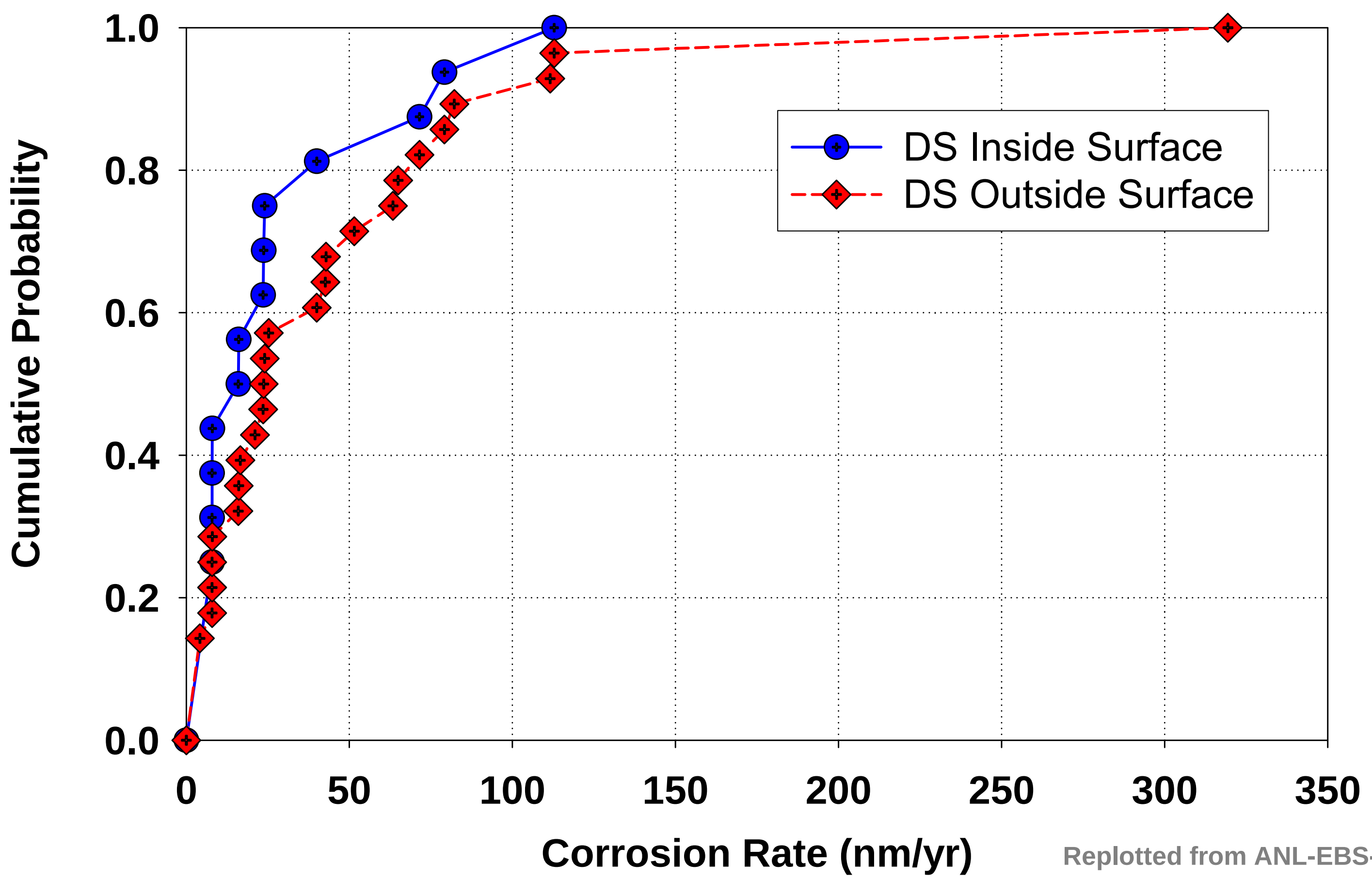


Sources of WP/DS EF

- Analyses under evaluation for WP and DS
- Considers the probability of processes occurring and not being detected such as
  - Base metal and weld flaws
  - Use of improper material
  - Improper heat treatment
  - Contaminants
  - Mislocated or missing welds
  - Handling damage
  - Administrative/operational error
- Strict fabrication controls will be used to minimize their occurrence

