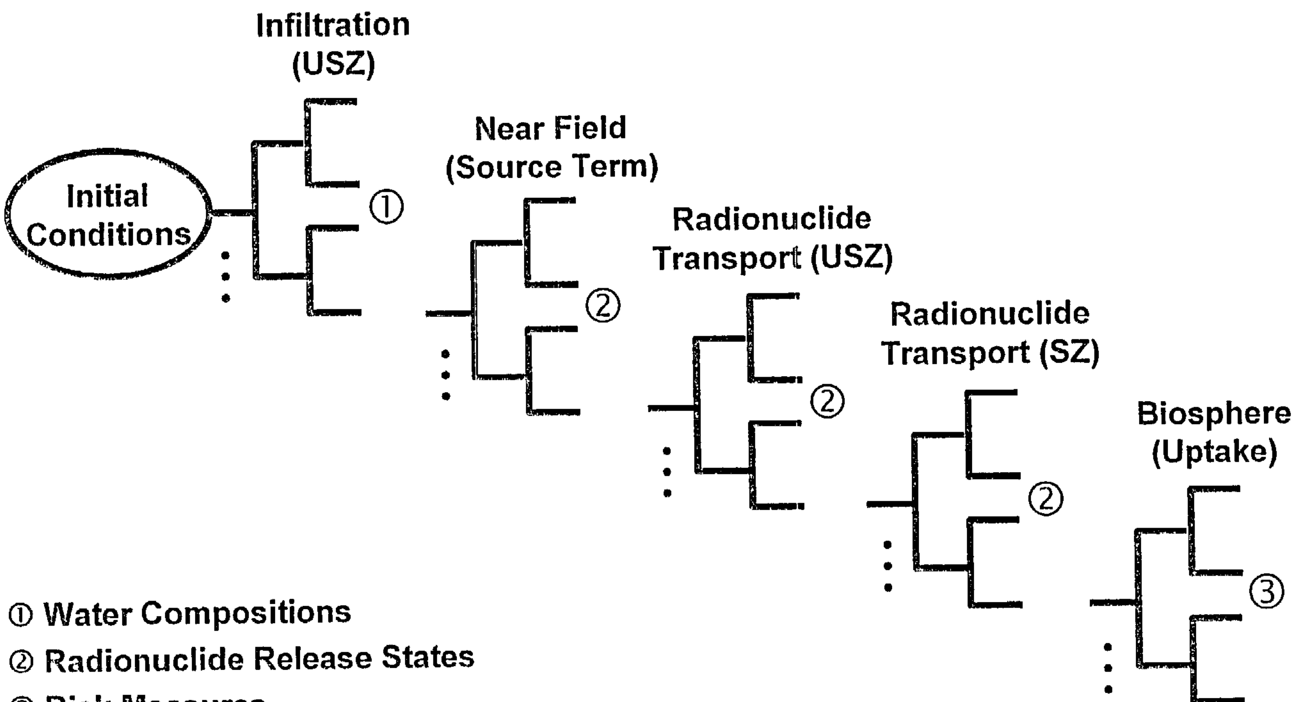
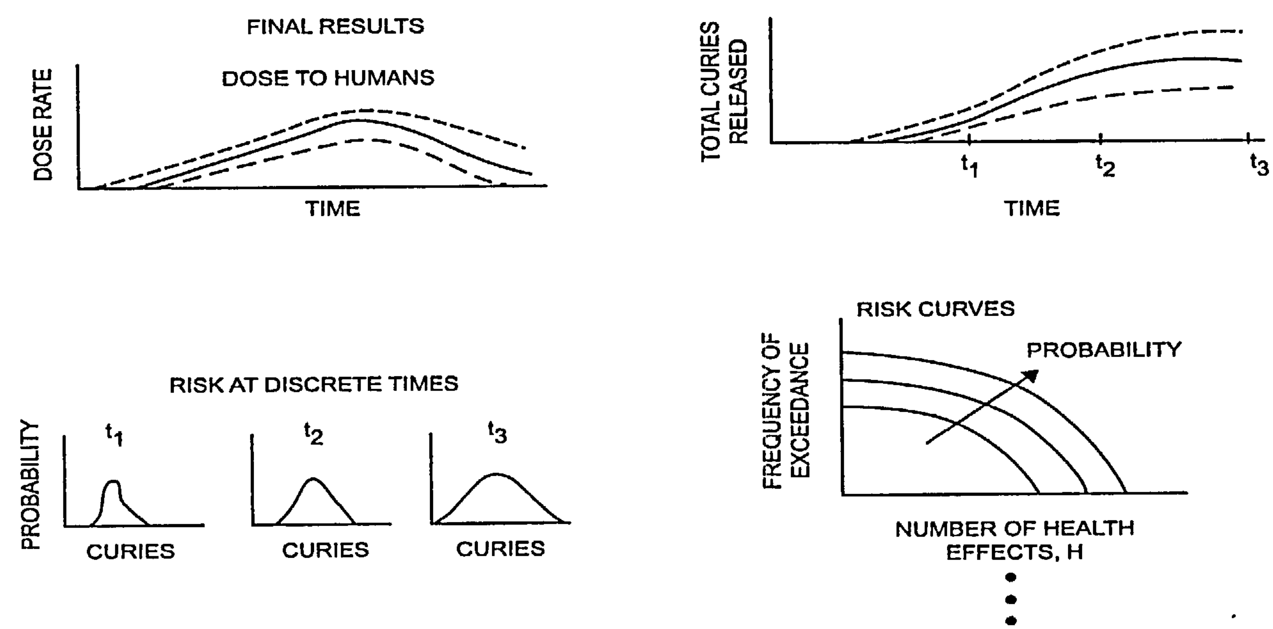
Modeling Stages for Quantitative Performance Assessment



① Water Compositions
② Radionuclide Release States
③ Risk Measures

B. John Garrick

Risk Measures for Performance Assessment of Nuclear Waste Repositories



B. John Garrick

United States Nuclear Regulatory Commission

Background and Role of NRC's Total-System Performance Assessment Capability

Andrew C. Campbell
Section Leader
Performance Assessment and Integration
Division of Waste Management
US Nuclear Regulatory Commission
301-415-6897
acc@nrc.gov

United States Nuclear Regulatory Commission

NRC's ROLE

- Pre-licensing Activities
  - Developing staff review capabilities
  - Understanding important features, events, and processes
  - Understanding Barriers
  - Interactions with DOE
  - Identifying information necessary to review a license application (agreements)

- Reviewing DOE license application

2

United States Nuclear Regulatory Commission

Historical Background

- Integrated performance assessment (IPA) modeling activities
- Development of Total-system Performance Assessment (TPA) code
- Interactions with DOE on TSPA
- Development of Key Technical Issue (KTI) framework

3

United States Nuclear Regulatory Commission

Role of NRC's TPA Code

- Independent review capability
  - Evaluate DOE's TSPA
  - Understand and evaluate DOE's models, assumptions, and data
  - Flexibility to evaluate completeness of DOE modeling approaches
- Enhance staff understanding
  - Identify key elements of repository system
  - Provide risk insights to help establish priorities
  - Integration of Evaluations of sub-system performance

4

United States Nuclear Regulatory Commission

Applications of TPA code

- Confirmatory analyses of DOE modeling approach and results
- Simplified calculations to support system performance analyses
- Uncertainty and sensitivity analyses
  - Identify uncertainties important to performance
  - Test relative importance of parameters, alternative conceptual models, and key assumptions
- Integration of processes and models into a comprehensive understanding of repository system
- Identify uncertainties in abstraction process
- Understanding importance of certain scenarios

5

United States Nuclear Regulatory Commission

Key Aspects of Estimating Nominal Performance

- Infiltration
- Near field
  - Engineered Barrier Degradation
  - Source Term
- Radionuclide Transport Through Geosphere
  - Unsaturated zone
  - Saturated zone
- Biosphere and Dose

6

United States Nuclear Regulatory Commission

Confidence Building for Performance Assessment

- Peer review of TPA 3.2
  - Areas evaluated
  - Key recommendations
  - Staff follow-up
- ~~Verification Testing of TPA 5.0~~
  - Purpose
  - Approach

7

United States Nuclear Regulatory Commission

Ongoing NRC Staff Activities and Path Forward in PA

- Risk Insights
  - Risk insights baseline
  - Risk Insights Report
  - Provide feedback to staff on agreements
- Interactions on DOE Risk Prioritization Approach
- Finalize development of TPA 5.0 prior to LA
- Developing IPA 4
- Update Risk Insights Baseline

8

United States Nuclear Regulatory Commission

Total-system Performance Assessment (TPA):
Approaches and Assumptions for Version 4.1

Christopher J. Grossman

Environmental and Performance Assessment Branch
Contact information: (301) 415-7658, cjg2@nrc.gov

Major Contributors: Sitakanta Mohanty, Richard Codell, Randy Fedors, Jim Winterle, Hans Arlt, Paul Bertetti, John Bradbury, Tae Ahn

Presented to: The Advisory Committee on Nuclear Waste, March 25-26, 2003

TPA: A Review Tool

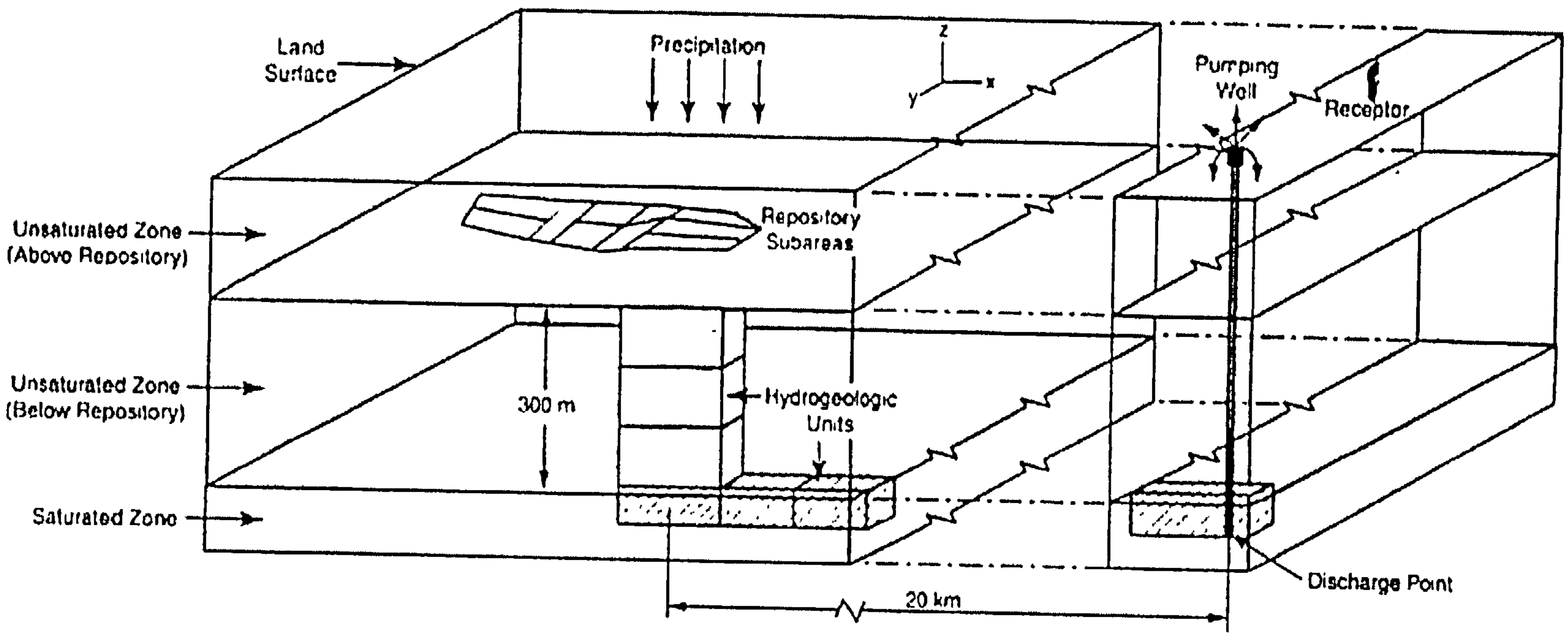
- TPA is an **independent** tool used to support review of both pre-licensing activities and a potential license application.
- TPA uses available **data** to construct approaches based on first principles.
- TPA uses approaches based on **fundamental principles** to simulate the repository behavior and allow for **computational efficiency** where warranted.
- TPA uses fundamental approaches to allow **flexibility** in independently evaluating of a license application for the proposed repository and support review capability.

TPA Approach

- TPA conducts probabilistic dose calculations for specified time periods, accounting for:
  - Essential features of the engineered and natural barriers,
  - Chemical and physical processes affecting degradation and release to the biosphere,
  - Uncertainties and spatial variability of system attributes, model parameters, and future states (scenario classes), and
  - Lifestyle characteristics of the reasonably maximally exposed individual (RMEI).
- Scenario classes include:
  - A nominal case including climate changes and seismic activity,
  - A disruptive case involving faulting, and
  - A disruptive case involving igneous activity.

United States Nuclear Regulatory Commission

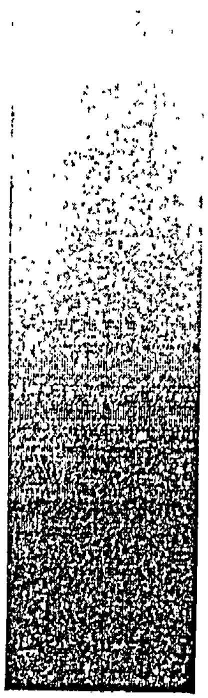
Repository Conceptualization

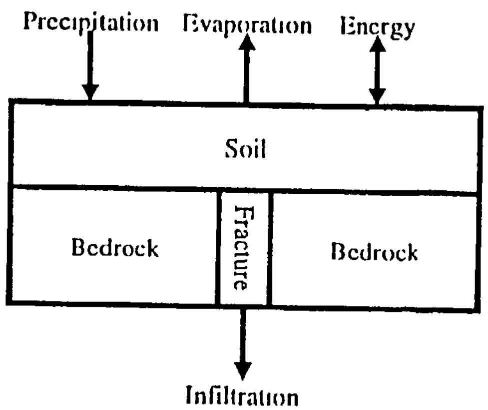


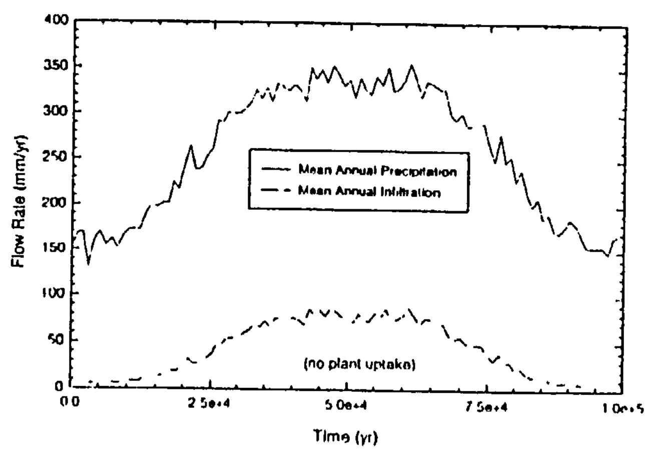
Water Movement Through the Repository

- Temperature and precipitation vary with glacial cycles.
- Process-level modeling, which incorporates climate, soil depth, and bedrock permeability, estimates the shallow infiltration flux for bare-soil conditions based on numerical solutions to the Richards equation.
- Deep percolation flux equal to the shallow infiltration flux.
- Water seeping into drifts varies with time during the first few thousand years largely because of coupled heat transfer and fluid flow processes such as vaporization, condensation, and refluxing.
- Large-scale diversion, as well as near- and in-drift diversion or focusing impact the water flux entering the failed waste package.

Shallow Infiltration







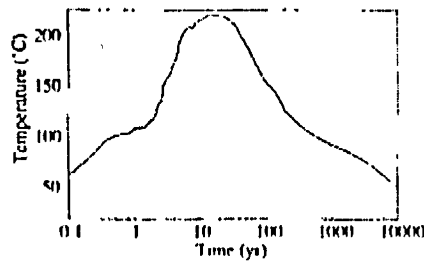
Variation of infiltration with climate change.

- Evidence suggests precipitation may have been 1.5-2.5 times larger than current climate conditions, while temperature may have been cooler by 5-10 ^{o}C at last full glacial maximum.

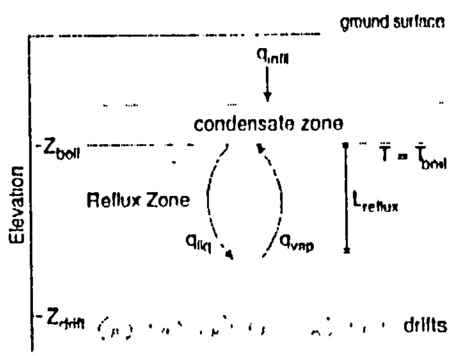
- Net infiltration for the modern climate is based on 1-D simulation results using a 15-year record of hourly meteorological data from Desert Rock, Nevada.

United States Nuclear Regulatory Commission

Groundwater Reflux



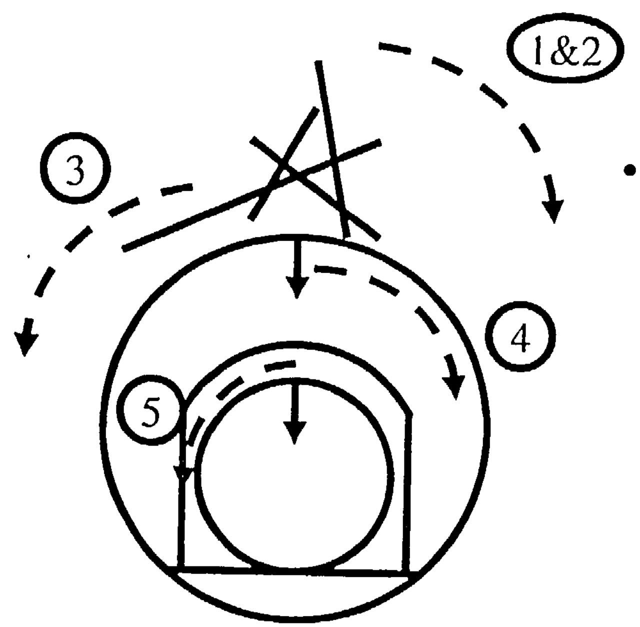
Temperature profile at the drift wall.



Conceptualization of drift-scale thermal hydrologic model.

- Process-level thermohydrologic modeling calculates the thickness of the dry out zone above the repository for TPA.
- Theory suggests water flowing down a fracture will penetrate a distance below the boiling isotherm before completely vaporizing.
- Water reaches the drift when the penetration distance exceeds the thickness of the dry out zone.
- TPA also incorporates two additional alternative conceptualizations to model groundwater reflux.

Flow Convergence/Divergence



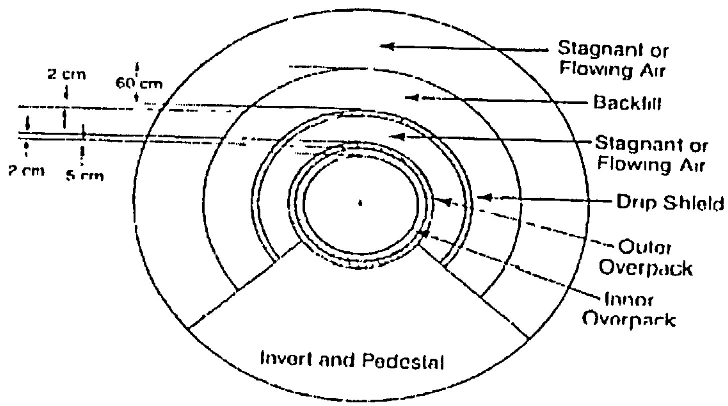
- TPA utilizes a simple and efficient approach to modify the percolation flux that reaches the waste package.
- Factors account for:
  1. Fraction of waste packages dripped on by flowing fractures,
  2. Focusing/divergence of deep percolation toward/away from drifts,
  3. Divergence due to capillary forces in unsaturated rocks,
  4. Film flow down the surface of the drift walls,
  5. Drips missing holes in the waste package, and the presence of corrosion products in the holes.

Degradation of the Engineered System

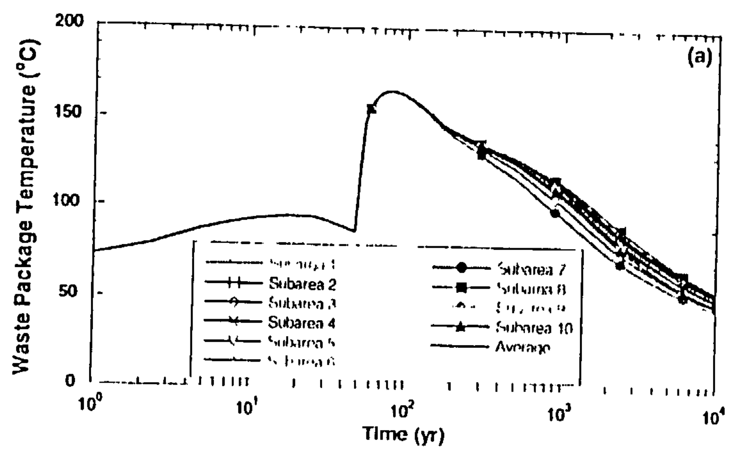
- Process-level modeling based on experimental evidence estimates the time of drip shield failure.
- TPA estimates initial failure of a small number of waste packages due to fabrication defects or emplacement damage.
- TPA simulates uniform or localized corrosion of the waste package depending on conditions (RH, T, [Cl^-], pH) in the near-field environment. TPA assumes the waste package fails with a single penetration of the outer (Alloy-22) and inner (316L SS) overpacks.
- TPA calculates the waste package surface temperature and relative humidity (RH) based on thermal output and the repository horizon temperature.
- Process-level modeling estimates the near-field chemical environment.

United States Nuclear Regulatory Commission

Thermal Modeling



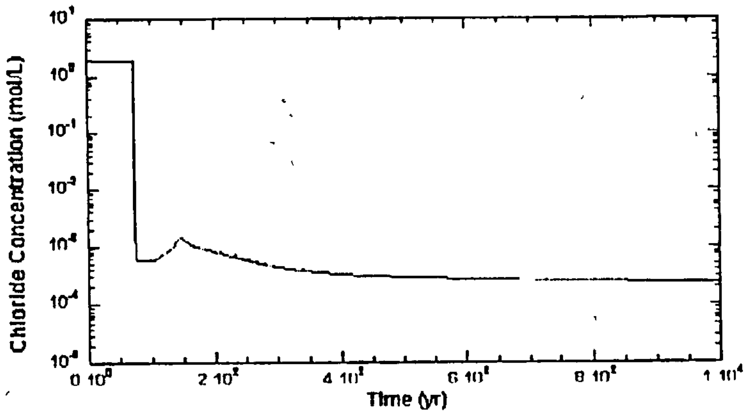
Idealization for thermal calculations.



Waste package surface temperatures.

- TPA calculates the temperature of the drift wall using a mountain-scale analytic conduction-only model.
- TPA calculates the waste package surface temperature and maximum temperature of the spent fuel using analytical approximations of multimodal heat transfer.
- TPA calculates RH as a function of drift wall and waste package surface temperatures and moisture present at closure.
- TPA can incorporate an alternative thermal model.

Near-Field Chemical Environment



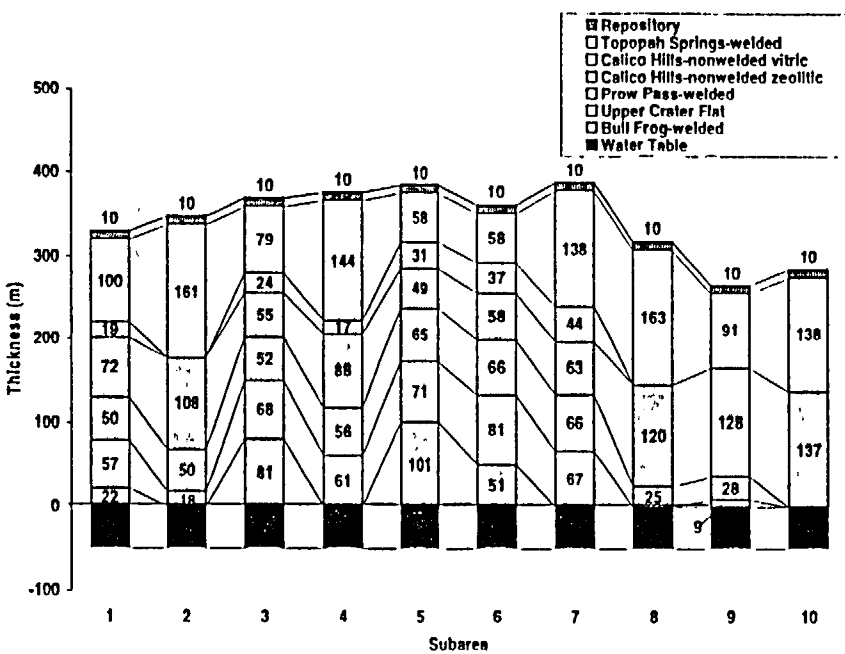
Chloride concentration at the drift wall.