Implementation—DS GC

- Titanium grade 7 drip shield plates
  - Empirical distributions for inside and outside surfaces
  - Epistemic uncertainty



Replotted from ANL-EBS-MD-000004

Corrosion During the Thermal Pulse

NWTRB Concerns on LC due to Dust Deliquescence

Jun. 06: “The Project maintains that potential localized corrosion of Alloy-22 at elevated temperatures can be excluded from its performance-assessment calculations. *The Board believes that the technical basis for the exclusion is not compelling, partly because only very limited corrosion data have been collected at temperatures above 150ºC and partly because data showing cessation (stifling) of localized corrosion at lower temperatures may or may not be relevant to all conditions under which localized corrosion could occur in the proposed repository*. The Board strongly urges the Project to continue collecting data that might justify its assumption that localized corrosion will not occur at temperatures as high as 200°C.”

Jan. 07: “The Board found that *significant uncertainties related to repository environments and to corrosion behavior at high temperatures persist* and that there are apparent contradictions among some of DOE’s experimental results.”

Will LC Initiate due to Deliquescence formed Brines?

1. ***Can multiple-salt deliquescent brines form at elevated temperature?*** **Yes**

2. ***If brines form at elevated temperature, will they persist?*** **Sometimes**

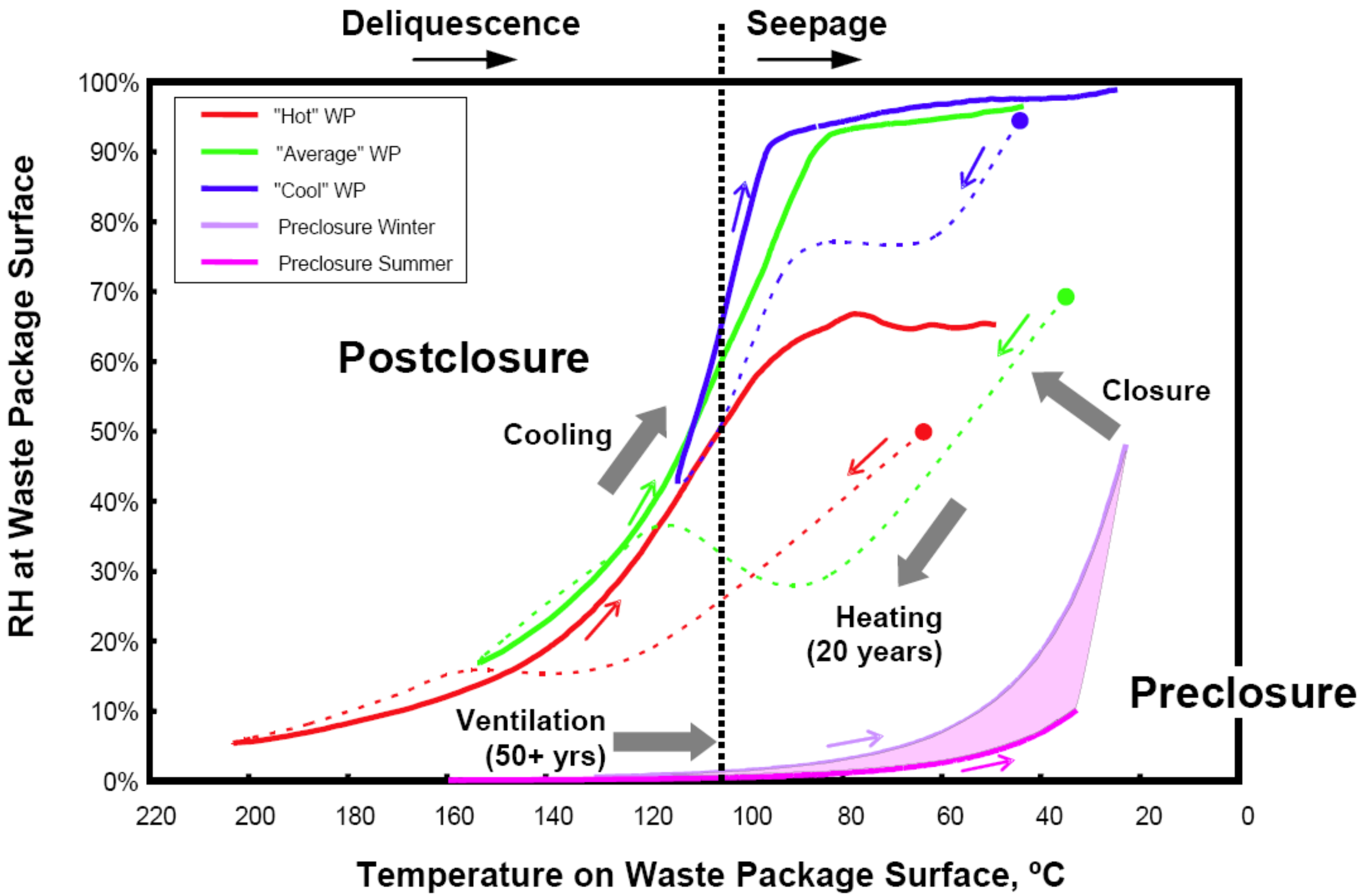
3. ***If deliquescent brines persist, will they be corrosive?*** **No, not under repository-relevant conditions**