- Currently, process-level modeling simulates the change in chloride concentration due to evaporation.
- TPA adjusts the chloride concentration to account for uncertainties and limitations of the modeling to represent the chemistry on the waste package surface.
- TPA fixes pH at 9 based on process-modeling.
- TPA 5.0 will add a new conceptual model to describe pO_2, pH, CO_3^{2-}, Cl, NO_3^{2-}, F^- evolution thereby improving realism in the corrosion modeling.

Radionuclide Release

- The quantity of water that enters the failed waste package, composition of water, and solubility of radionuclides impact the transfer of radionuclides from spent fuel into water for transport.
- TPA considers two models, a bathtub and flow-through model, for advective transport of radionuclides from the waste package. TPA 5.0 will add a diffusion transport model.
- Experimental evidence supports the spent fuel dissolution rate model. TPA includes 3 additional alternative dissolution rate models.
- TPA incorporates two spent fuel surface area models, a particle model and a grain model.
- TPA 5.0 will add a high-level waste glass source term model.
- Cladding can reduce the fraction of total spent fuel surface area exposed to water entering the waste package.

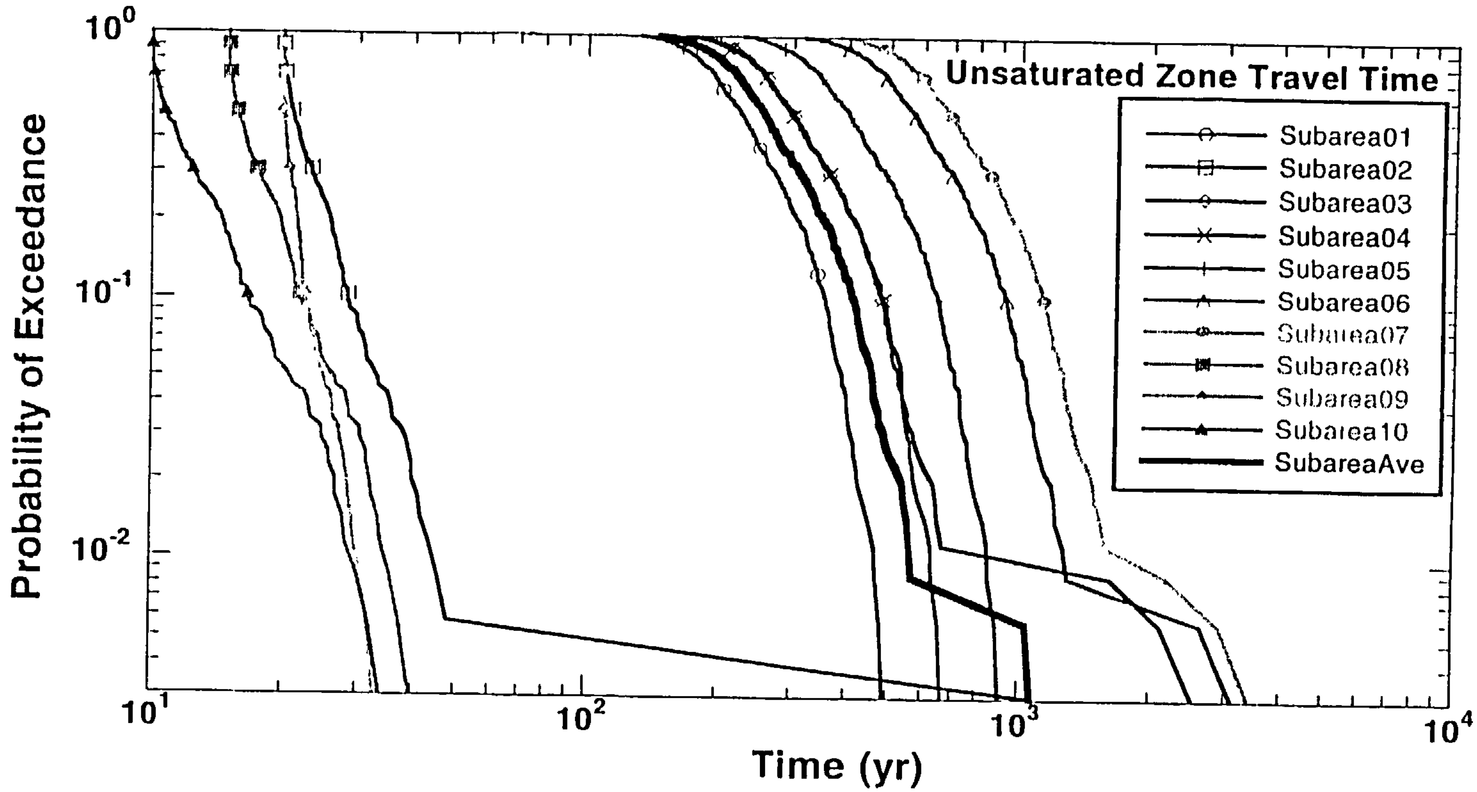
Unsaturated Radionuclide Transport



- TPA utilizes a simple 1-D vertical flow field through hydrostratigraphic layers whose thicknesses were derived from the Geologic Framework Model 3.1.
- UZ flow occurs in fractures when the percolation flux exceeds the matrix hydraulic conductivity for a given tuff layer.
- Due to large uncertainty and long run time, TPA does not include diffusion of radionuclides from fast flowing fractures into near-stagnant matrix pores.
- TPA models retardation in the rock matrix.

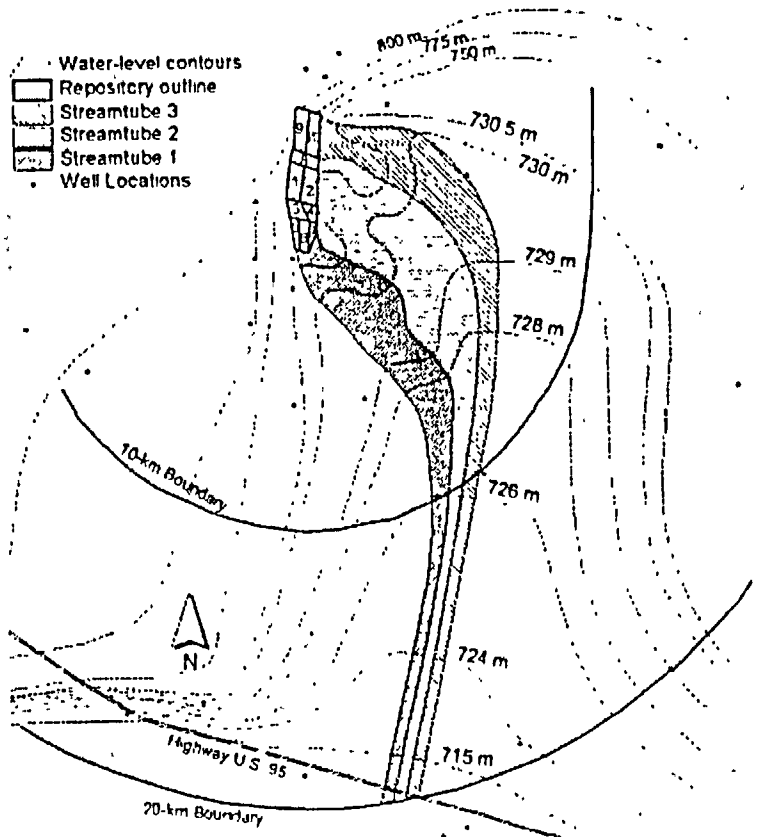
United States Nuclear Regulatory Commission

Unsaturated Radionuclide Transport



Unretarded unsaturated zone travel time.

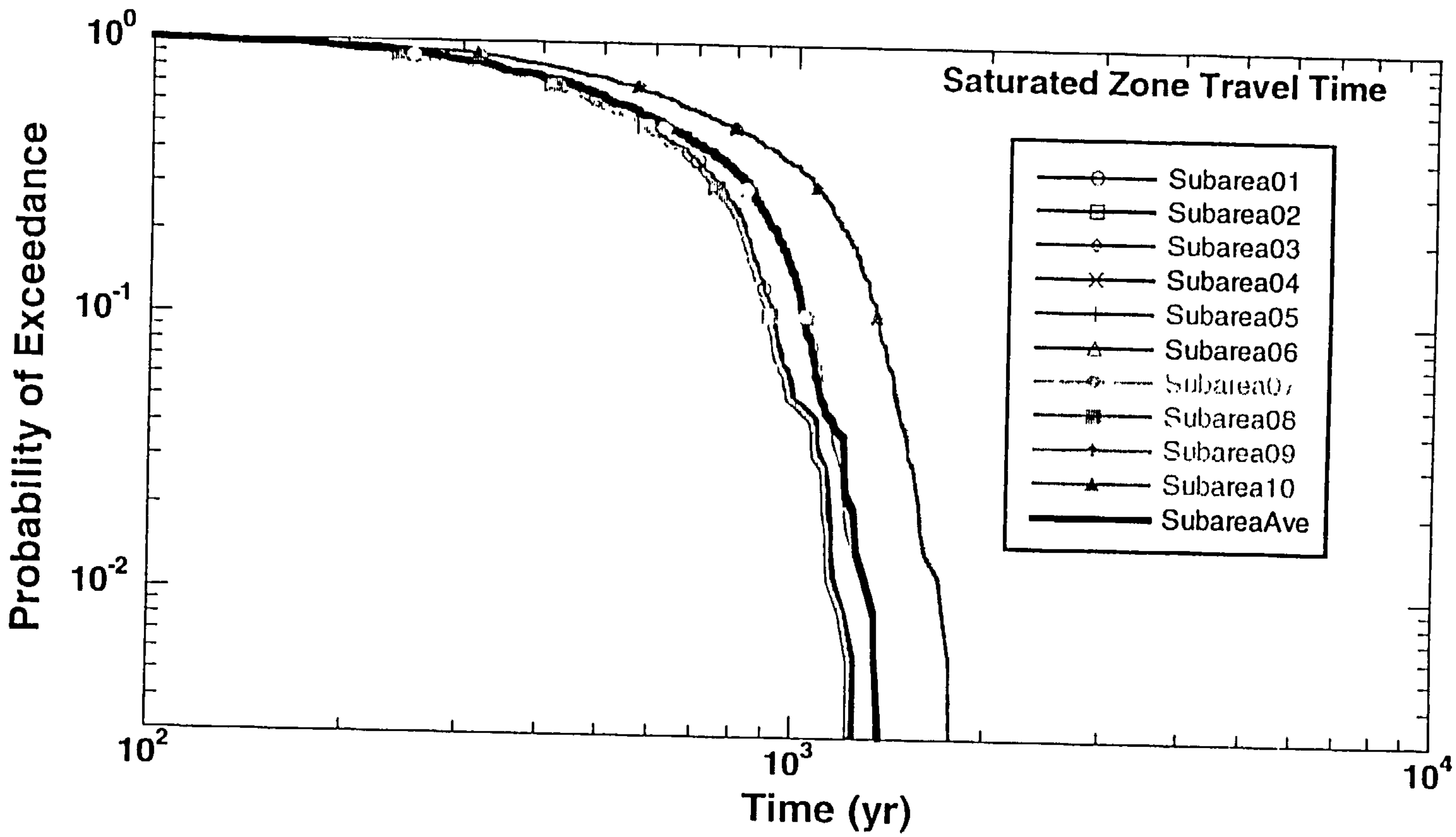
Saturated Radionuclide Transport



- TPA models 3 streamtubes based on a 2-D horizontal flow-net interpretation of hydraulic gradients in the uppermost aquifer.
- Water level data from area wells provides basis for hydraulic gradient and transmissivity.
- TPA samples tuff-alluvium interface.
- TPA models sorption in alluvial aquifer and tuff matrix.
- Radionuclides can diffuse from fractures into matrix in the tuff aquifer.

United States Nuclear Regulatory Commission

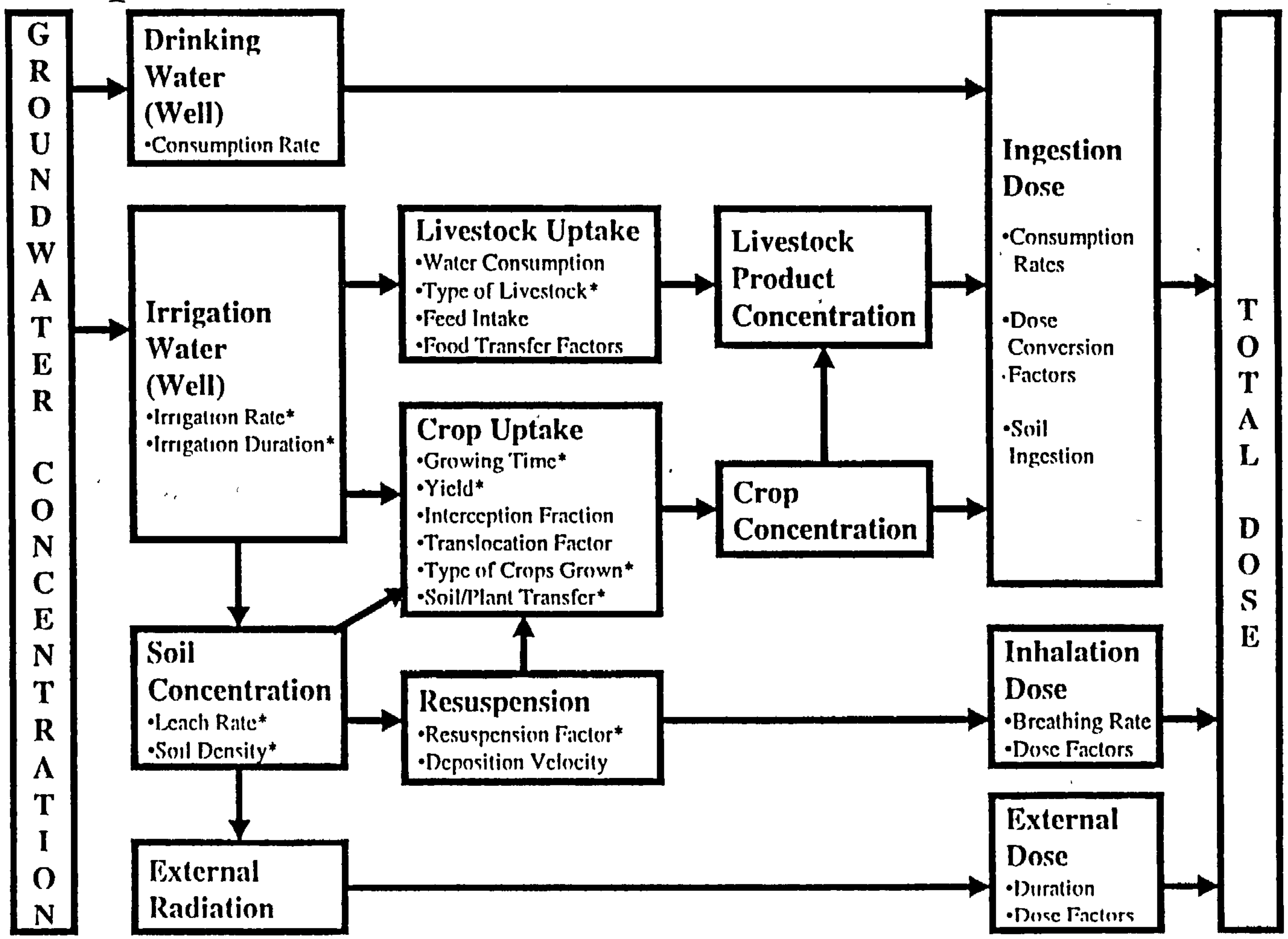
Saturated Radionuclide Transport



Unretarded saturated zone travel time.

United States Nuclear Regulatory Commission

Biosphere



* Examples of Site-Specific Parameters

Disruptive Events

- TPA predicts the number of waste package failures caused by falling rocks resulting from seismic activity that mechanically load and deform the waste package.
- TPA models waste package failure resulting from movements along undetected or new faults that exceed a displacement threshold.
- TPA accounts for waste package failures caused by both extrusive and intrusive igneous events. TPA models airborne releases of radionuclides for volcanic eruptions.

Afterword

- TPA provides a **flexible** framework to **independently** review pre-licensing activities and a license application for the proposed repository at Yucca Mountain.
- TPA uses approaches based on **fundamental principles**, where possible, to simulate the repository behavior and allow for some **computational efficiency**.
- Where possible, the approaches are based on available **data**.

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

YUCCA MOUNTAIN PROJECT

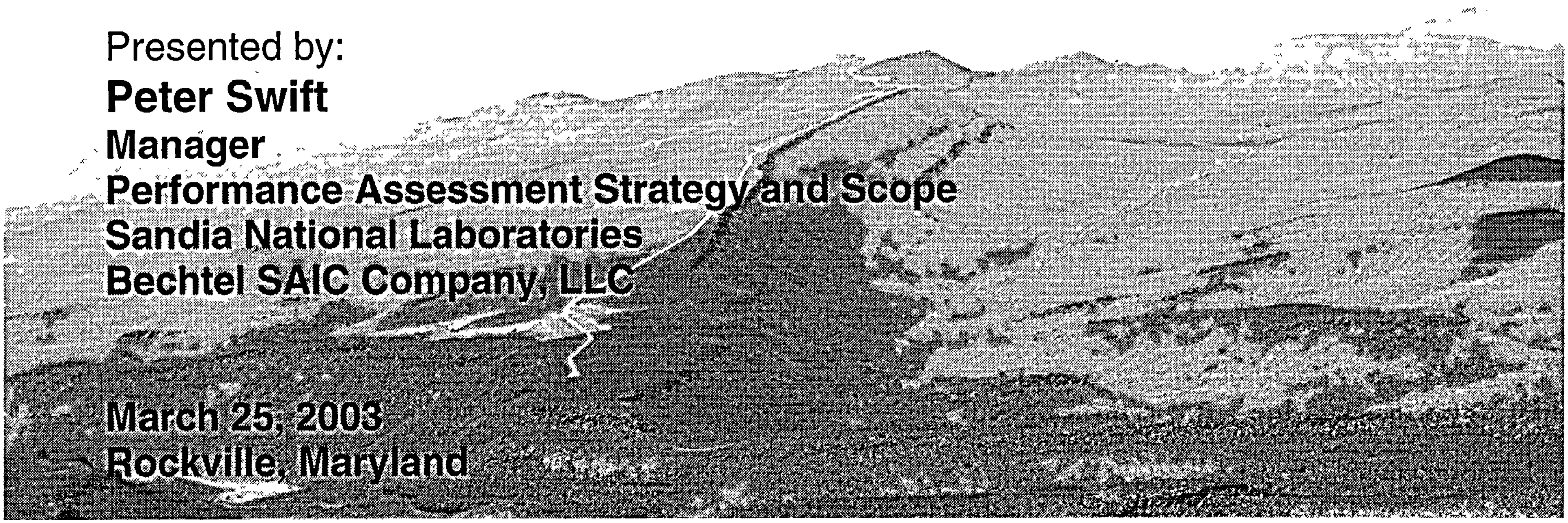
Overview of the U. S. Department of Energy Total System Performance Assessment Model

Presented to:
Advisory Committee on Nuclear Waste

Presented by:

Peter Swift
Manager
Performance Assessment Strategy and Scope
Sandia National Laboratories
Bechtel SAIC Company, LLC

March 25, 2003
Rockville, Maryland



Outline

- Current Status of the Total System Performance Assessment
- Summary of Total System Performance Assessment methodology
- Summary of the major model components
  - Mapping of workshop topics to DOE Total System Performance Assessment model components
  - Process models and abstractions
    - Source term discussed separately in later presentation
  - Linkage in Total System Performance Assessment model

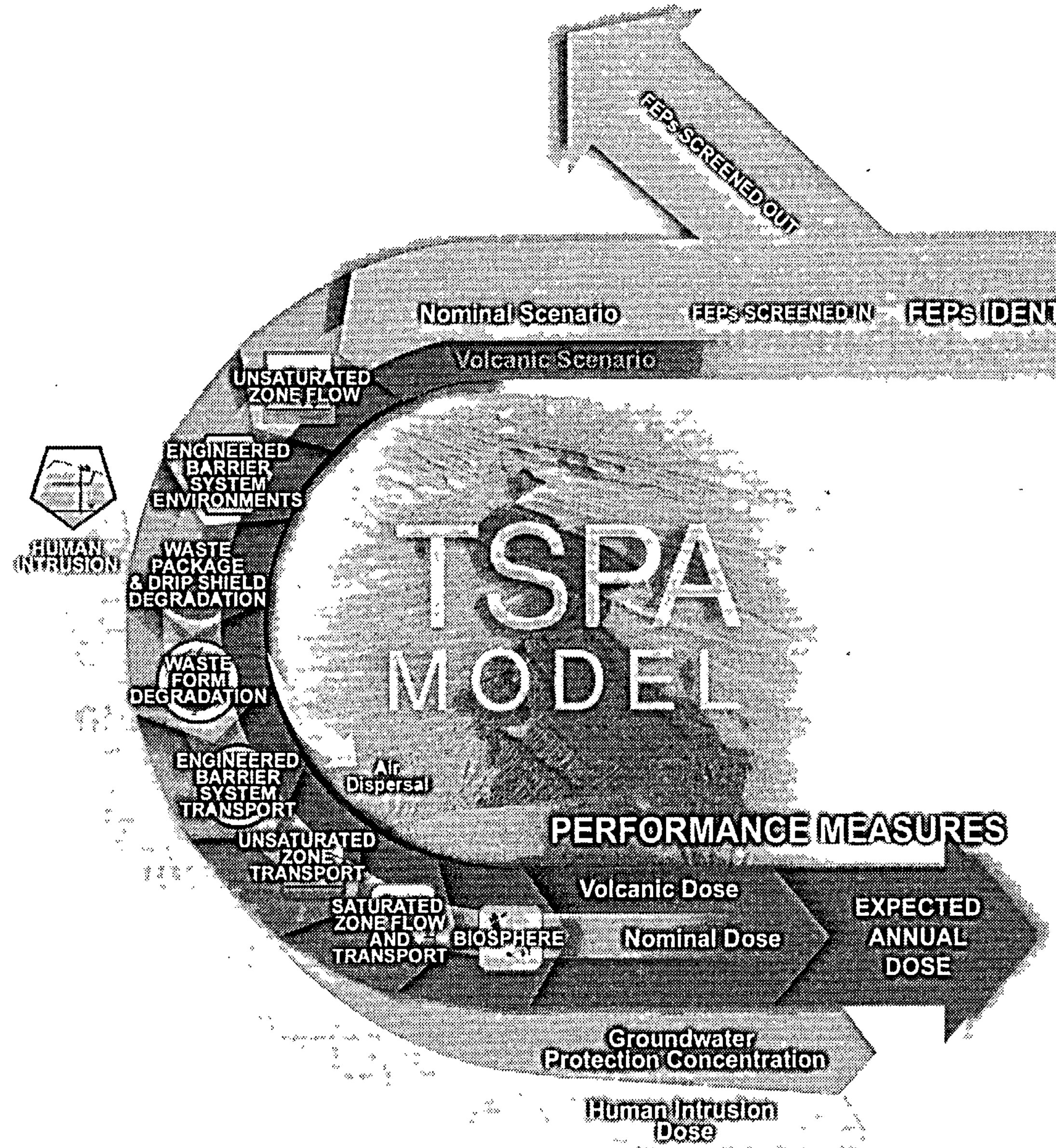
Status of Total System Performance Assessment Analyses

- **All DOE Total System Performance Assessment information used at this workshop is from existing Total System Performance Assessment analyses**
  - December 2000: Total System Performance Assessment for the Site Recommendation
  - July 2001: FY01 Supplemental Science and Performance Analyses
  - September 2001: Revised Supplemental Total System Performance Assessment to support the Final Environmental Impact Statement and Site Suitability Evaluation
  - Additional analyses completed in 2002
    - "One-off" analyses to support risk-based prioritization
    - "One-on" analyses to provide insight into barrier performance
- **Models and analyses that will support the License Application are currently under development**

Total System Performance Assessment Process

- Screen features, events and processes to determine those that must be retained in performance assessment
- Develop models, along with their scientific basis, for each process included in Total System Performance Assessment
- Identify uncertainty in models and parameters
- Construct integrated Total System Performance Assessment model using all retained processes
  - "Nominal" performance model contains all features, events and processes likely to occur
  - "Disruptive event" performance model contains low-probability events (e.g., volcanism)
  - Stylized human intrusion model, as specified by regulation
- Evaluate total-system performance (individual protection, groundwater protection, and human intrusion standard) considering uncertainty through Monte Carlo simulation

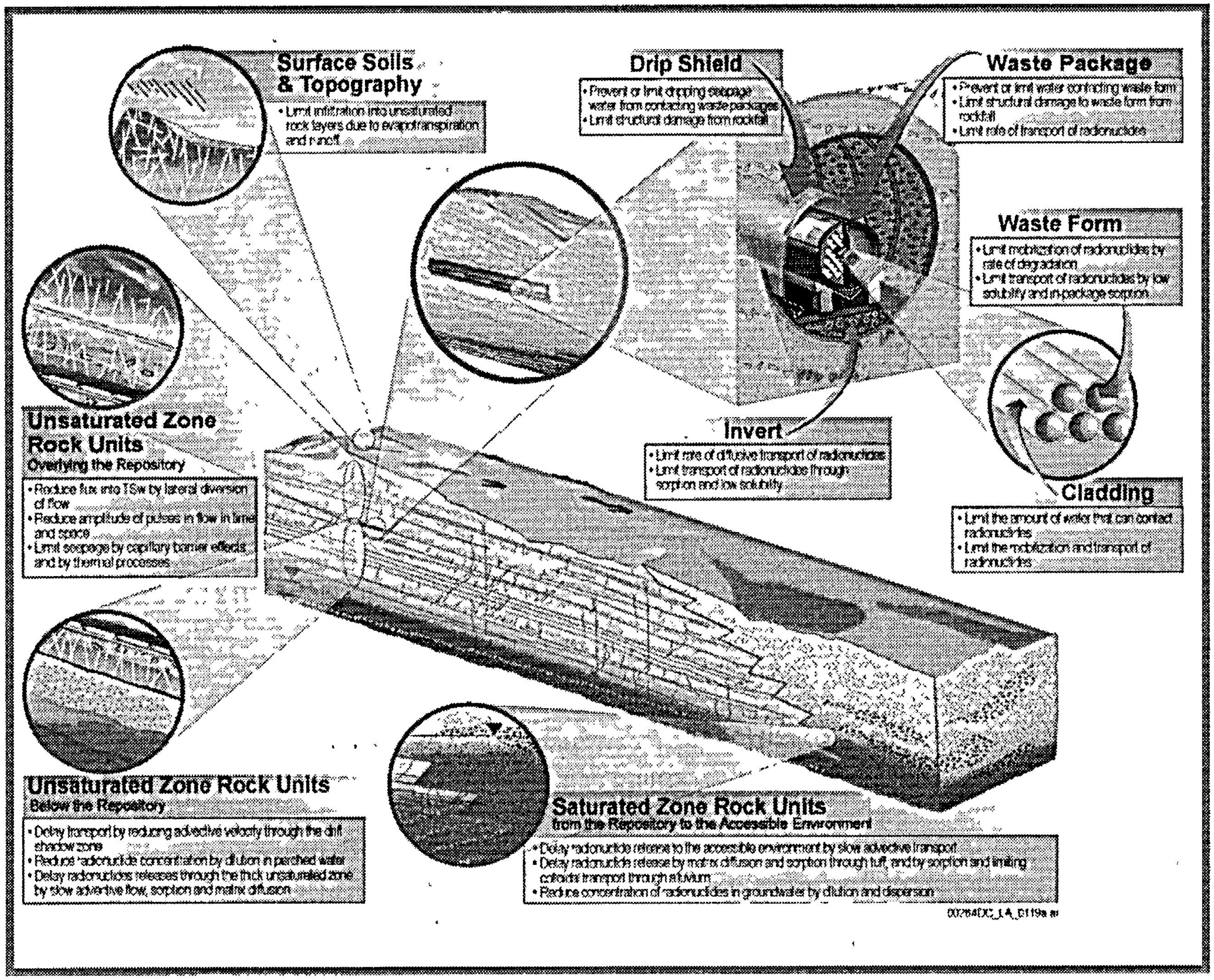
Total System Performance Assessment Process



Nominal Performance Model Components

Workshop Groupings	DOE Total System Performance Assessment Components
Infiltration/Tunnel Dripping	Climate, Infiltration, Unsaturated Zone Flow, Thermal Effects, Seepage
Source Term	Drip Shield, Waste Package, Cladding, Waste Form
Near Field	Transport in the Engineered Barrier System, including Invert
Unsaturated Zone	Flow and transport in the Unsaturated Zone below the Repository
Saturated Zone	Flow and transport in the Saturated Zone
Biosphere	Biosphere

Nominal Performance Model Components Organized by Barriers



- Surface soils and topography (includes climate, infiltration)
- Unsaturated zone above (seepage, drift effects)
- Drip shield
- Waste package
- Cladding
- Waste form
- Invert
- Unsaturated zone below (transport)
- Saturated zone

Total System Performance Assessment Model Components

(Nominal Performance)

- Radionuclide Inventory
- In-Package Chemistry
- Cladding Degradation
- CSNF Degradation
- DSNF Degradation
- DHLW Degradation
- Solubility Concentration Limit
- Colloid Concentration

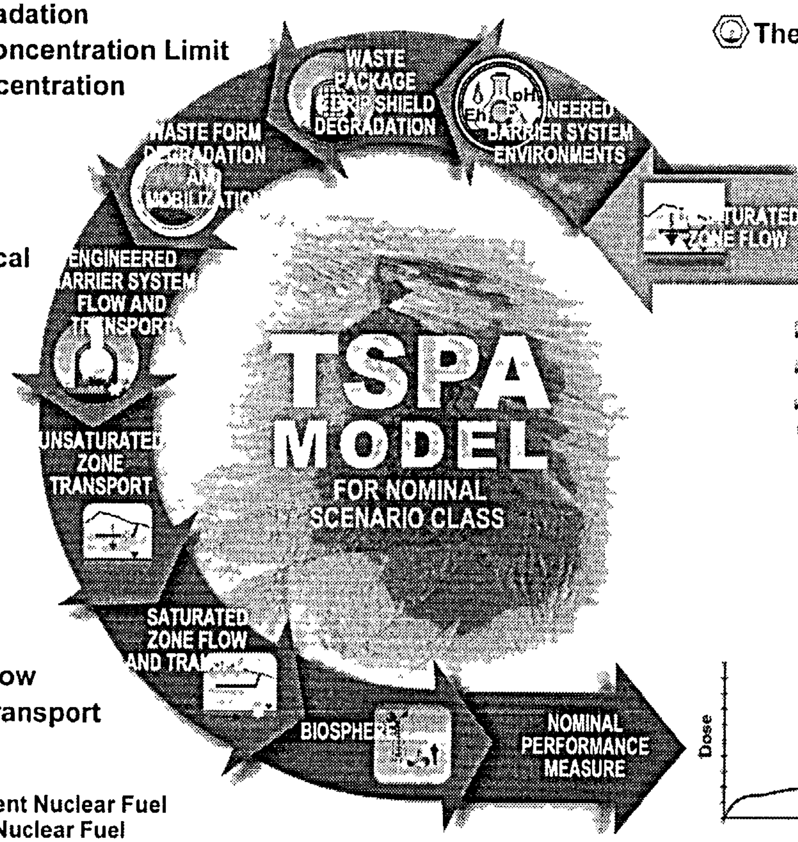
- Waste Package Degradation
- Drip Shield Degradation

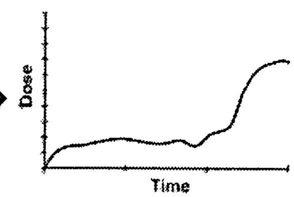
- Chemical Environment
- Thermal Hydrologic Environment

- EBS Physical Chemical Environment
- EBS Radionuclide Transport

- Climate
- Net Infiltration
- UZ Flow
- Seepage

- UZ Transport





00185DR_Figure 1 ai

- SZ Flow
- SZ Transport

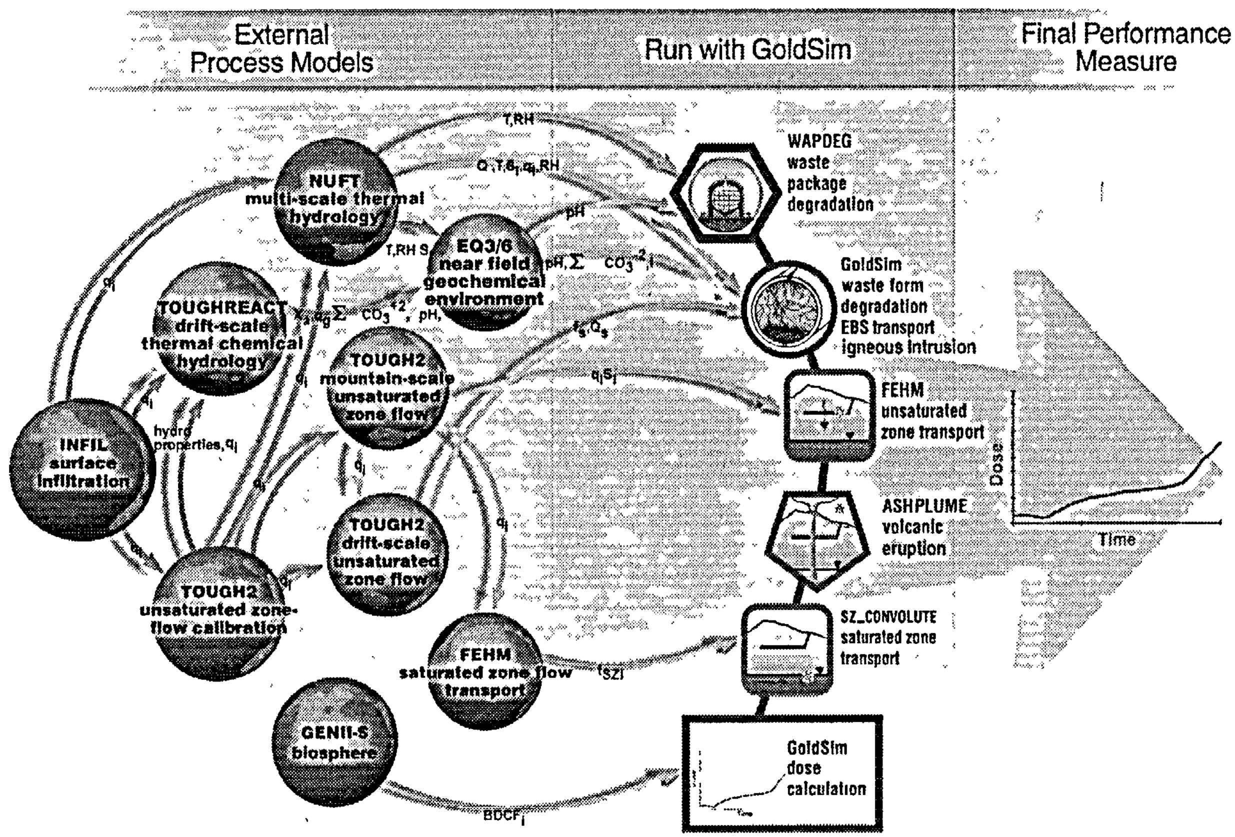
LEGEND

CSNF	Commercial Spent Nuclear Fuel
DSNF	Defense Spent Nuclear Fuel
DHLW	Defense High-Level Waste
EBS	Engineered Barrier System
SZ	Saturated Zone
UZ	Unsaturated Zone

- Biosphere Dose Conversion Factor
- Reasonably Maximally Exposed Individual Behavior

Overview of Model Linkage

(Total System Performance Assessment - Site Recommendation)



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		
ΣCO_3^{-2}	Carbonate Concentration	q_i	Infiltration Flux		

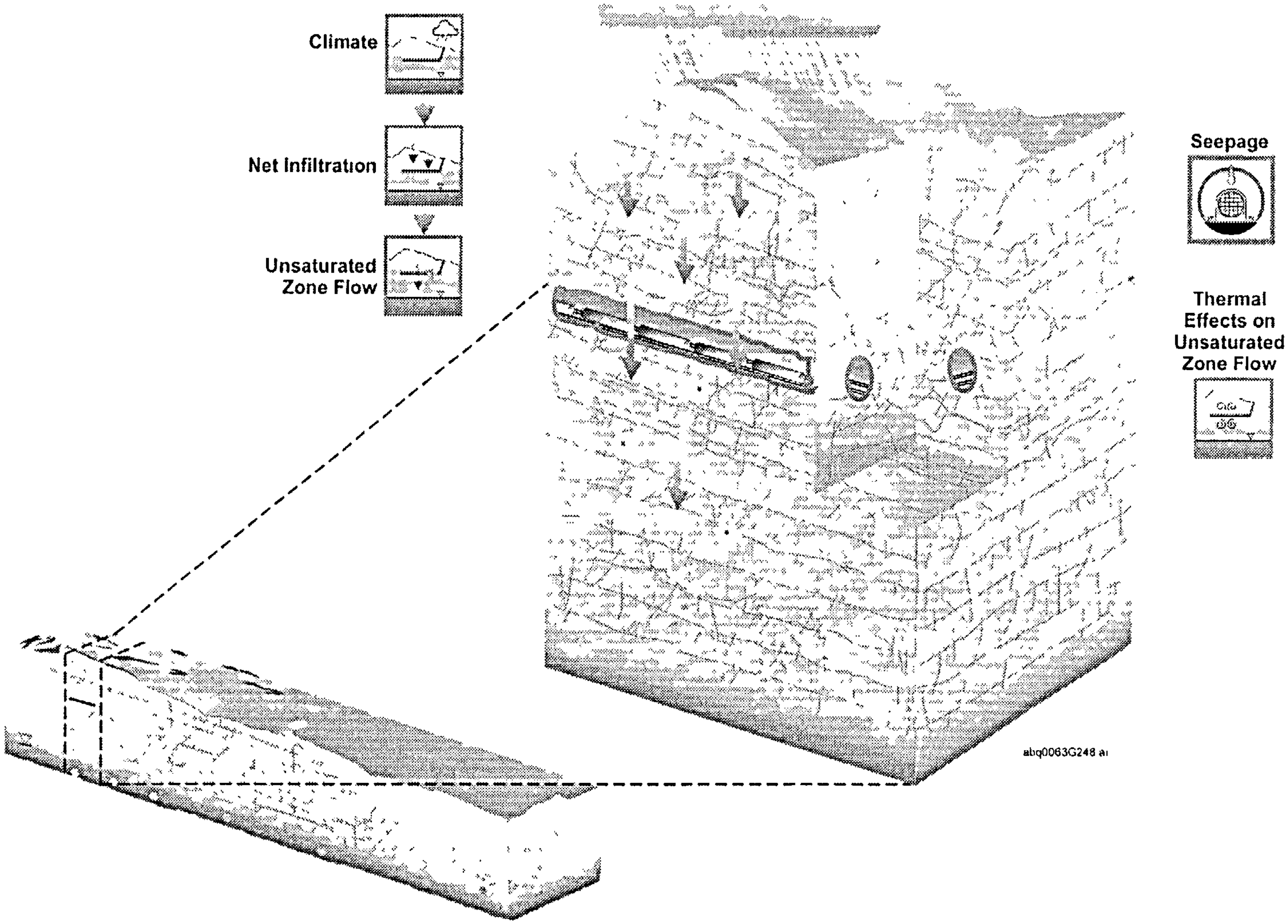
Legend

Response Surface Between Process Models

Response Surface from Process Model to GoldSim

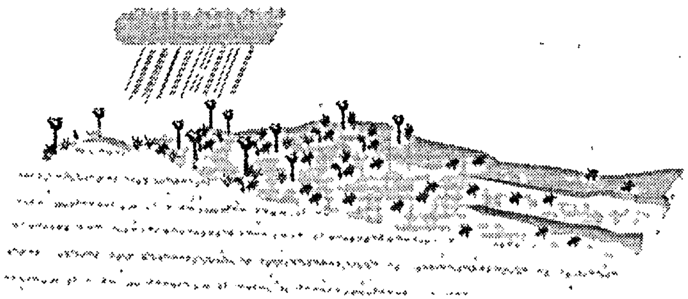
00185DR_Figure 2 ai

Components Related to Infiltration/Tunnel Dripping



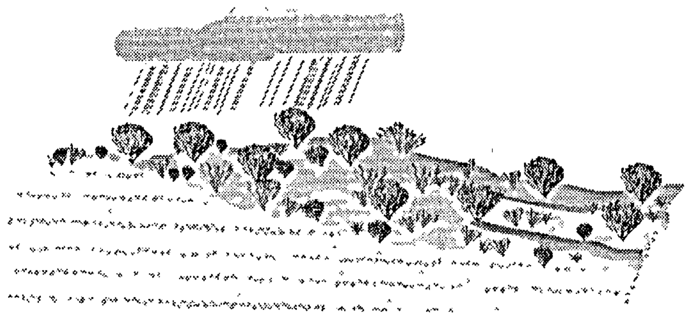
Climate

Total System Performance Assessment Abstraction and Linkage



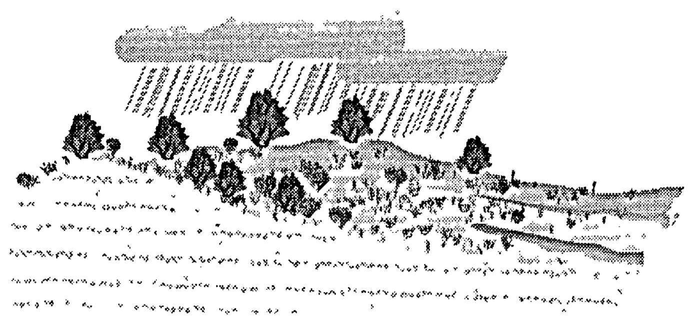
Present Day

Yucca Mountain



Monsoon

Lower-bound analog Yucca Mountain
Upper-bound analog. Nogales, AZ
Higher precipitation and temperature than present-day



Glacial Transition

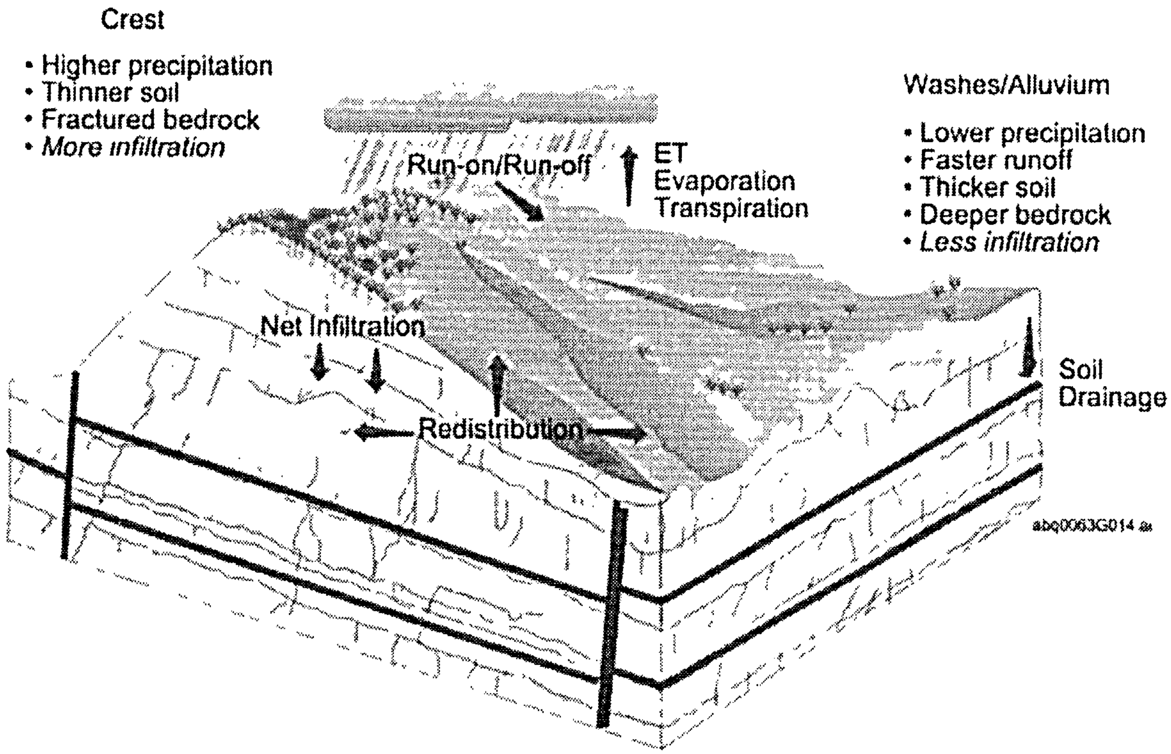
Lower-bound analog Delta, UT
Upper-bound analog· Spokane, WA
Higher precipitation and lower temperature than present-day

abq0063G052 al

- **Present climate and two future states based on paleoclimate data and modern analogs**
  - **Timing of climate changes is fixed**
  - **Uncertainty in magnitude of changes in precipitation and temperature is included through the infiltration model**
- **Outputs**
  - **To infiltration model**
    - **Mean annual temperature and precipitation, timing of changes**
  - **To unsaturated zone transport model**
    - **Water table rise with wetter climates shortens transport path**
  - **To saturated zone flow and transport model**
    - **Wetter climates increase flow rates, breakthrough curves calculated for present flow field are scaled accordingly**

Infiltration

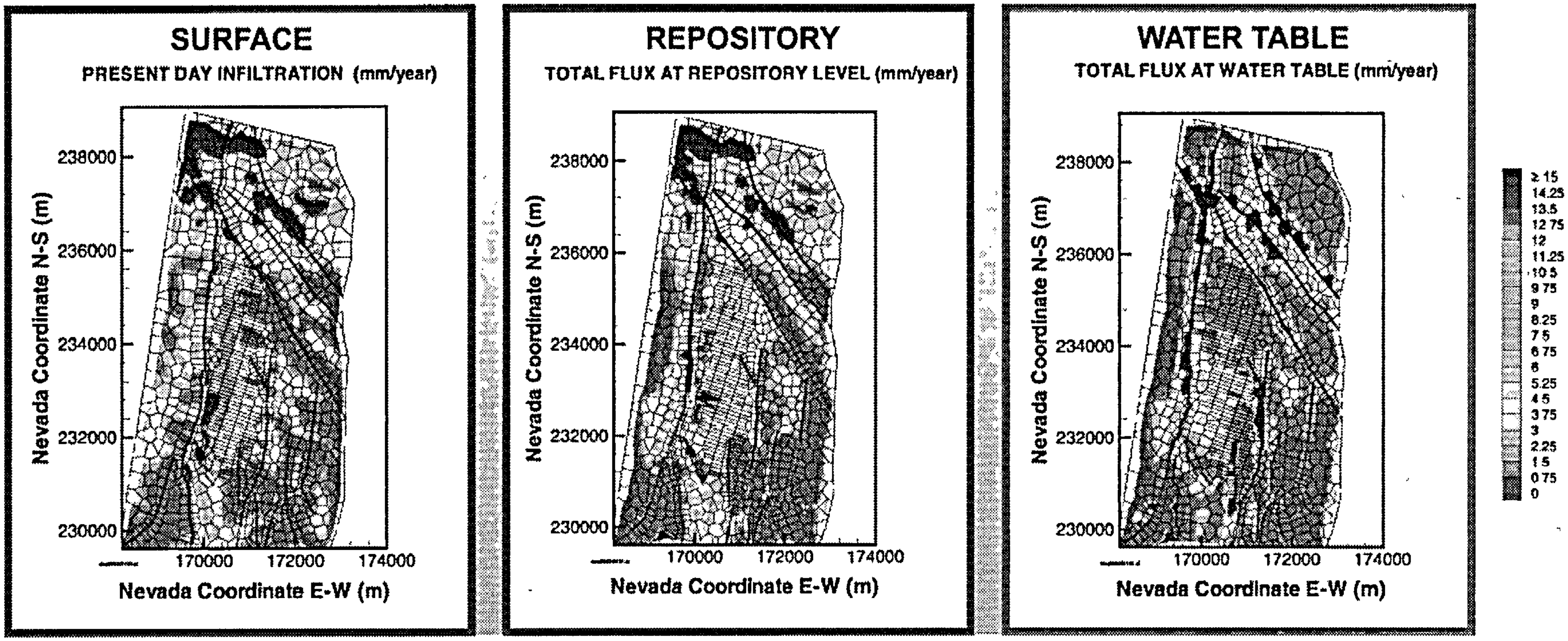
Total System Performance Assessment Abstraction and Linkage



- **Inputs from climate model, site and analog data**
- **Process model includes precipitation, temperature, evapotranspiration, insolation, run-on, run-off, soil storage**
- **Abstraction implements three detailed net infiltration maps (high, medium, low) calculated for each climate state**
- **Output**
  - **Infiltration flux maps to mountain scale flow model and thermal hydrology model**
  - **Probability of infiltration maps to Total System Performance Assessment for binning waste packages and source term**