4. ***If deliquescent brines are potentially corrosive, will they initiate LC?*** **No, not under repository-relevant conditions**

5. ***Once initiated, will LC penetrate the WP outer barrier?*** **No**

- **On this basis, LC due to dust deliquescence is screened out due to low consequence**

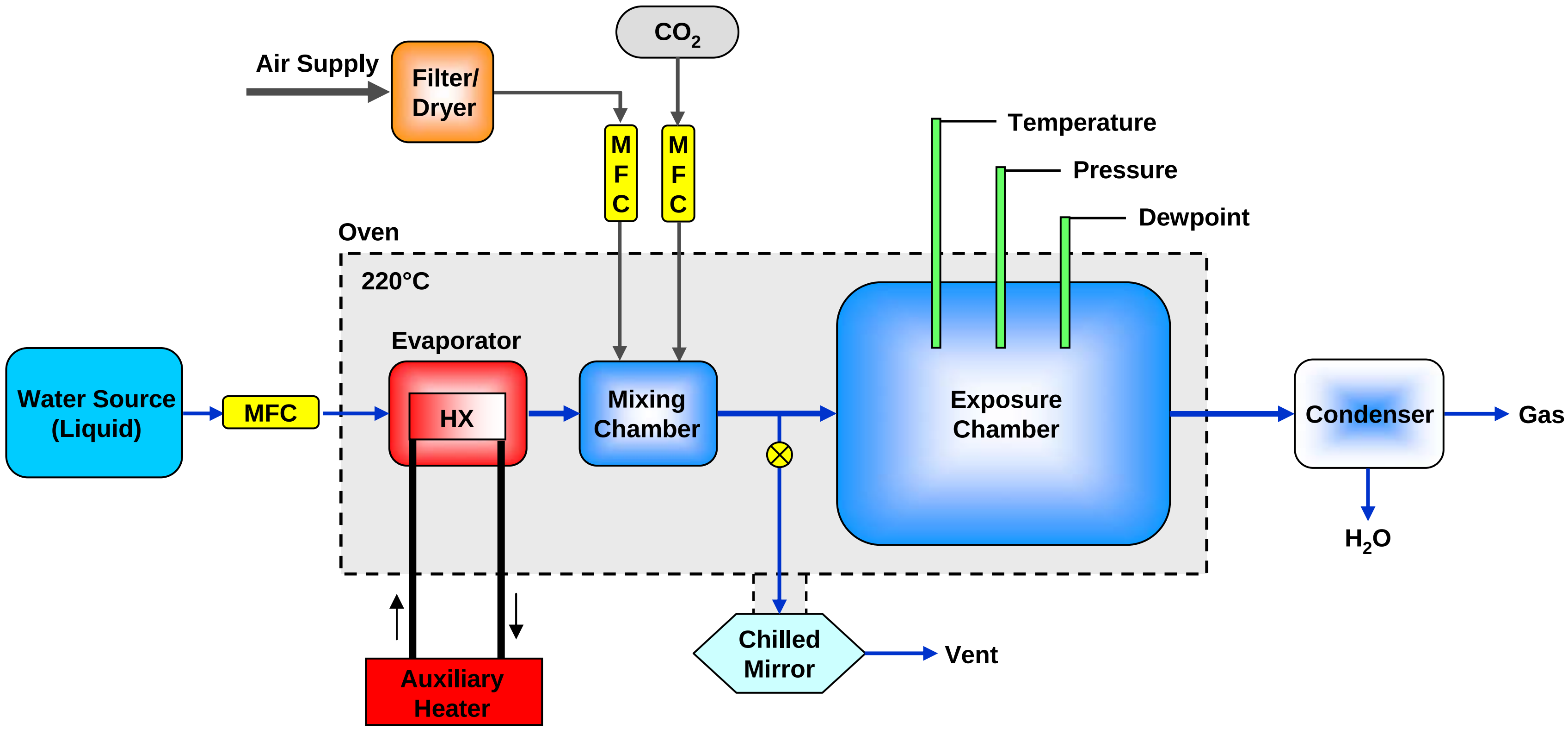
Post-Closure Waste Package Surface Temperature