Mountain Scale Unsaturated Zone Flow

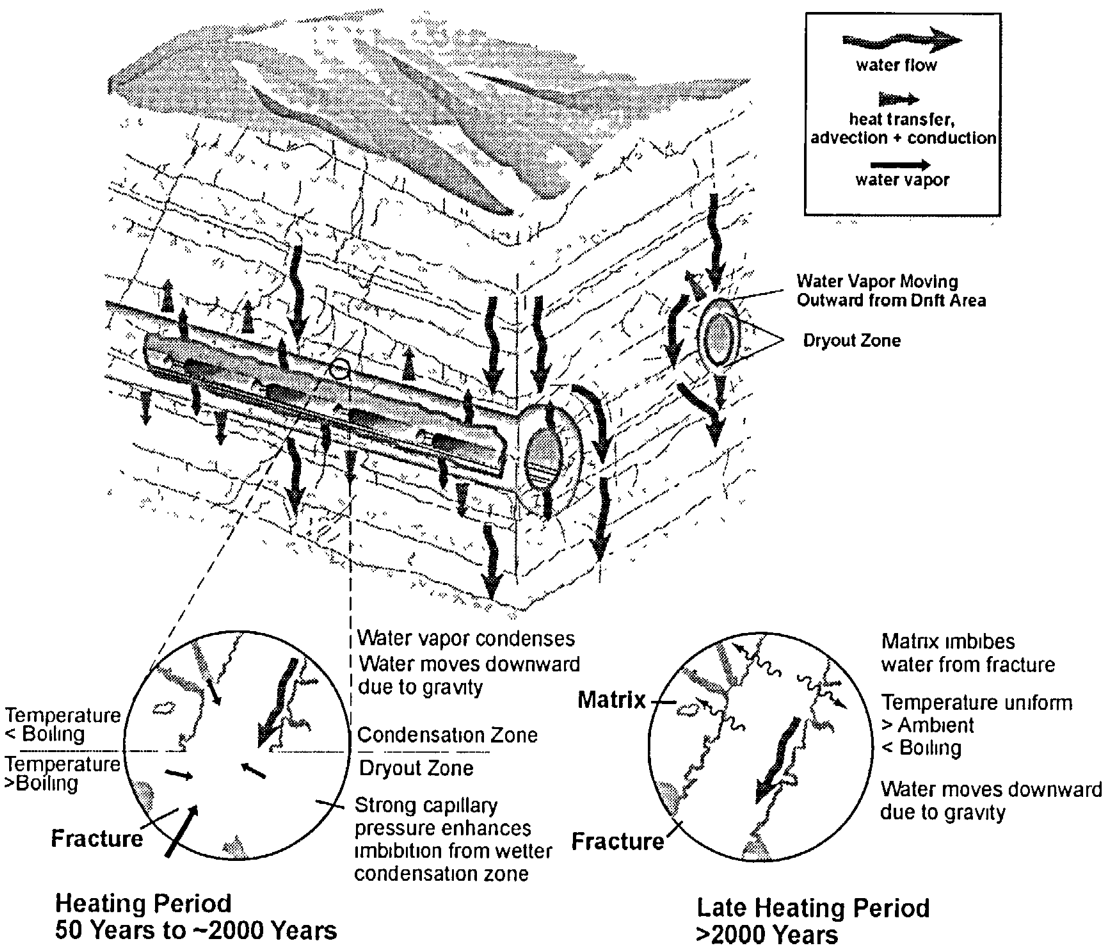
Total System Performance Assessment Abstraction and Linkage



- Inputs from infiltration model, site data
- Process model calculates 3-D steady state isothermal flow in an unsaturated dual permeability medium
- Abstraction implements a flow field for each infiltration map
- Outputs
  - Hydrologic properties to thermal hydrology model
  - Flow fields for unsaturated zone transport model

Thermal Hydrologic Environments

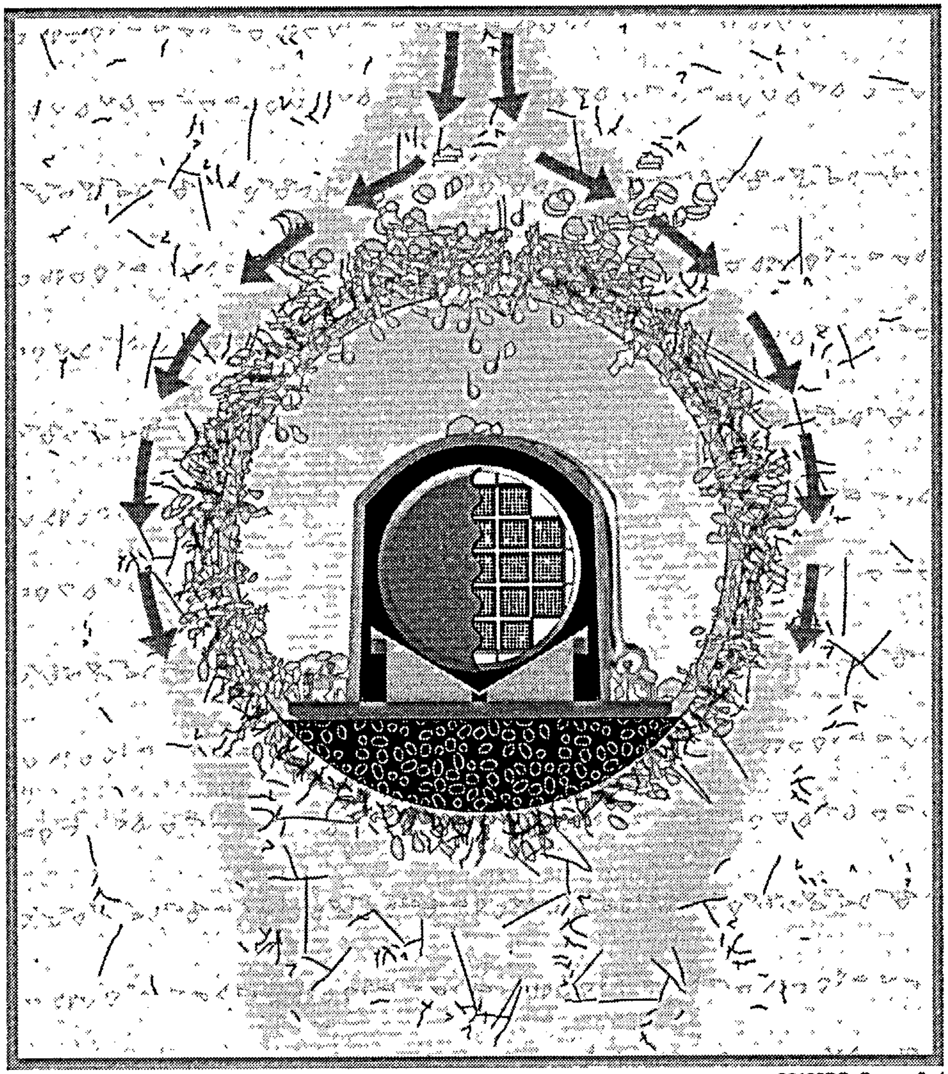
Total System Performance Assessment Abstraction and Linkage



- **Thermal hydrology model**
  - Inputs: drift layout and heat loading from repository design; hydrologic properties from mountain scale flow model; water flux from infiltration model
  - Outputs: percolation flux to seepage model; environmental conditions in drift and adjacent rock
- **Thermal hydrologic chemistry model**
  - Inputs: initial water chemistry, temperature history from thermal hydrology model
  - Outputs: water chemistry entering drift

Seepage

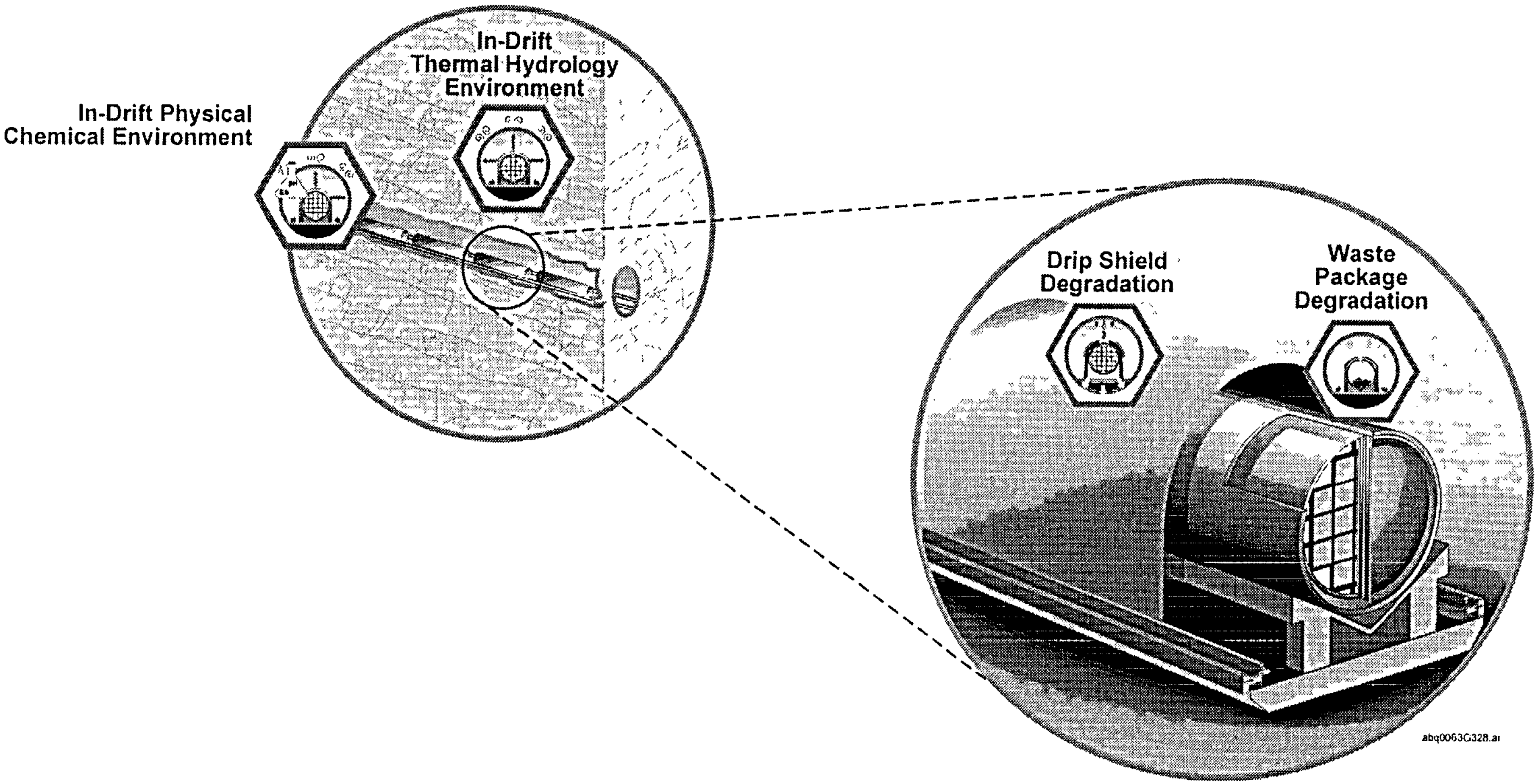
Total System Performance Assessment Abstraction and Linkage



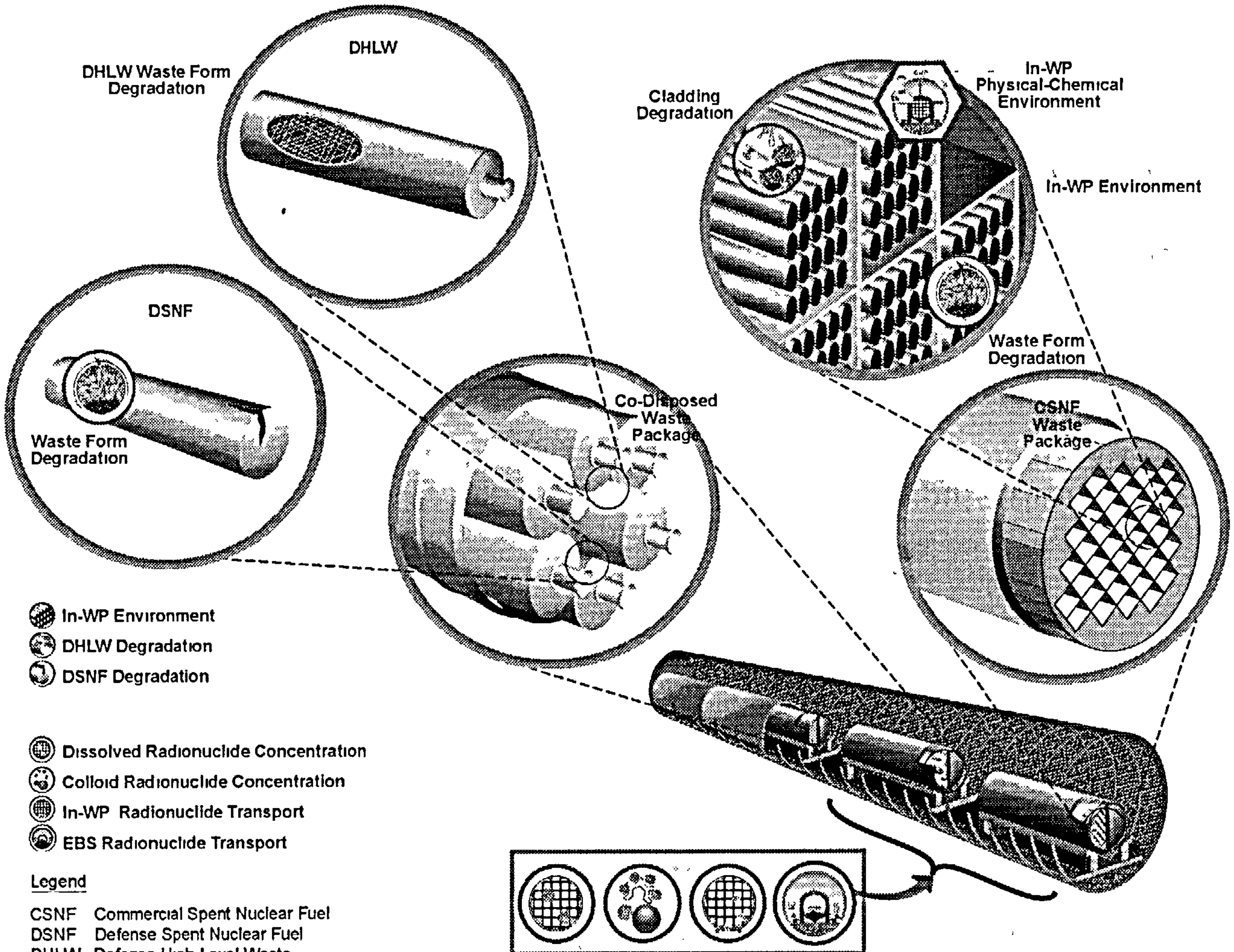
00185DR_Figure_5 ai

- Process model calculates 3-D fracture-only flow, includes flow focusing effects, drift degradation
- Inputs are thermal hydrology flux, drift design, rock properties
- Abstraction uses thermal hydrology flux 5 m above drift as input
- Outputs are seepage fraction (overall 13% for Total System Performance Assessment - Site Recommendation, 48% for Supplemental Science and Performance Analyses and Final Environmental Impact Statement), seep rate (with uncertainty) for different waste package bins (i.e., waste type, infiltration states)

Components Related to the Source Term
Waste Package and Drip Shield Degradation



Components Related to the Source Term Radionuclide Release From the Waste Form

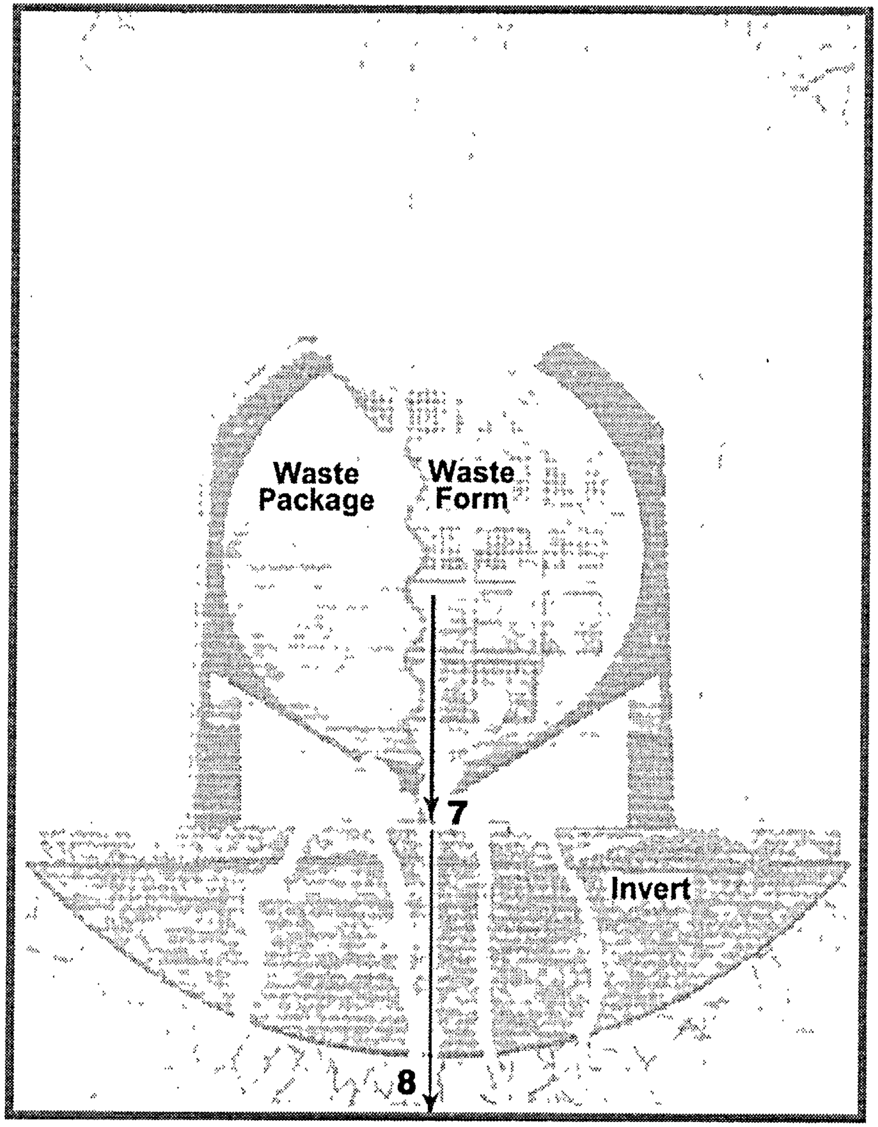


Legend

CSNF Commercial Spent Nuclear Fuel
DSNF Defense Spent Nuclear Fuel
DHLW Defense High-Level Waste
EBS Engineered Barrier System
WP Waste Package

abq0063G322_a ai

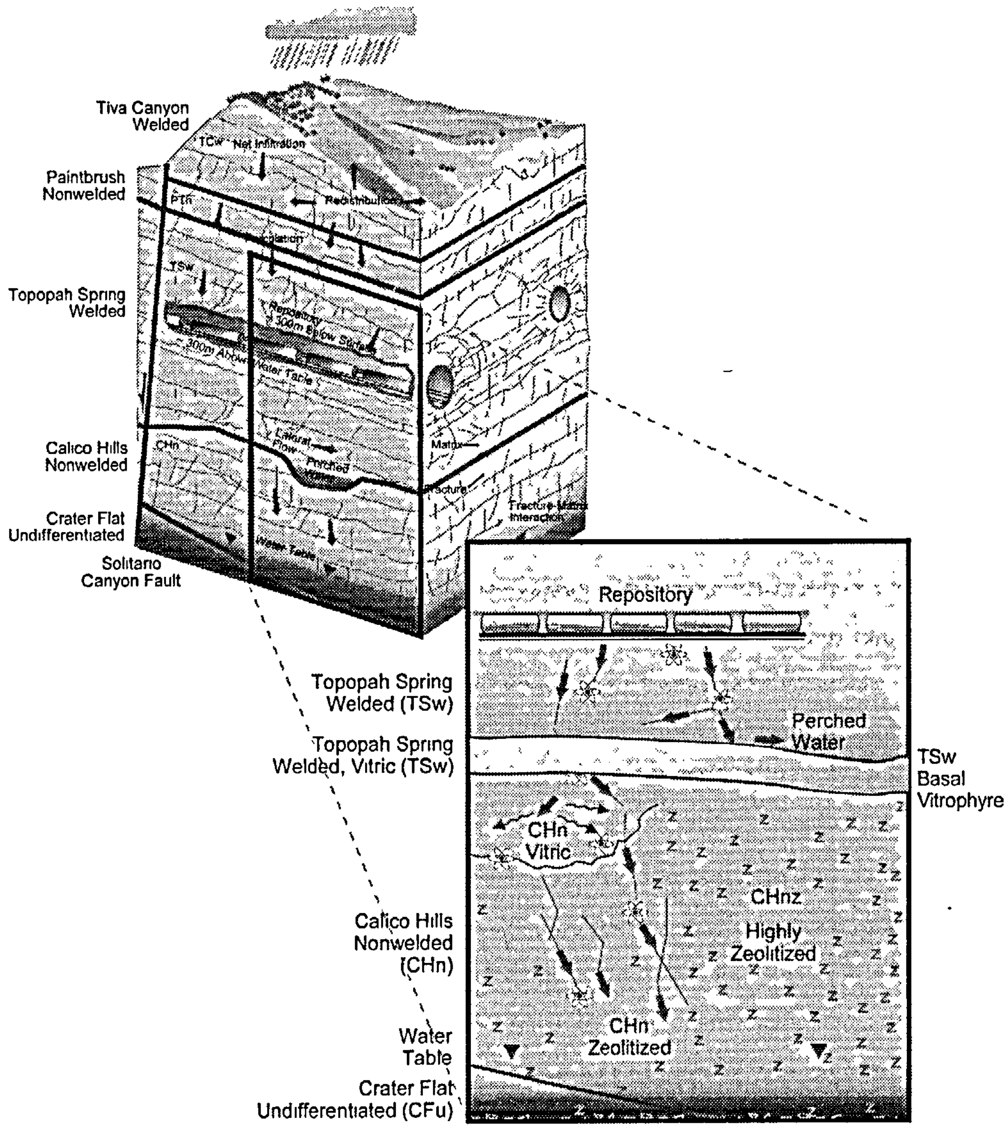
Components Related to the Near Field Radionuclide Transport in the Drift



- **Engineered barrier system flow**
  - 1-D flow model uses input from thermal hydrology, seepage, waste package (source term)
- **Engineered barrier system chemistry**
  - Inputs include water chemistry, flux, temperature
  - Outputs: invert water chemistry to engineered barrier system transport model
- **Engineered barrier system transport**
  - Advective and diffusive transport
  - Inputs from engineered barriers system flow, waste package
  - Outputs: radionuclide flux to unsaturated zone transport model

Unsaturated Zone Transport

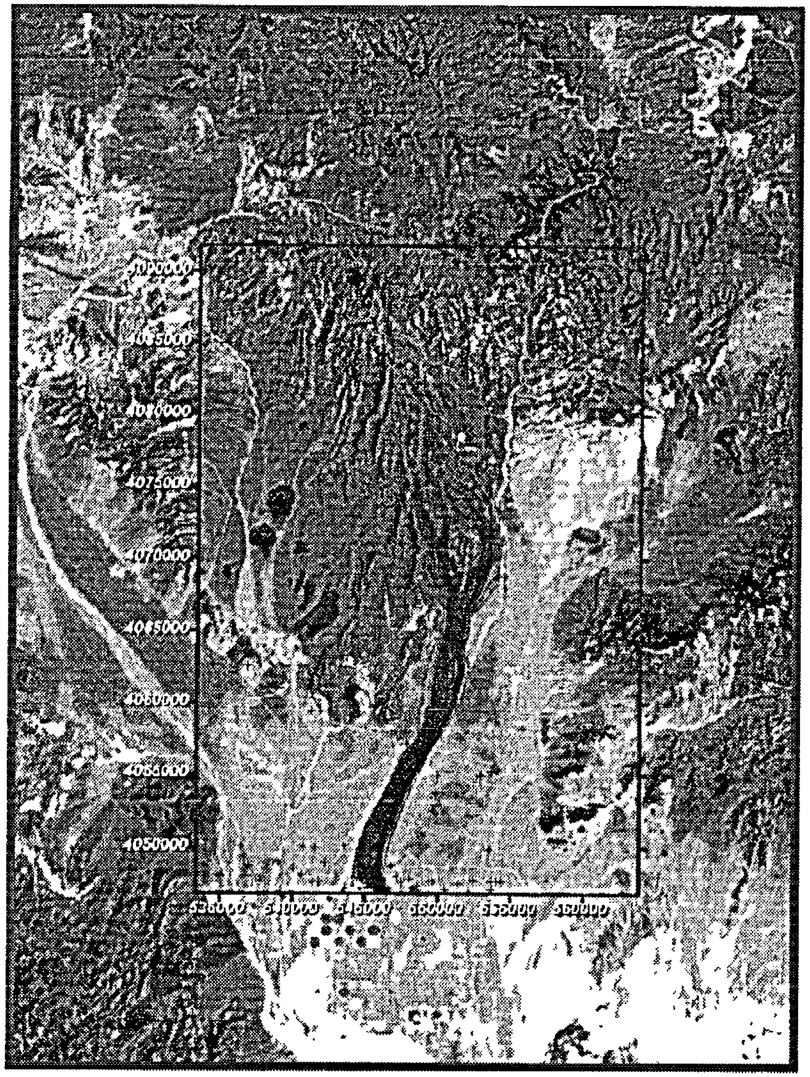
Total System Performance Assessment Abstraction and Linkage



- 3-D steady-state particle tracker, dual-continuum transport with sorption, reversible and irreversible colloids
- Implemented directly in Total System Performance Assessment
- Inputs:
  - Flow fields from mountain scale flow model
  - Radionuclide fluxes from engineered barrier system transport model
  - Time and magnitude of climatic changes in water table elevation
- Outputs: radionuclide flux to saturated zone transport model

Saturated Zone Flow and Transport

Total System Performance Assessment Abstraction and Linkage

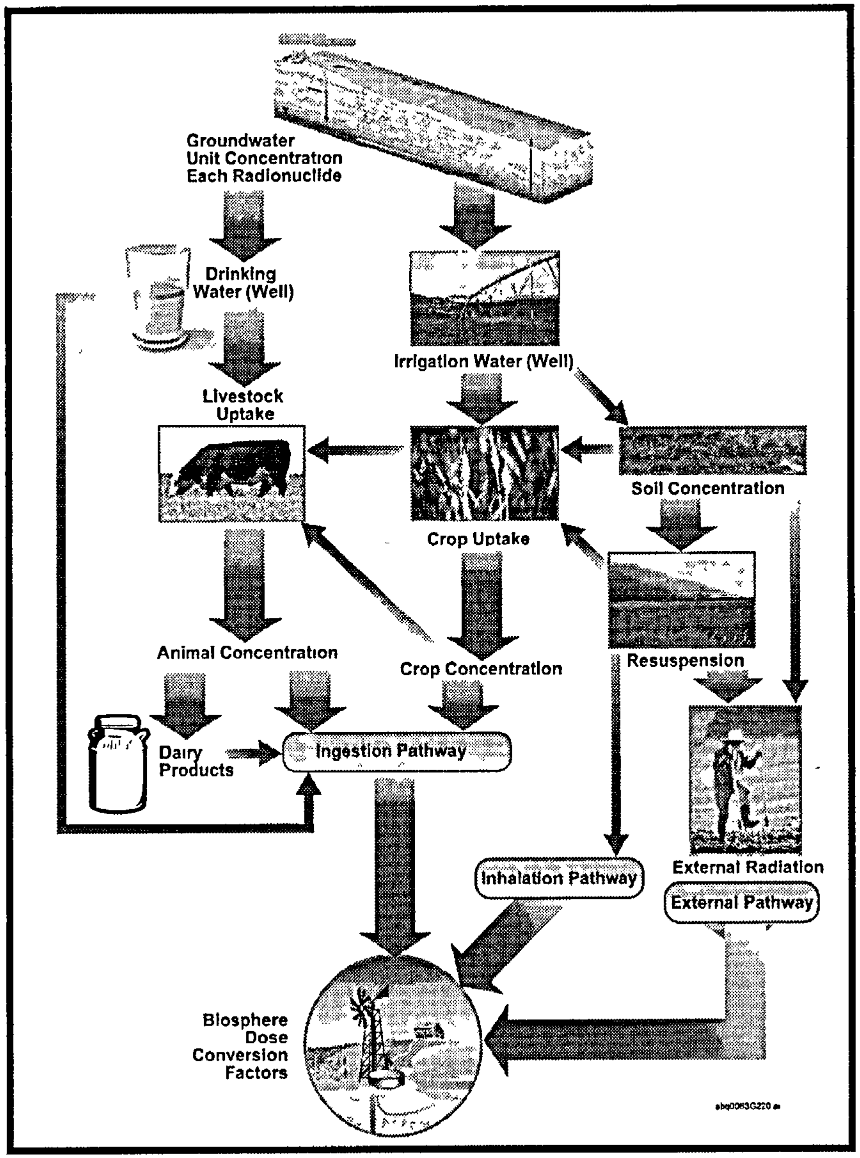


00135DR Figure 3 a

- **Process model calculates site-scale 3-D steady-state flow**
  - Inputs include hydrogeologic framework regional model, boundary and recharge fluxes, future flux climate scaling factors
  - Calibration to water table data
- **Transport calculated as breakthrough curves for release at initial time**
  - Includes sorption, reversible and irreversible colloids
- **Total System Performance Assessment abstraction uses convolution integral approach to apply breakthrough curves to releases at all times, scaling for climate effects and accounting for radioactive decay/ingrowth**
- **Output to biosphere model: radionuclide flux into the withdrawal well**

Biosphere

Total System Performance Assessment Abstraction and Linkage



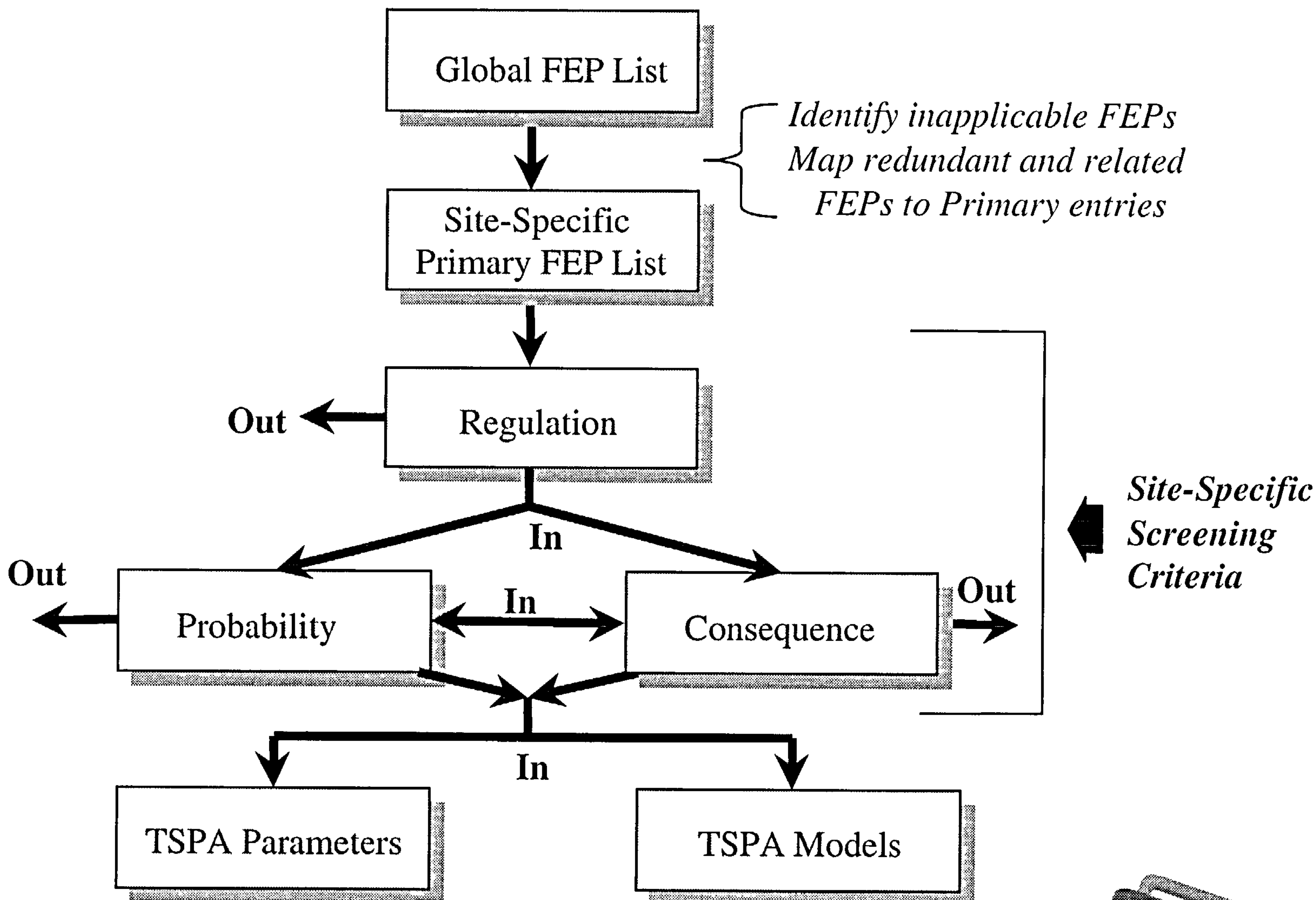
- Exposure pathways include food and water ingestion, dust inhalation, external exposure to contaminated soil
- Human lifestyles and groundwater pumping consistent with regulatory requirements
- Dose methodology based on the International Commission on Radiological Protection 30 standards
- Inputs are radionuclide concentrations in groundwater, human lifestyle data
- Outputs to Total System Performance Assessment are biosphere dose conversion factors

Summary

- Detailed models characterize water flow, radionuclide transport, and other important processes through the major components of the system
- Total System Performance Assessment links these models, simplified where appropriate and necessary, to provide estimates of system performance
- Total System Performance Assessment and process models can be used to examine behavior of individual components within the system, to be discussed in subsequent presentations

Backup

Screening Features, Events, and Processes



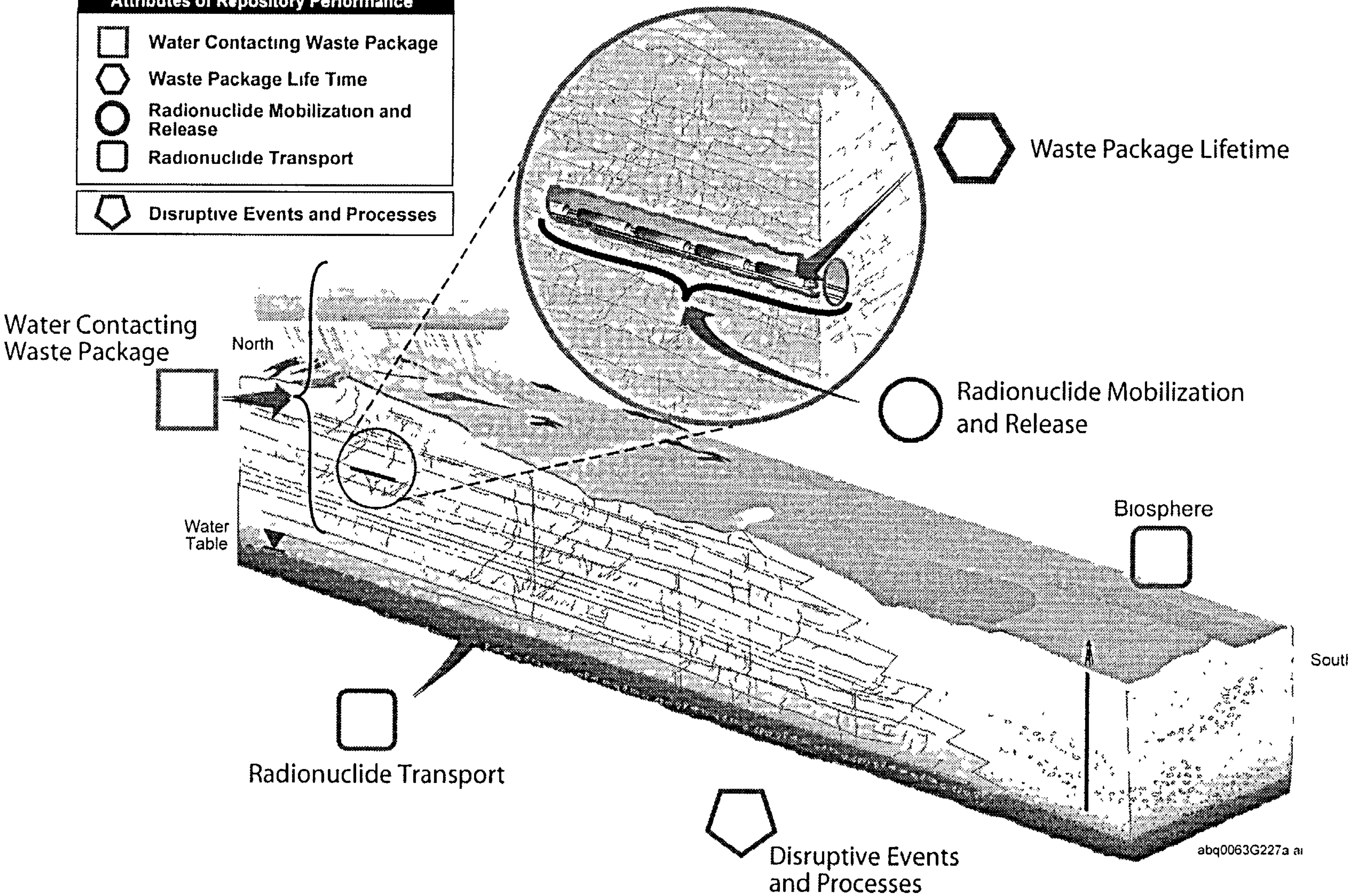
Screening Features, Events, and Processes Screening Criteria

- From 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."

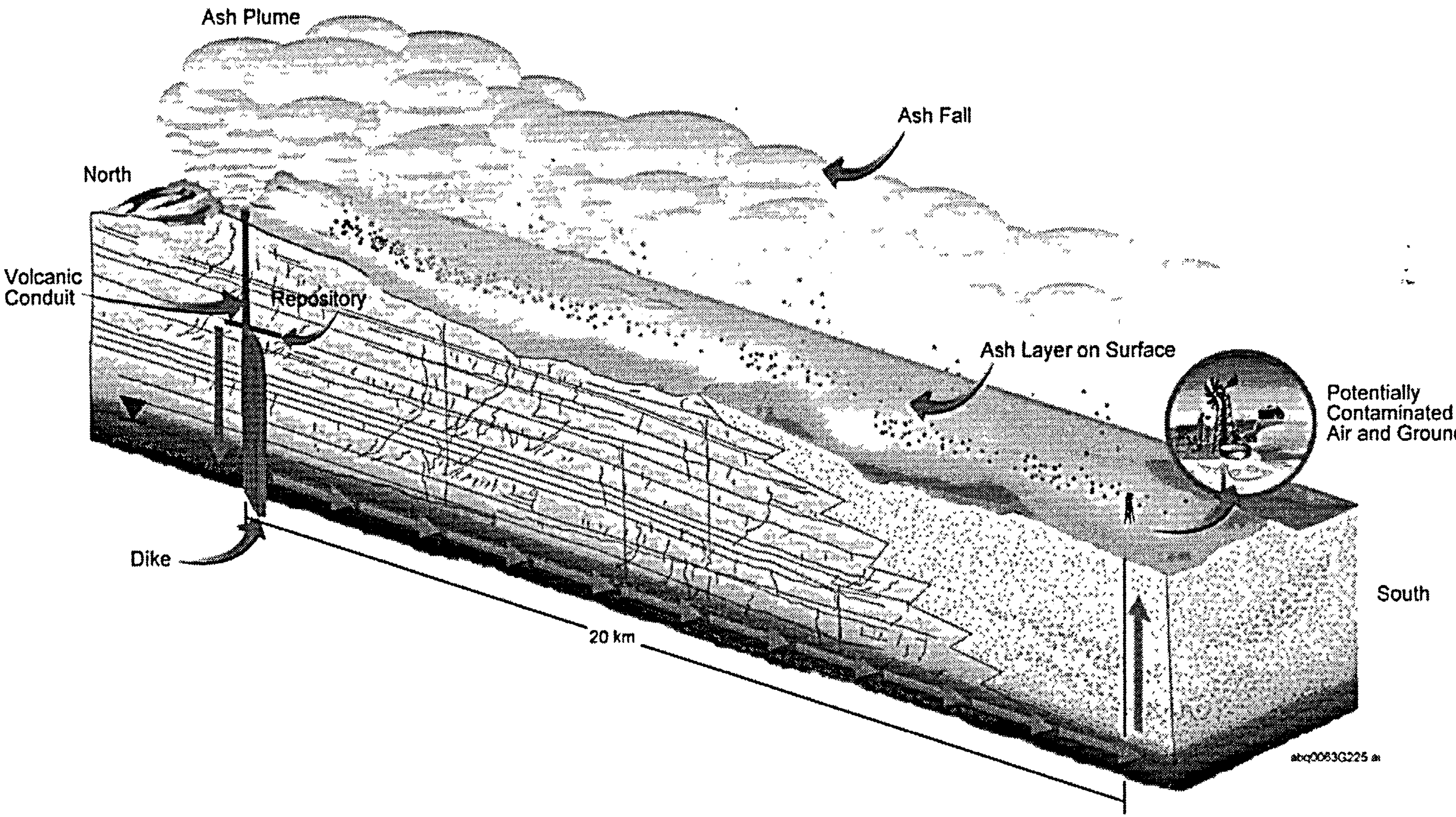
Nominal Performance Scenario Class

Attributes of Repository Performance
Water Contacting Waste Package
Waste Package Life Time
Radionuclide Mobilization and Release
Radionuclide Transport

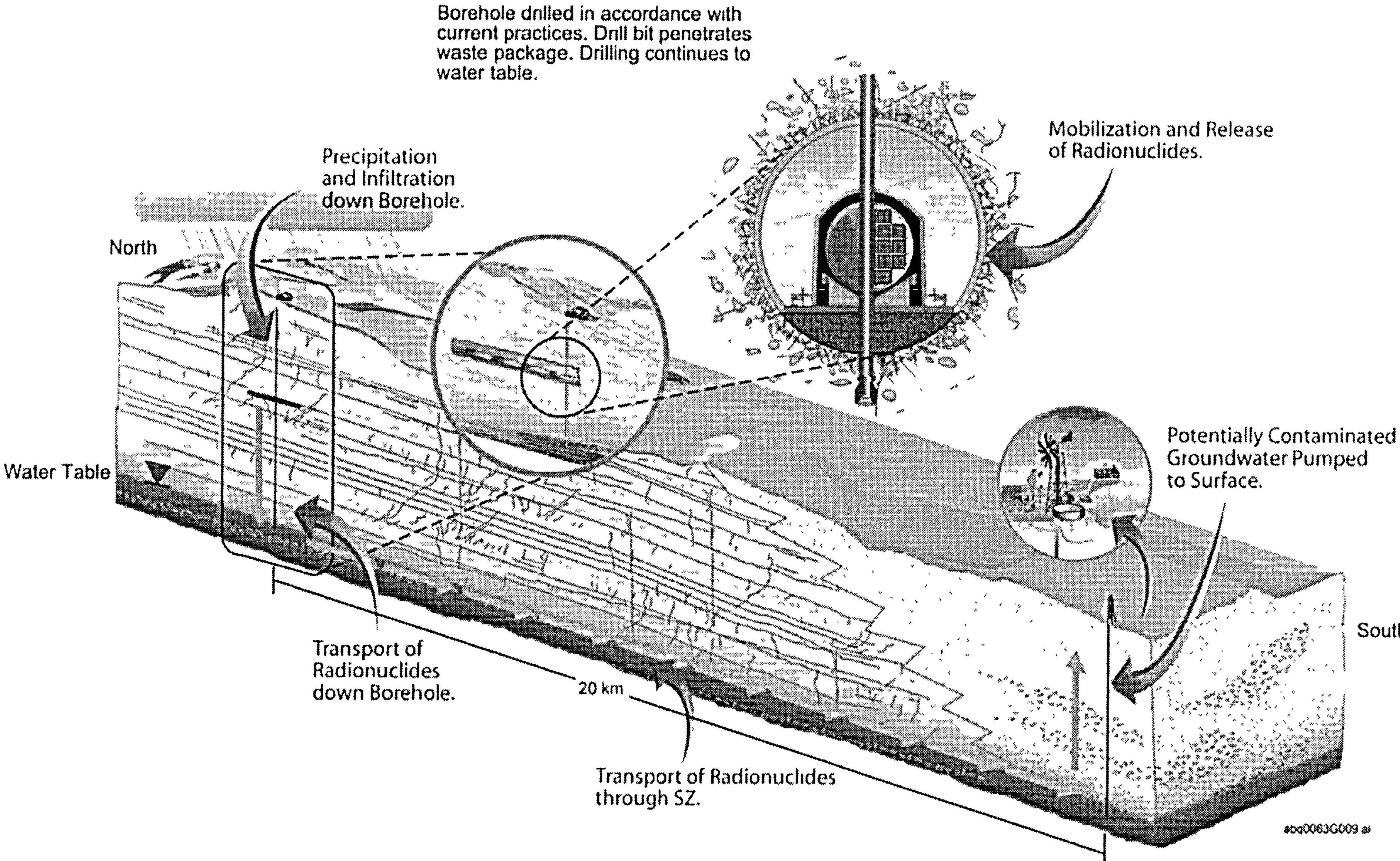
Disruptive Events and Processes



Igneous Disruption Scenario Class

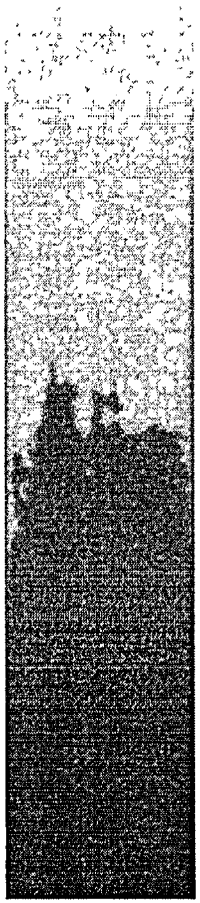


Human Intrusion Scenario



References

- "Total System Performance Assessment - Site Recommendation"
  - CRWMS M&O 2000. *Total System Performance Assessment for the Site Recommendation.* TDR-WIS-PA-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001220.0045
- "Total System Performance Assessment - Supplemental Science and Performance Analysis"
  - BSC (Bechtel SAIC Company) 2001. *FY01 Supplemental Science and Performance Analyses, Volume 2: Performance Analyses.* TDR-MGR-PA-000001 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010724.0110
- "Total System Performance Assessment - Final Environmental Impact Statement"
  - Williams, N.H. 2001. "Contract No. DE-AC08-01RW12101 – Total System Performance Assessment – Analyses for Disposal of Commercial and DOE Waste Inventories at Yucca Mountain – Input to Final Environmental Impact Statement and Site Suitability Evaluation REV 00 ICN 02." Letter from N.H. Williams (BSC) to J.R. Summerson (DOE/YMSCO), December 11, 2001, RWA:cs-1204010670, with enclosure. ACC: MOL.20011213.0056 (SL986M3, Rev. 00)
- "One-Off Analyses"
  - BSC (Bechtel SAIC Company) 2002. *Risk Information to Support Prioritization of Performance Assessment Models*, TDR-WIS-PA-000009 Rev. 01 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20021017.0045
- "One-On Analysis"
  - Saulnier, G. J., 2002. *Use of One-on Analysis to Evaluate Total System Performance.* Las Vegas, NV: Bechtel SAIC Company. ANL-WIS-PA-000004 Rev. 00 ICN 00



United States Nuclear Regulatory Commission

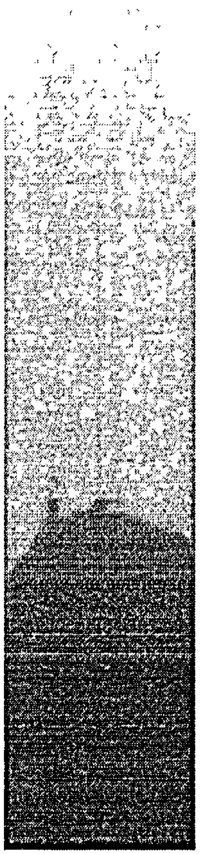
Source-Term Modeling and Support

David W. Esh, Ph.D.