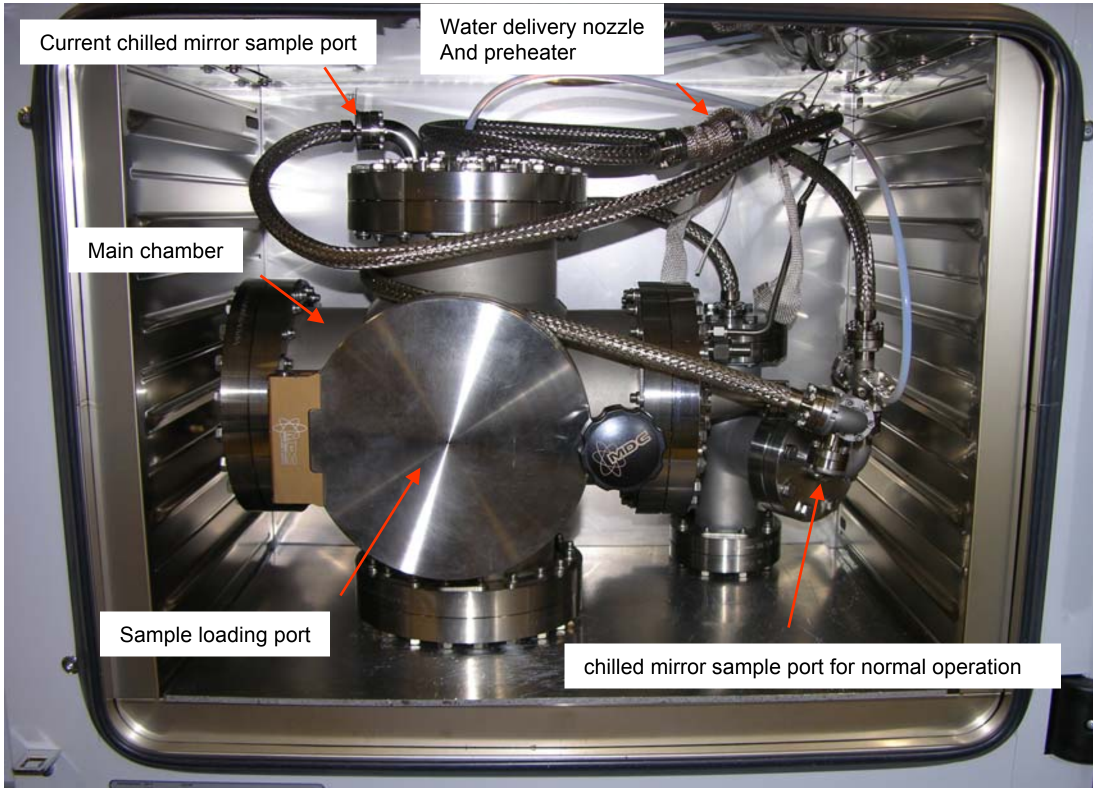
DTN: SN0508T0502205.015

Generation of a High Dewpoint Environment (95°C+) at Atmospheric Pressure

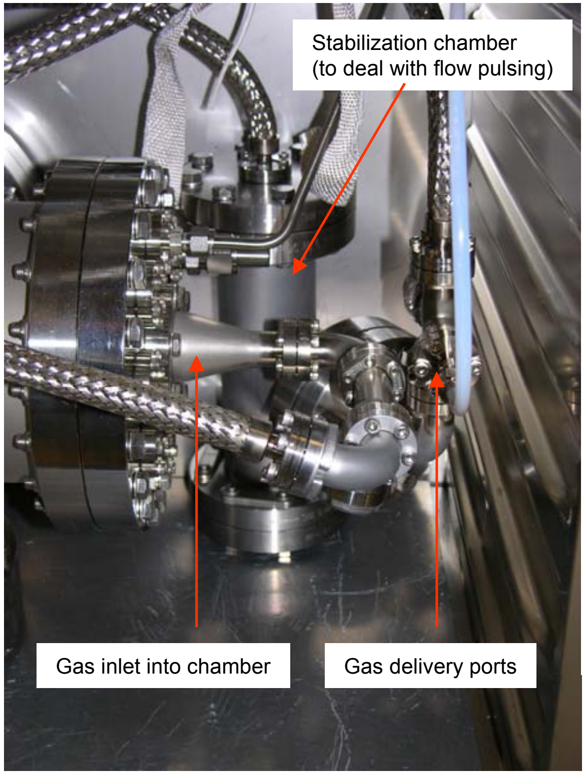
- Schematic of High-T, controlled moisture content system

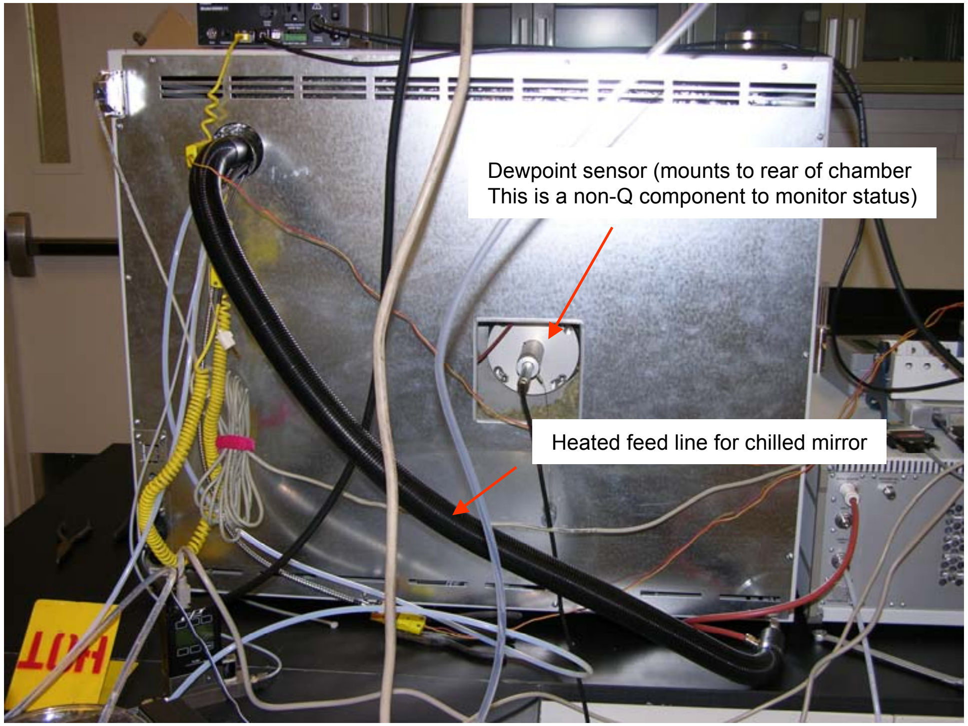


Status Update: High Temperature, Controlled Dewpoint System construction



Status Update: High Temperature, Controlled Dewpoint System construction





Quantitative Assessment of Corrosion Stifling Process via Resistance Measurements

Goal: Establish if localized corrosion of Alloy 22, once initiated due to a limited quantity of contaminant, will stifle with time due to the consumption (including physical sequestration) of the aggressive component