Environmental and Performance Assessment Branch
Contact info: (301) 415-6705, dwe@nrc.gov

<u>Main Contributors:</u> Tae Ahn, Gustavo Cragnolino, Vijay Jain, Richard Codell, Osvaldo Pensado, Roberto Pabalan, Sitakanta Mohanty

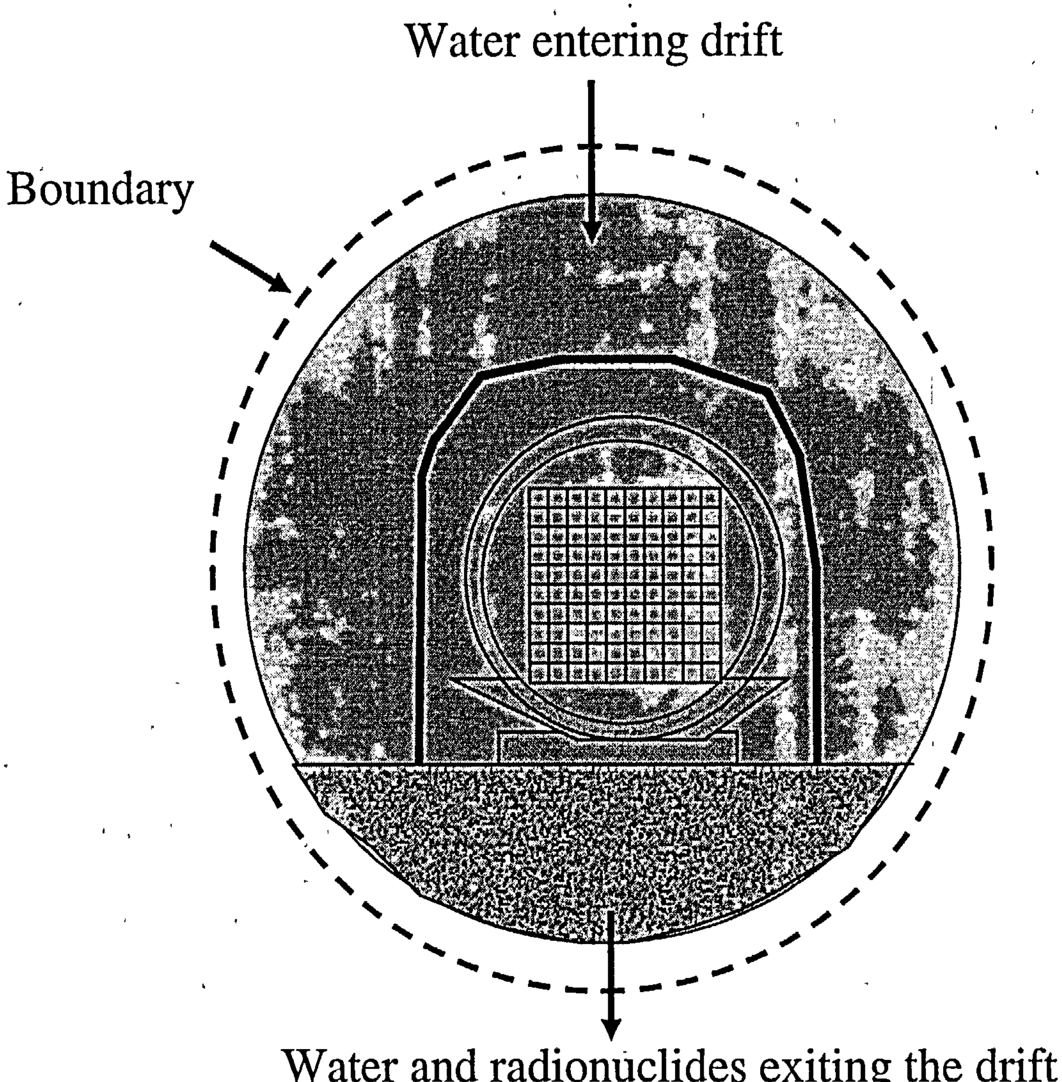
<u>Presented to:</u> The Advisory Committee on Nuclear Waste, March 25-26, 2003



Overview- NRC Source-Term Modeling

- **"Data"-based** (as much realism as practical)
- Based on **simple** concepts
- **Flexible** - to enable review considering uncertainty
- Development **independent** of DOE
- Computationally **efficient**
- **Alternatives** represented (conceptual models)

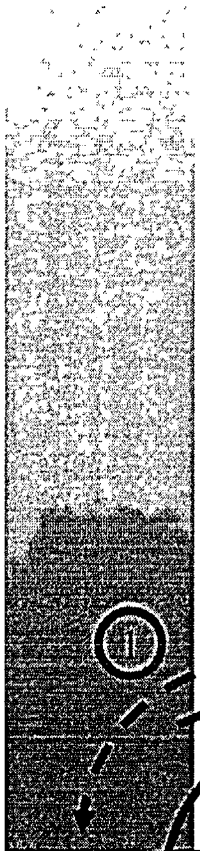
United States Nuclear Regulatory Commission



- Seepage and water contacting waste
- Drip shield corrosion
- Waste package corrosion
- Spent fuel degradation
- Glass degradation
- Cladding failure
- Radionuclide release

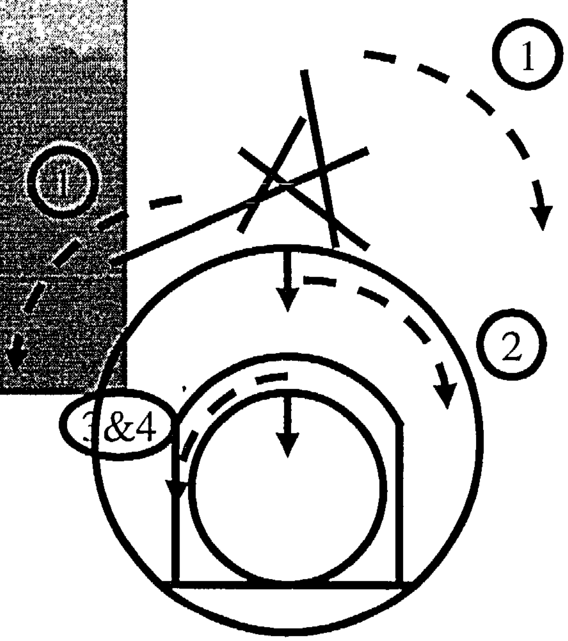
United States Nuclear Regulatory Commission

Seepage and water contacting waste



<u>POTENTIAL DRIPPING TO ENGINEERED BARRIERS:</u>

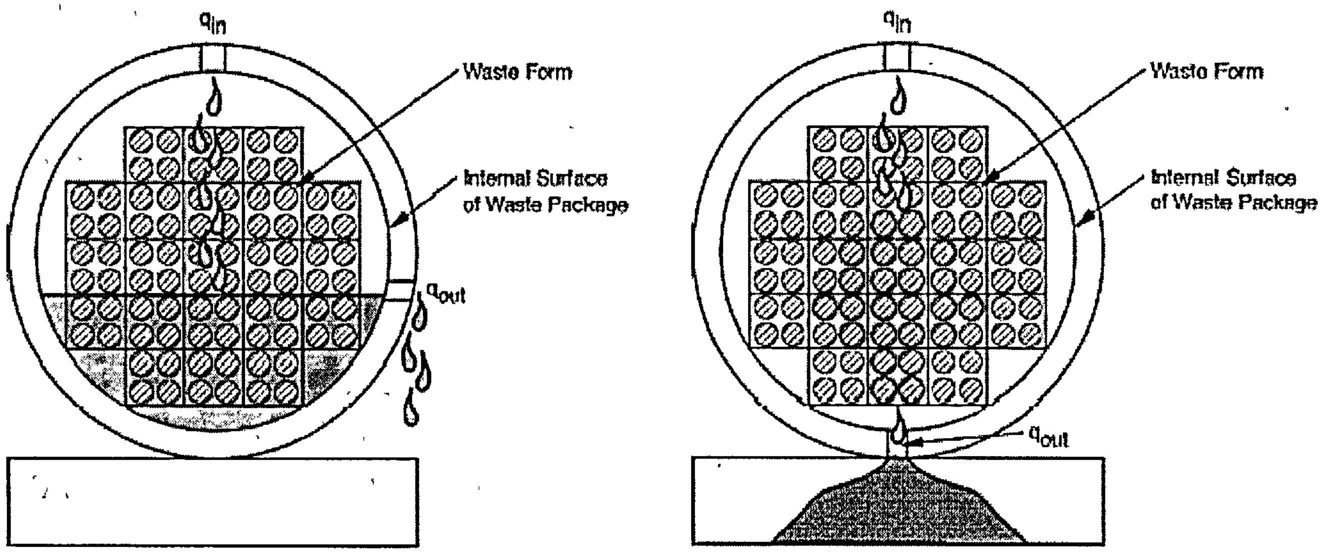
- Account for variability in dripping water
- Spatial variability in both infiltration and hydraulic conductivity
- Variability in the fraction of engineered barriers getting wet and the amount of flow
- Many parameters correlated to prevent unphysical results



<u>FRACTION OF DRIPPING ENTERING WASTE PACKAGE (F_{mult}):</u>

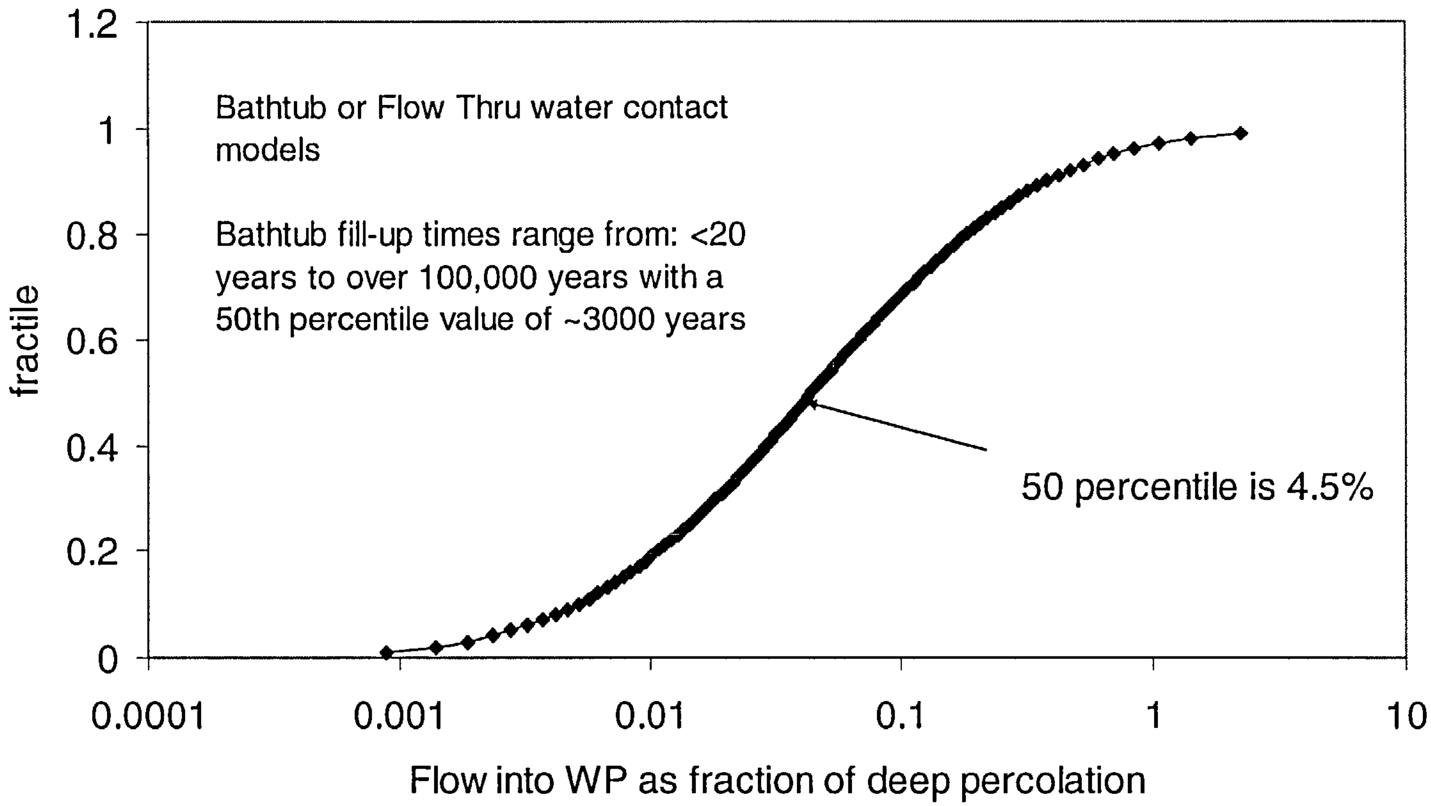
- Assumes thru-going holes in WP
- Multipliers for diversion of water by:
  (1) diversion around drift by capillarity
  (2) water running down walls
  (3) water not impacting holes
  (4) diversion from holes because of corrosion products

Conceptual Models for Water Contact



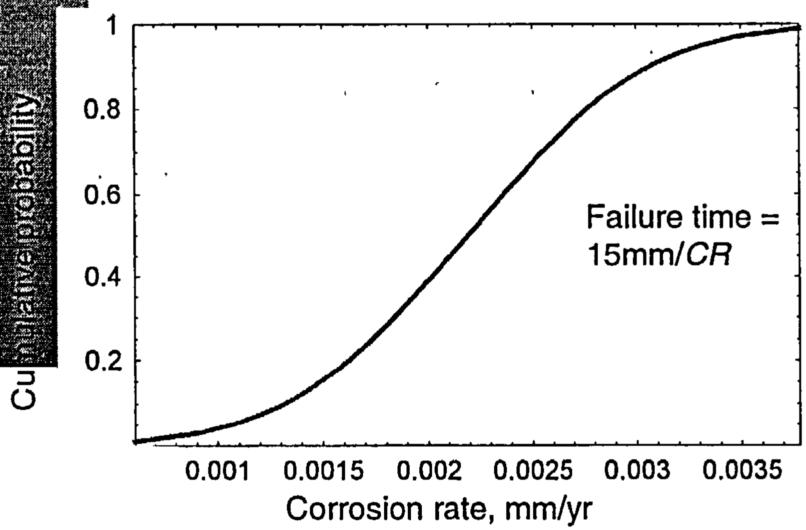
- Bathtub and flow-through conceptual models for water contacting the waste.
- Bathtub modeled as a stirred-tank and solubility limits are applied.

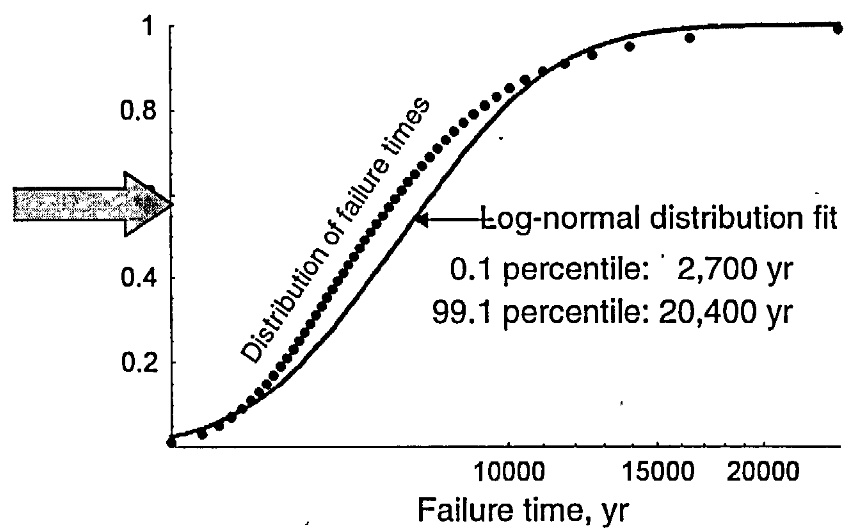
Seepage and water contacting waste



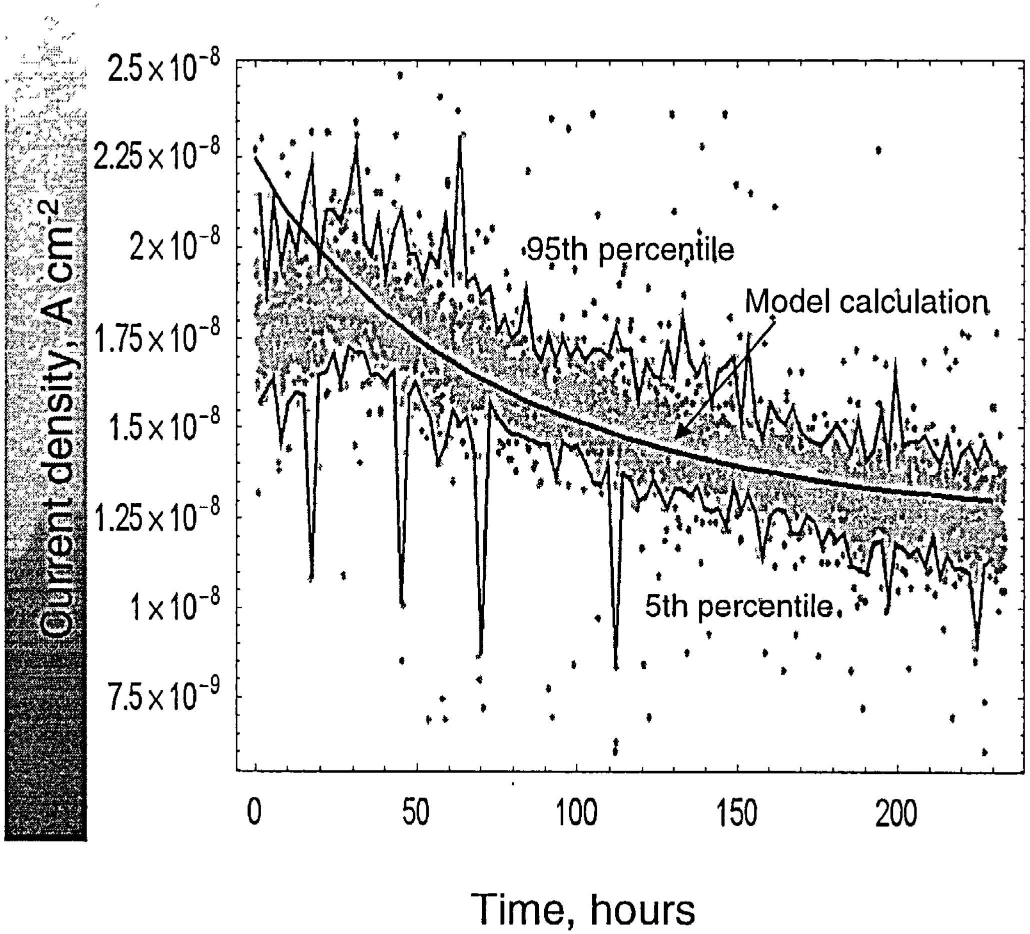
Drip shield corrosion

- Ti Grade 7 current densities in the range 10^{-8} to 5×10^{-7} A/cm^2 (pH range 2.1 to 10.7, [Cl] range 0.1 to 1M, 95°C)
- Corrosion rates ranging from 8.7×10^{-5} to 4.3×10^{-3} mm/yr (assumed 0.1 and 99.9 percent quantile values of a normal distribution)
- Assumptions: general corrosion occurs from only one side of the drip shield, general corrosion is the only degradation mechanism





Waste package – uniform corrosion



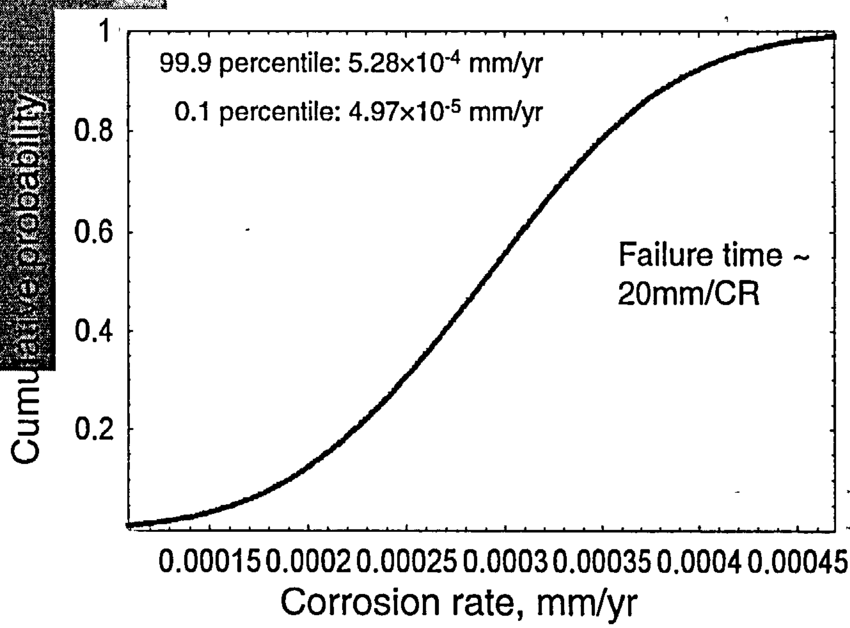
- Extension of Point Defect Model to ternary alloy system based on Cr_2O_3-rich passive film with Ni, Cr, and Mo (interstitial cations) as predominant charge carriers
- Vacancies created by alloy dissolution and accumulated at the metal-film interface lead to a passive current density (i_{pass}) decrease until steady state is reached
- Breakdown of passivity or enhanced dissolution for extended periods is unlikely

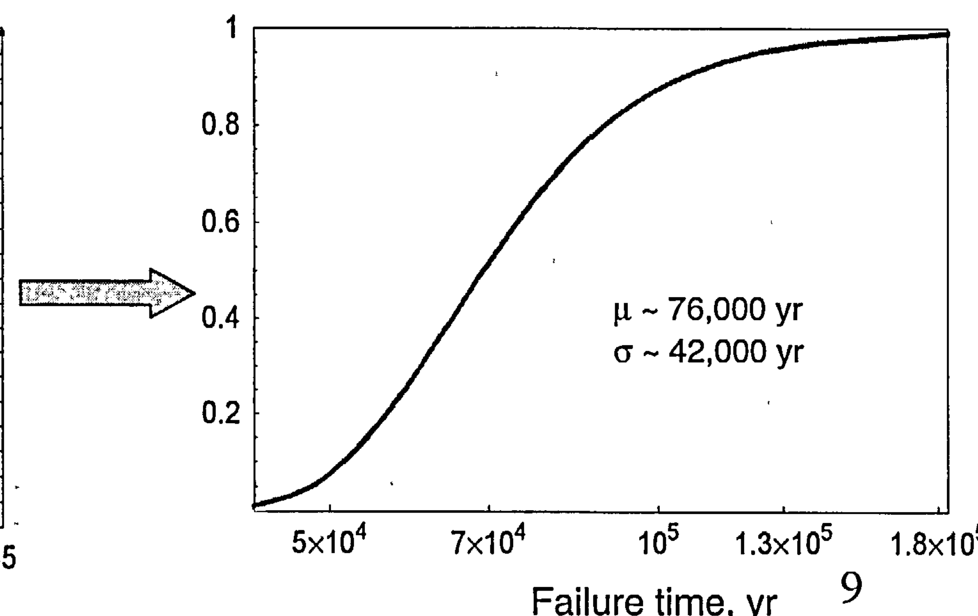
Measured in 0.028M Chloride solution at 95 °C

United States Nuclear Regulatory Commission

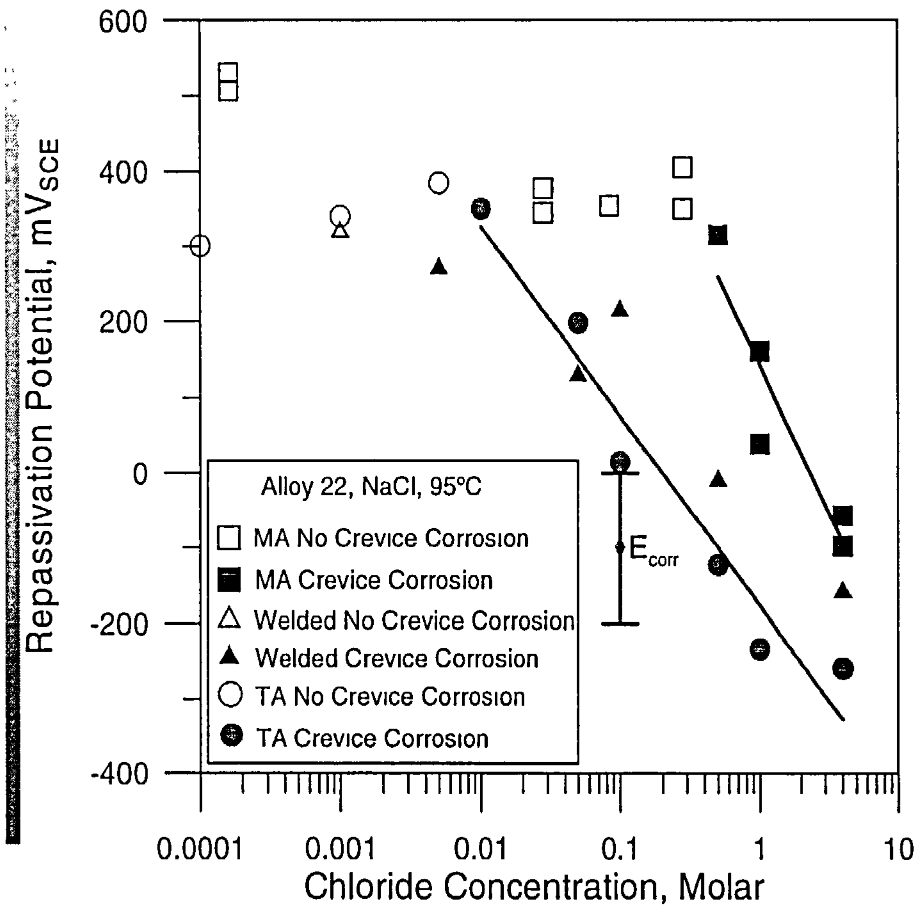
Waste package – uniform corrosion

- Passive current densities in the range 5×10^{-9} A/cm^2 to 5.4×10^{-8} A/cm^2 (pH range 2.7 to 8, [Cl] range 0.028 to 4 M, 95°C)
- The corrosion rate in the code is computed using Faraday's law.
- Corrosion rates ranging from 4.97×10^{-5} to 5.28×10^{-4} mm/yr (assumed 0.1 and 99.9 percentiles of a normal distribution)
- Assumptions: breach defined to occur as complete penetration of the waste package wall thickness by the corrosion front