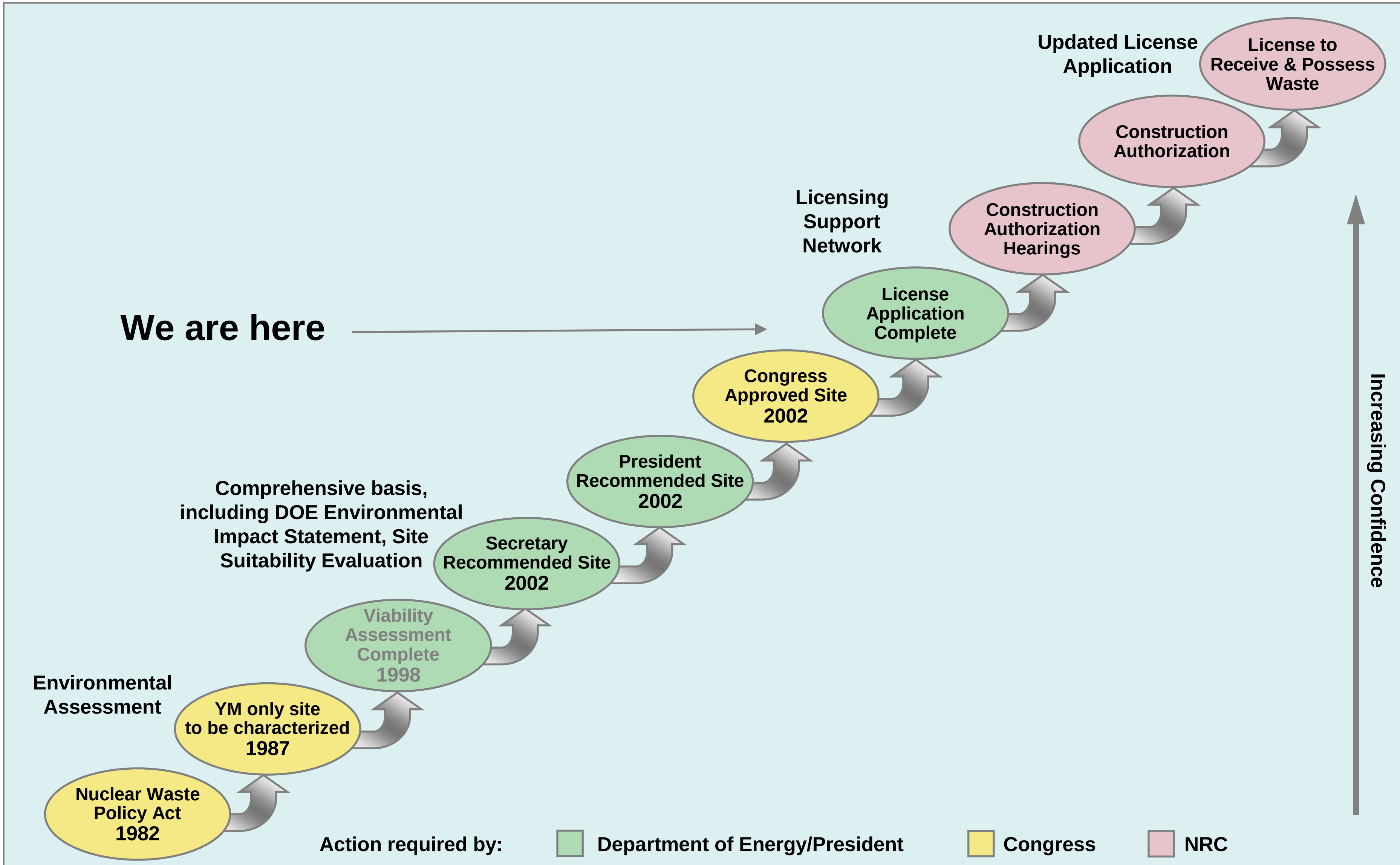
- Four-point resistance measurements, analogous to DCPD
- Resistance change function of degree of attack.
  - Limitations
    - General view of sample
    - Potentially limited sensitivity
  - Alloy 22 and less corrosion resistant analogs
  - Re-initiation, impact of crevice former, etc.

Propagation and Stifling Processes for Localized Corrosion under Dust Deliquescence Conditions

Goal: Understand the kinetics of the crevice corrosion process for atmospherically exposed samples under YMP relevant conditions

- Fine pitch, segmented electrodes will be used to simulate a bulk (continuous) material (similar to work of Scully, et. al.)
- Traditional MCA (Al_2O_3 or ZrO_2) will be used to form the occluded geometry over a portion of the electrodes.
- Samples will be electrochemically stressed, and the kinetics of the corrosion and repassivation/stifling processes within the crevice monitored.
  - Impact of T, [contaminants], dewpoint
  - Re-initiation via re-inoculation with contaminant, changing environment, etc. will be explored.

Repository Timeline



Conclusions

- The technical basis for long-term performance at Yucca Mountain includes quantitative estimates of barrier capability and system performance
- Confidence in the quantitative estimates comes from
  - Understanding components and their capabilities
  - Understanding system performance
  - A clear display of uncertainty
  - Following a process that demonstrates completeness
- Current scientific understanding will support a license application in June 2008