Waste package – localized corrosion



MA – Mill Annealed
TA – MA + Aged 5 minutes at 870 °C
Welded – MA + Welded

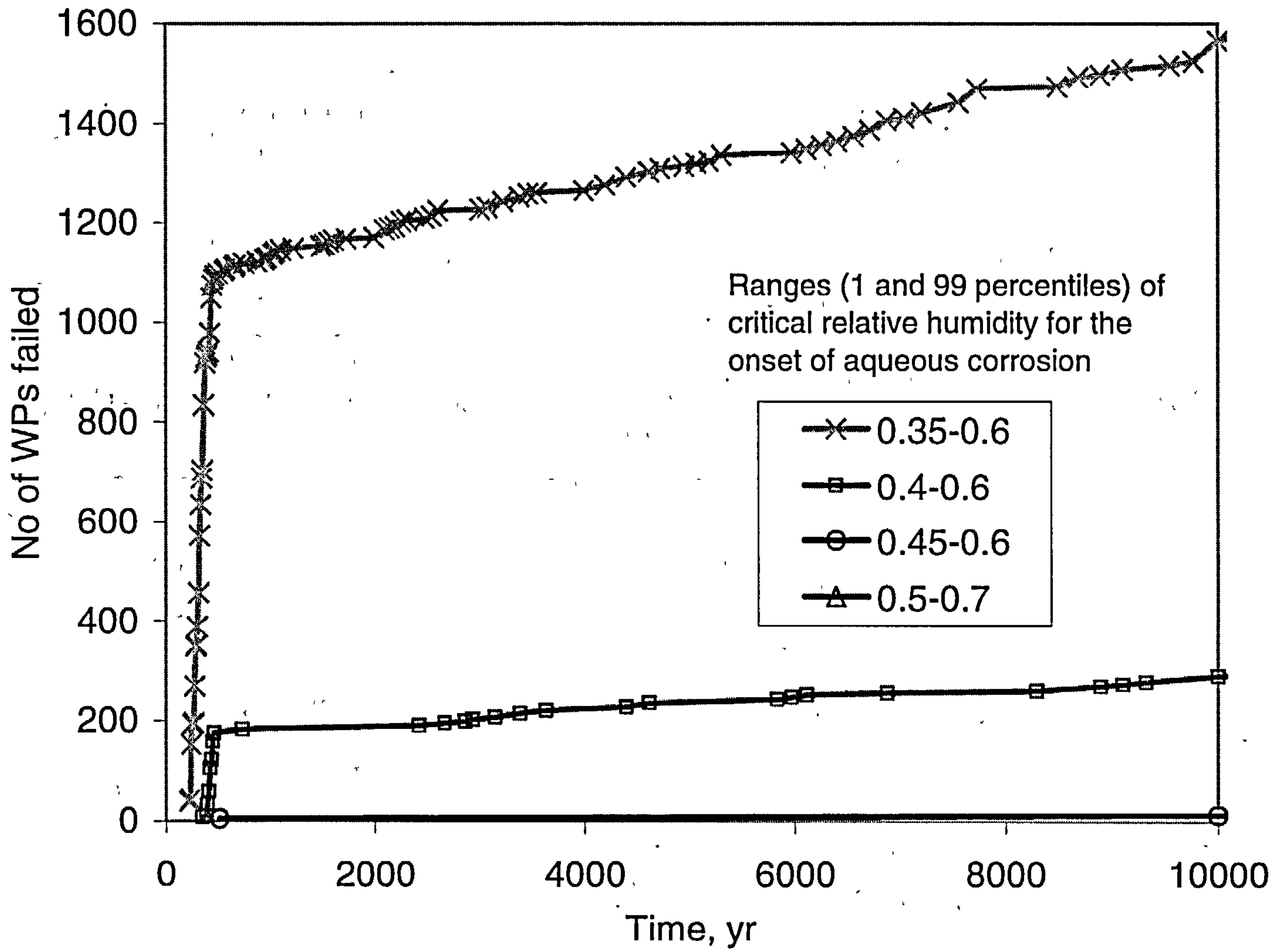
- Localized (crevice) corrosion occurs when the corrosion potential (E_{corr}) is higher than the crevice corrosion repassivation potential (E_{rcrev})

$$E_{rcrev} = E^o_{rcrev}(T) + B(T)\log[Cl^-]$$

where $E^o_{rcrev}(T)$ and $B(T)$ are linear functions of temperature

- As a result of welding and post-welding processes, E_{rcrev} may become lower than E_{corr}, facilitating the occurrence of localized corrosion at Cl^- concentrations lower than those required for the MA alloy
- These effects, as well as the inhibiting effect of NO_3^-, can be introduced in the code through changes in the E_{rcrev} expression

Waste package – localized corrosion



Waste package – stress corrosion cracking (SCC)

Test conditions and results for the testing of Alloy 22 precracked double cantileverbeam (DCB) specimens

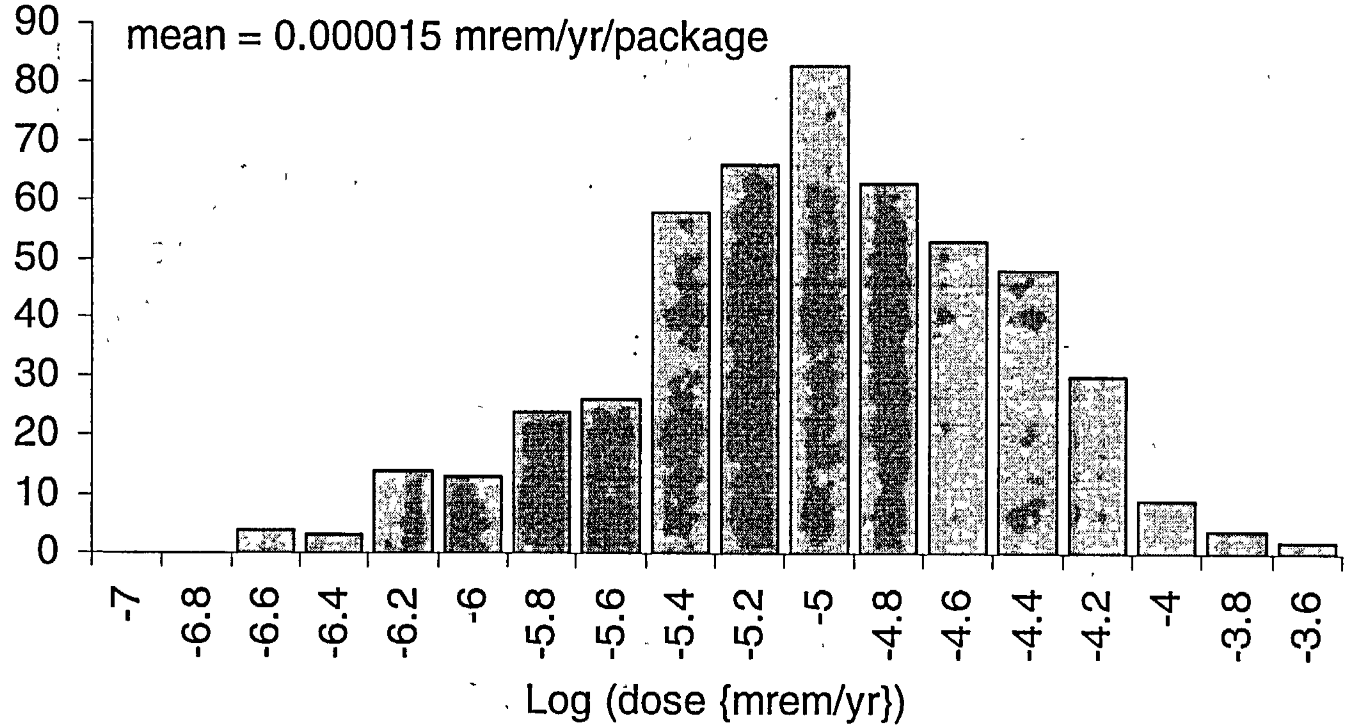
Specimen ID (Orientation)	Test Solution and Temperature	Potential (mVSCE)	Duration (hr)	Results
22-1 (T-L)	0.9 molal Cl^- (5% NaCl), pH 2.7 90 °C, N_2 deaerated	-330 to -310 (OC)	9,264 (386 days)	No crack growth
22-2 (T-L)	14.0 molal Cl^- (40% $MgCl_2$), 110 °C	-280 to -260 (OC)	9,264 (386 days)	No crack growth Grain boundary attack
22-7 (S-L)	14.0 molal Cl^- (40% $MgCl_2$), 110 °C	-270 to -250 (OC)	9,264 (386 days)	No crack growth Minor secondary cracking

T-L – Transverse-Longitudinal; S-L – Short tranverse-Longitudinal; OC – Open Circuit

- For the conditions evaluated and types of tests performed, stress corrosion cracking has not been observed.
- It appears that $E_{corr} < E_{SCC}$ and/or $K_i < K_{iscc}$, which seems to be high for Alloy 22

Waste package – SCC

- The TPA 4.1 code does not have an SCC abstraction.
  - experimental observations
  - additional analyses for risk impacts



Wasteform - spent nuclear fuel (SNF)

Select Representative Spent Fuel Dissolution Rates

Dissolution Rate (mg/m2-day)	Sample	Solution (pH)	Test Method	Reference
0.2 - 1.0 ~ 1/140 for partially clad fuel	Spent fuel	J-13 (8.4)	Immersion	Wilson, 1990
$3 \times (10^{-2} - 1)$	UO_2	$NaHCO_3 + CaCl_2$ +Silicic Acid (8.4)	Flow Through	Gray and Wilson, 1995
$(0.8 - 2.5) \times 10^{-2}$	UO_2	Silicate Solution (Near Neutral)	Flow Through	Tait, 1997
0.07 36 (initial, will decrease)	Spent fuel	Allard Synthetic Groundwater (8.1) (2.0)	Immersion	Forsyth, 1997
2.7	Spent fuel	J-13 (8.4, down to 3.2)	Drip	ANL, Finch et al., 1999
10 (Factor 1/30 at pH 3 wrt pH 8)	UO_2	HCO_3 (3) Reducing	Flow Through	Bruno et al., 1991

Wasteform - spent nuclear fuel (SNF)

- The NRC has 4 different models in TPA for SNF dissolution.

- Models based on experimental data for different conditions (model 1 and model 2), natural analogs (model 3), and secondary mineral formation [schoepite] (model 4).

- Base case is Model 2 (T=25 to 85 °C, J-13 and carbonate solutions)

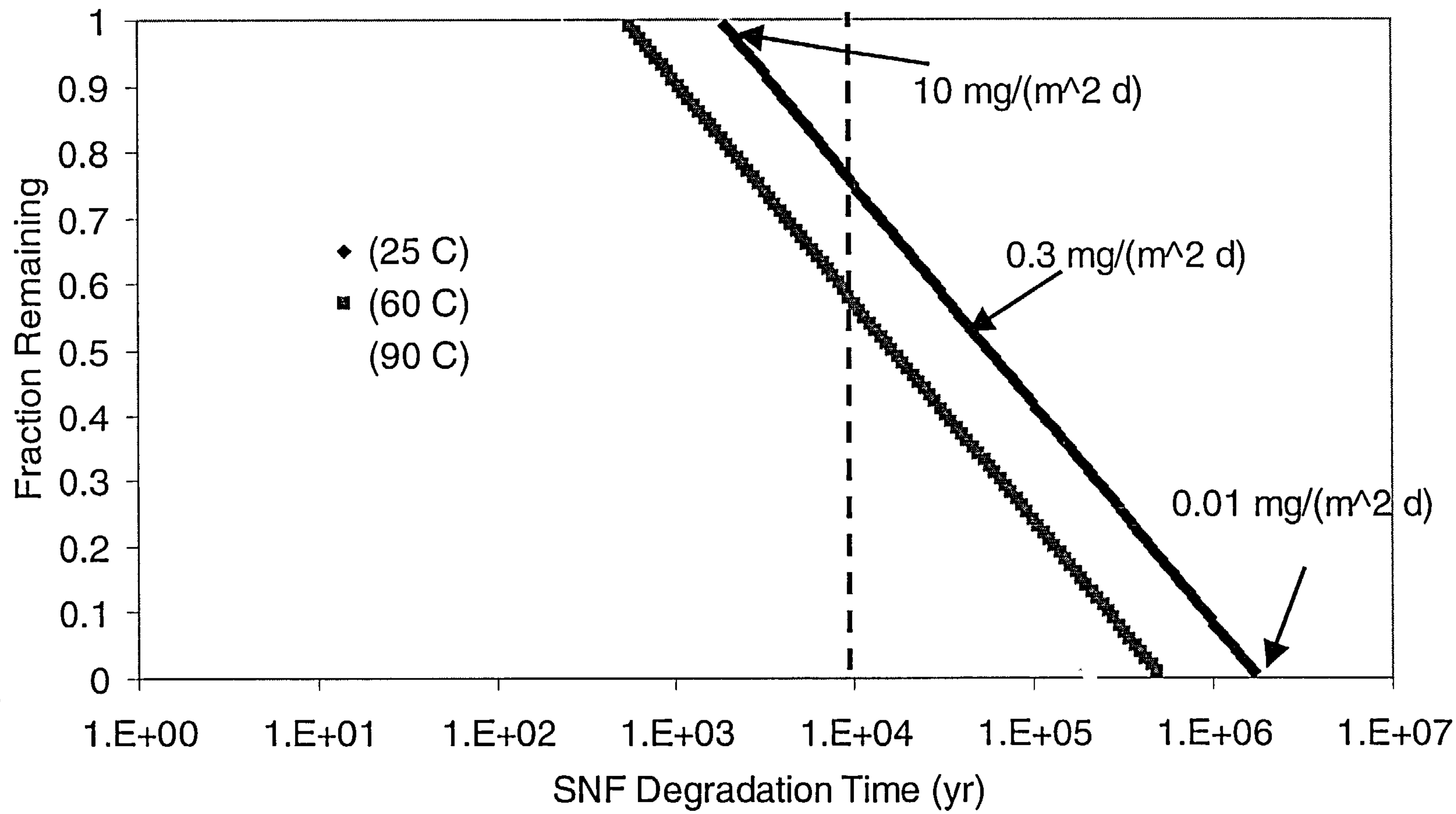
- Temperature dependence from spent fuel tests under immersion and flow through conditions at 25 and 85 °C (Wilson 1990; Gray et al. 1992)

- Two models for SNF surface area: particle and grain.

$$r = r_o \exp[-E_a/RT]$$

E_a=activation energy [kJ/mol]
r_o=preexponential coefficient [mg/m^2-d]
R=universal gas constant [kJ/mol-K]
T= WP temperature [K]

Wasteform - spent nuclear fuel (SNF)



Wasteform – high-level waste glass*

- Estimated glass dissolution rates can be dependent on many variables (e.g., glass formulation, testing methods, test conditions)
- MANY experiments completed to determine dissolution rates
- Typical rate expression:

$$\text{Rate} = S\{\, k\,[1-(Q/K)]\}$$

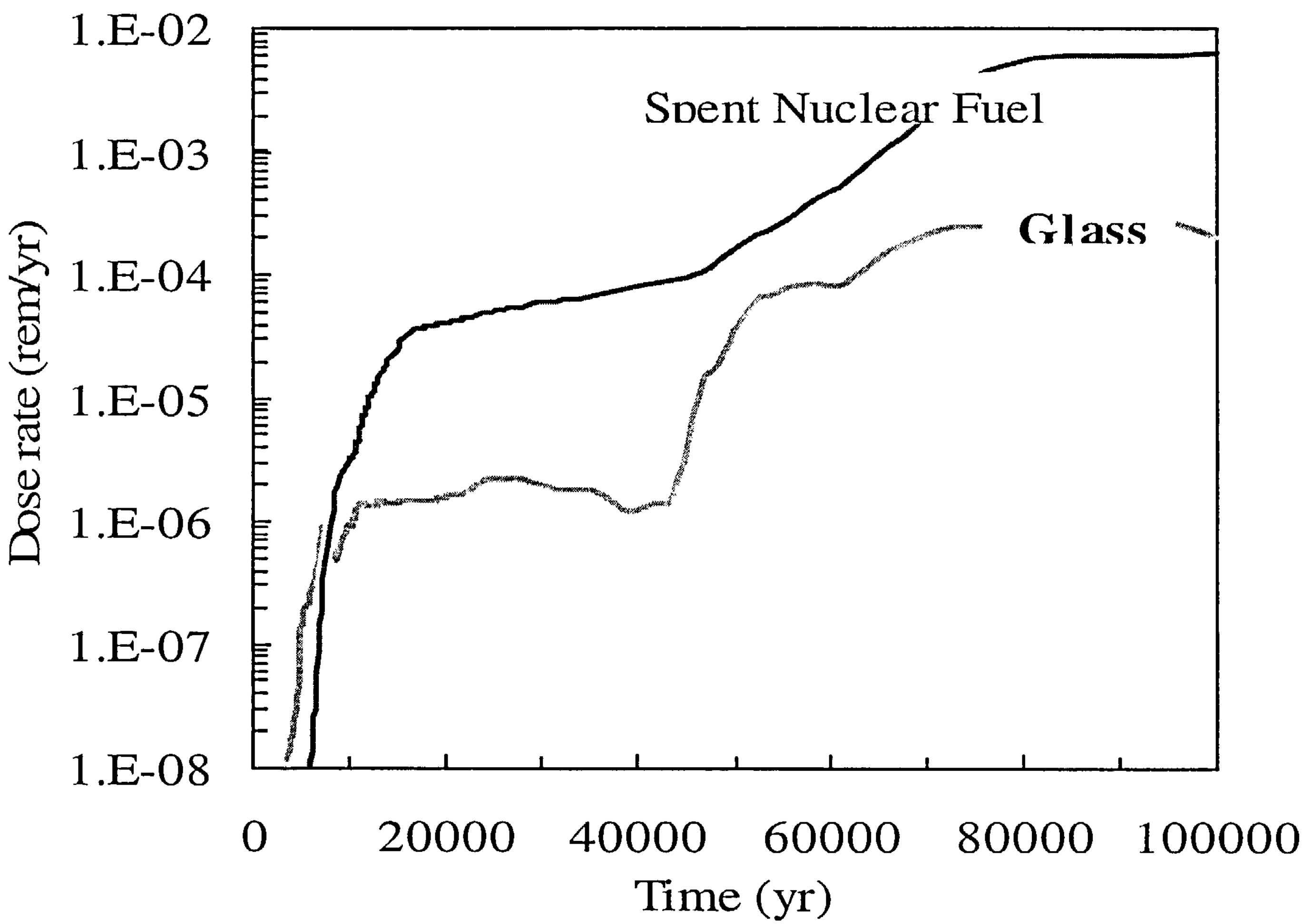
$$k = k_o\, 10^{\eta\, \text{pH}} \exp(-E_a/RT)$$

S - surface area of glass immersed in solution
k - forward dissolution rate
Q - concentration of dissolved silica in the solution
K - a quasi-thermodynamic fitting parameter equal to the apparent silica saturation value for the glass

k_o - intrinsic dissolution rate in g/m^2-day
η - pH dependence coefficient
E_a - activation energy in kJ/mol
R - gas constant (8.314 kJ/mol-K)
T - temperature in Kelvin

* New for TPA 5.0

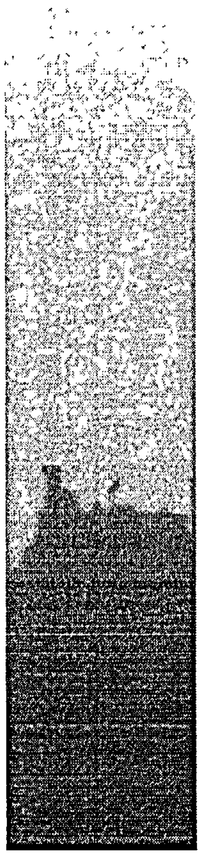
Wasteform – high-level waste glass



Wasteform – cladding

- The failure mechanisms of cladding include (i) mechanical failure by external forces, (ii) localized corrosion, (iii) creep, (iv) hydrogen-induced failure, (v) splitting by matrix volume expansion, (vi) uniform corrosion, (vii) creep, and (viii) stress corrosion cracking.
- TPA4.1j has a factor (CladdingCorrectionFactor) to represent the fraction of the spent fuel surface area protected by cladding.
- CladdingCorrectionFactor is set by the code user for complete to no protection (can be time dependent in TPA 5.0).
- Approach allows flexibility and ease of use.

Wasteform – cladding



- To assess the performance of spent fuel cladding as a metallic barrier to radionuclide release is as complicated as assessing the performance of the waste packages without the flexibility offered by improvements in design

- Complications arise largely from uncertainties associated with in-package chemistry. To assess the incidence of localized corrosion and external stress corrosion cracking, better estimates of concentrations of chloride, ferric ion, and radiolysis products, as well as pH, are needed

- To assess the possibility of hydride embrittlement and creep, better estimates of hoop stresses and temperatures profiles are required for upper range of fuel burn-ups

Release and transport out of the package

Advective Transport

- Requires flow out of WPs carrying dissolved radionuclides.

Diffusive Transport (for TPA 5.0)

- Transport out of WP by diffusion in films of water inside and outside of WP.
- User defines lengths and thickness of films.
- Zero concentration boundary at outer surface of WP, and solubility limit at terminus of film inside WP.

Release and transport out of the package

- Two models for aqueous release of radionuclides are available for selection by the user: bathtub and flow-through.
- Bathtub can have variable height, modeled as well-stirred tank with solubility limits applied.
- Flow-through model is the same, but doesn't allow buildup of fluid. The fraction of fuel wetted is independent:

$$M_{out}[i]=Q \cdot C[i]$$

where Q is the water flow rate and C[i] is the concentration of radionuclide i in solution determined by solubility limits.

- Solubility limits abstraction is based on (i) the likely solid phase precipitated or coprecipitated and (ii) the chemistry of the fluid that reacts with the solid phase.

Release and transport out of the package

- For a number of radioelements (C, Cs, Cl, I, Se, Tc) solubility limits are set to 1.0 M because no solubility-limiting solids are estimated to form.
- The range and probability distributions of solubility limits for many other elements in TPA are based on and elicitation of experts conducted by DOE in 1993 (Wilson et al., 1994, CWRMS M&O, 1998).
- The assumptions behind the expert panel's distributions are:
  - the UZ water composition is bounded by that of J-13 well water and well UE-25p#1.
  - the solubility limits are determined by far-field groundwater environment.
  - the environment is oxidizing.
- TPA has a model for transport through the invert (simple advection/retardation/diffusion model) and a factor to bypass transport through the invert.

Conclusions

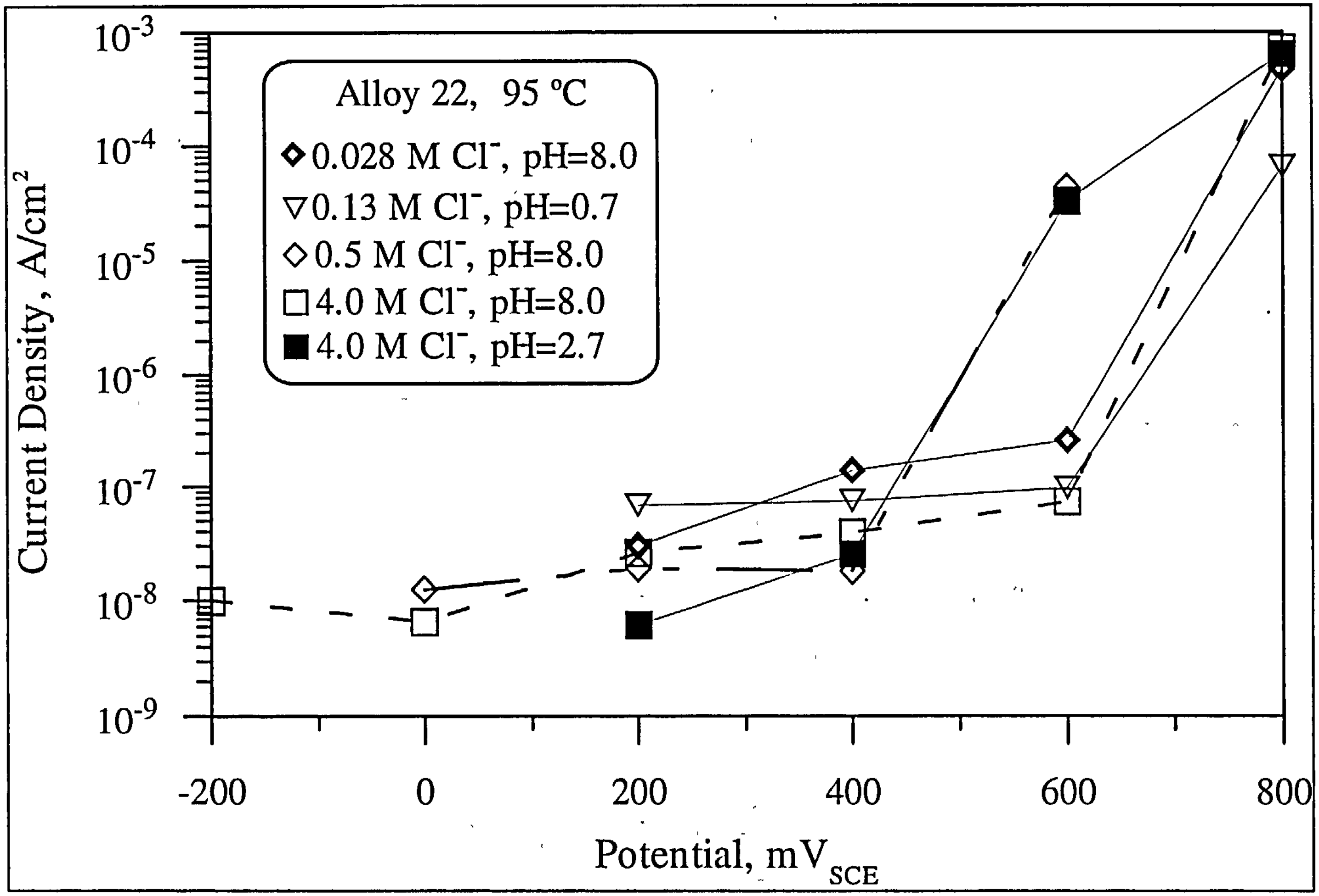
- To extent practical, NRC models are **"data"-based**
- Based on **simple** concepts
- TPA provides NRC reviewer's the **flexibility** to complete review considering uncertainty

Backup Slides

Waste package – uniform corrosion (TPA 5.0)

- Range of corrosion rates will be redefined in TPA 5.0 (mean close to ~4×10-8 A/cm^2 (3.9×10-4 mm/yr) at 95°C).
- The definition for failure will be reconsidered in TPA 5.0:
  - Mechanical damage of partially corroded engineered barriers (need to consider the Type 316L inner container).
  - There is stochastic variability in the corrosion rates that could produce an irregular corrosion front. More flexibility in the consideration of distributed failures.
- Refinements in TPA 5.0 are not anticipated to change the conclusion indicating that waste packages will not breach in 10,000 years solely due to general corrosion.

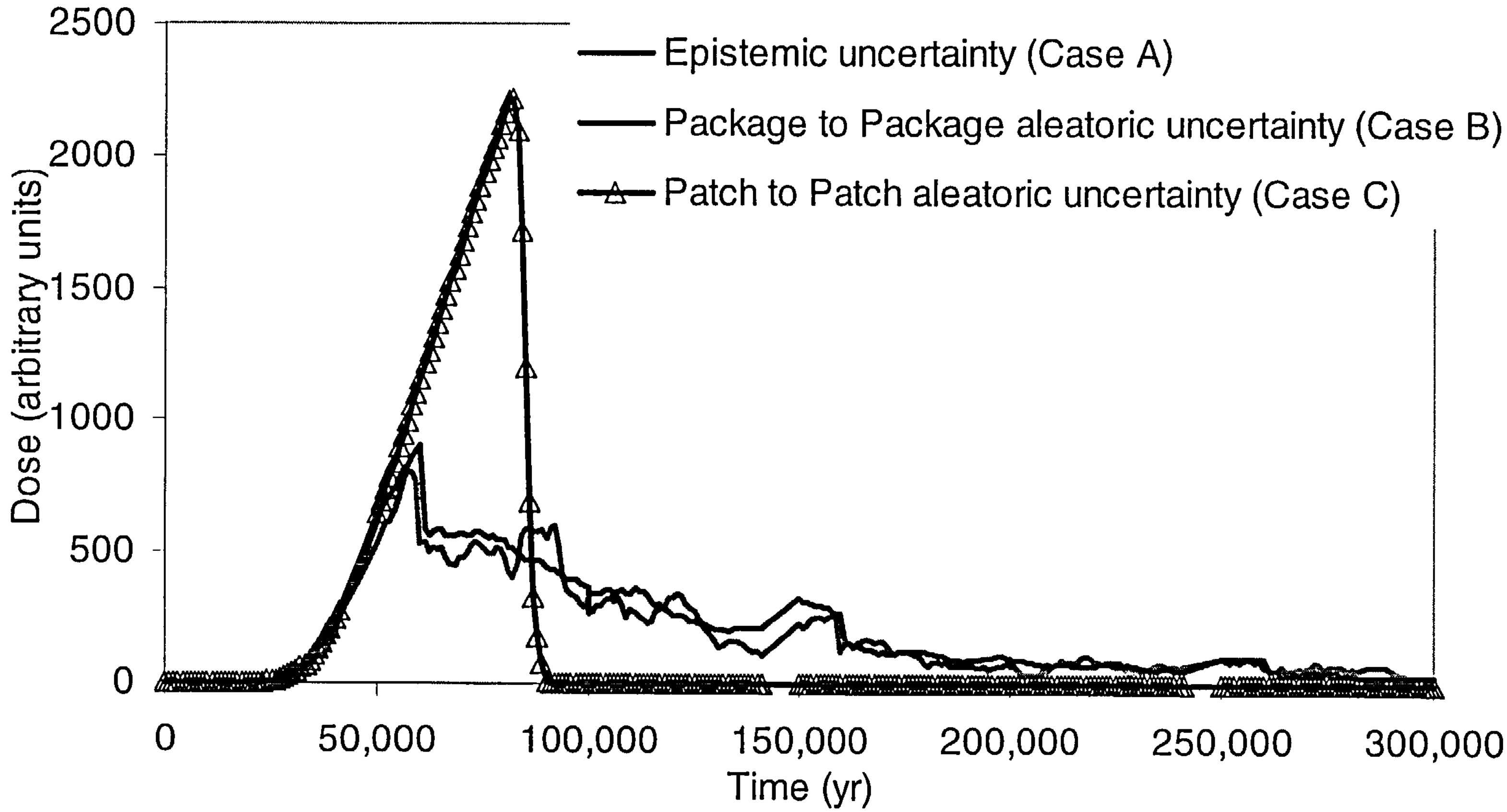
Waste package – uniform corrosion



Anodic current density of Alloy 22 measured under potentiostatic conditions for a period of 48 hours.

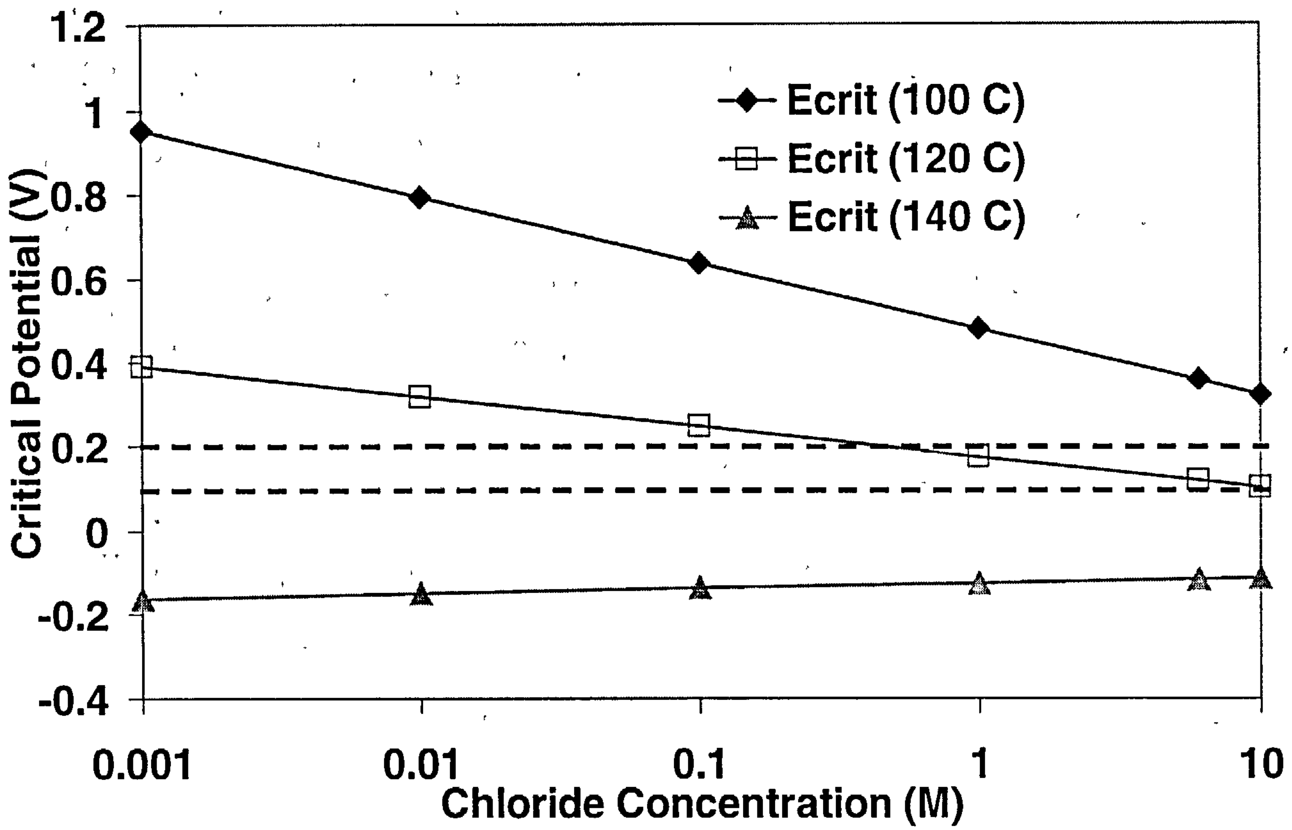
United States Nuclear Regulatory Commission

Waste Package Distributed Failure



Analysis by Codell et al. (2001 SRA) investigated the impacts on risk of the conceptual model to represent distributed waste package failure.

Waste package – localized corrosion

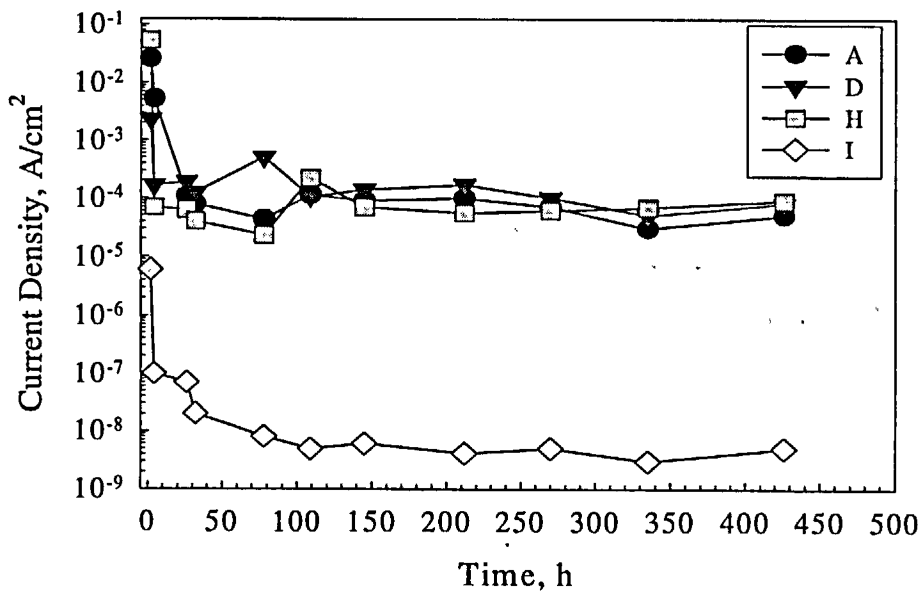


Corrosion potential range shown by dashed lines, localized corrosion only predicted by the model for temperatures at or above boiling and concentrated solutions.

Drip shield corrosion (TPA 5.0)

- Influence of fluoride on corrosion rate disregarded in TPA Code Version 4.1j, because:
  - Amount of fluoride is possibly limited in Yucca Mountain system (fluoride forms Ti complexes and it is consumed in the corrosion reactions).
  - A mechanism is needed to accumulate fluoride on the drip shield surface (water tends runs off the drip shield surface).
- Nonetheless, the influence of fluoride on drip shield corrosion rate will be included in TPA 5.0
  - A multiplication factor, function of the fluoride concentration, will affect the corrosion rate.
- Mechanical failure of the drip shield will also be incorporated into TPA 5.0.

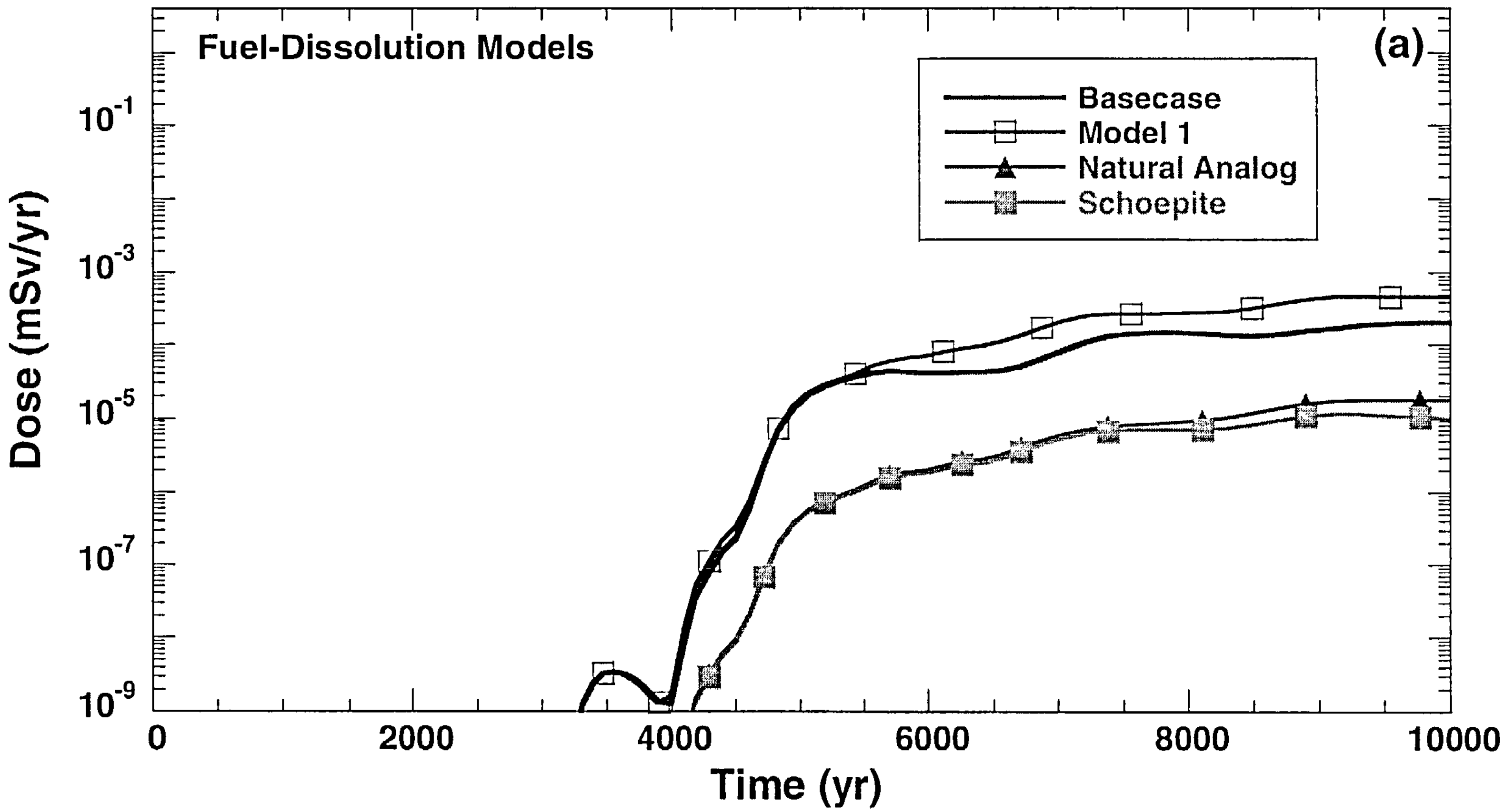
Drip shield – flouride effects



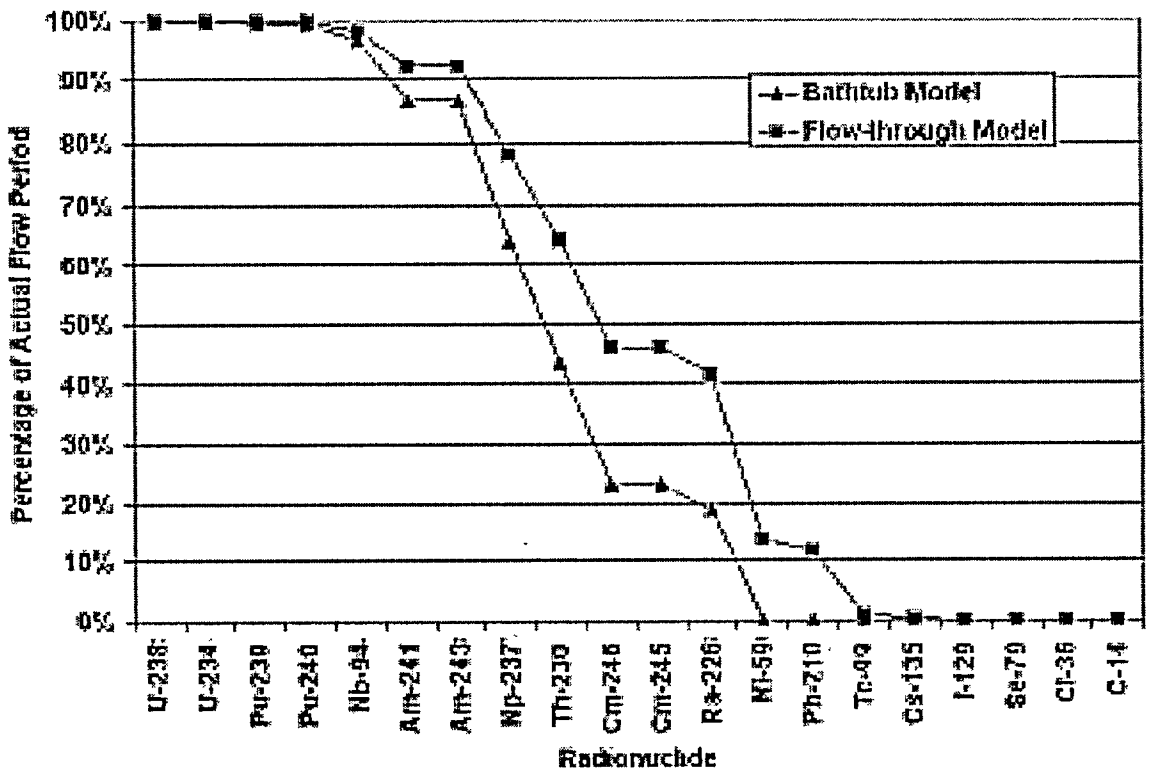
A = 1M Cl^-, 0.1M F^-, 0.55M NO_3^-, 0.92M SO_4^{2-}
D = 3.84M Cl^-, 0.07M F^-, 2.32M NO_3^-, 0.15M SO_4^{2-}
H = 1M Cl^-, 0.1M F^-, 0.0M NO_3^-, 0.0M SO_4^{2-}
I = 1M Cl^-, 0.0M F^-, 0.0M NO_3^-, 0.0M SO_4^{2-}.

Effects of fluoride under passive current density of Ti Grade 7 in various deaerated solutions containing chloride, nitrate, and sulfate at 95 C and an applied potential of of 0 V_{SCE}.

Spent Fuel Dissolution Model Sensitivity Analysis



Solubility Limits Sensitivity Analysis



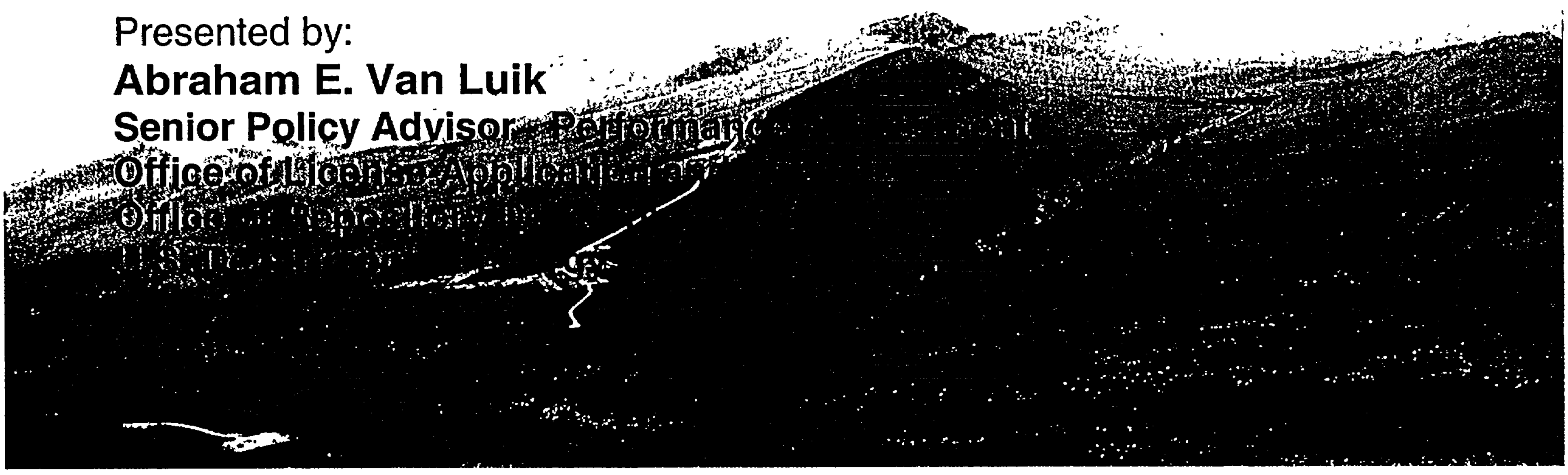
From Mohanty, Adams, Pabalan (MRS Fall 2002 Meeting), '*The Role of Solubility as a Barrier to Radionuclide Release*'

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

YUCCA MOUNTAIN PROJECT

Total System Performance Assessment for the License Application - Credibility and Realism Issues

Presented to:
Advisory Committee on Nuclear Waste



Presented by:
Abraham E. Van Luik
Senior Policy Advisor - Performanc
Office of License Applicatio
Office of Repository
U.S.

Overview

- NRC requirements and guidance - treatment of uncertainty
  - 10 CFR Part 63
  - Yucca Mountain Review Plan
- Summary of DOE's approach to realism and conservatism
- Total System Performance Assessment - License Application development schedule

Meeting Nuclear Regulatory Commission Requirements

- 10 CFR Part 63 specifies requirements for the performance assessment used to demonstrate compliance with 63.113 (b and c) postclosure performance objectives
- The Yucca Mountain Review Plan, Rev. 2, specifies the approach to judging adequacy of the performance assessment in terms of meeting 10 CFR Part 63 requirements

10 CFR 63 Requirements

§63.304–Reasonable Expectation

- *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:
  - Requires less than absolute proof because absolute proof is impossible to attain for disposal due to the uncertainty of projecting long-term performance
  - Accounts for the inherently greater uncertainties in making long-term projections of the performance of the Yucca Mountain disposal system
  - Does not exclude important parameters from assessments and analyses simply because they are difficult to precisely quantify to a high degree of confidence
  - 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

§63.304 Implications for DOE's Performance Assessments

- The DOE should:
  - Evaluate uncertainties
  - Include parameters of importance even if not precisely known
  - Evaluate full range of distributions but be reasonable (goal is likely performance, not unlikely performance for tails of distributions–see next slide)

10 CFR 63 Requirements

§63. 303–Implementation of Subpart L

DOE must demonstrate that there is reasonable expectation of compliance with this subpart before a license may be issued. In the case of the specific numerical requirements in § 63.311 this subpart, and if performance assessment is used to demonstrate compliance with the specific numerical requirements in §§ 63.321 and 63.331 this subpart, compliance is based upon the mean of the distribution of projected doses of DOE's performance assessments which project the performance of the Yucca Mountain disposal system for 10,000 years after disposal.

§63.303 Implications for DOE's Performance Assessments

The mean dose is to be evaluated using full range of distributions as discussed in §63.303.

10 CFR 63 Requirements

§63. 342–Limits on Performance Assessments

DOE's performance assessments shall not include consideration of very unlikely features, events, or processes, i.e., those that are estimated to have less than one chance in 10,000 of occurring within 10,000 years of disposal. DOE's assessments for the human-intrusion and ground-water protection standards shall not include consideration of unlikely features, events, and processes, or sequences of events and processes, i.e., those that are estimated to have less than one chance in 10 and at least one chance in 10,000 of occurring within 10,000 years of disposal. In addition, DOE's performance assessments need not evaluate the impacts resulting from any features, events, and processes or sequences of events and processes with a higher chance of occurrence if the results of the performance assessments would not be changed significantly.

§63.342 Implications for DOE's Performance Assessments

- Performance assessments not to consider very unlikely features, events, or processes
- Assessments for human-intrusion and groundwater protection not to consider unlikely features, events, and processes

10 CFR 63 Requirements

§63.114–Requirements for Performance Assessment

- **Any performance assessment used to demonstrate compliance with § 63.113 must:**
  - Include data related to the geology, hydrology, and geochemistry (including disruptive processes and events) of the Yucca Mountain site, and the surrounding region to the extent necessary, and information on the design of the engineered barrier system used to define parameters and conceptual models used in the assessment
  - Account for uncertainties and variabilities in parameter values and provide for the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment
  - Consider alternative conceptual models of features and processes that are consistent with available data and current scientific understanding and evaluate the effects that alternative conceptual models have on the performance of the geologic repository
  - Consider only events that have at least one chance in 10,000 of occurring over 10,000 years

10 CFR 63 Requirements

§63.114–Requirements for Performance Assessment

(Continued)

- Provide the technical basis for either inclusion or exclusion of specific features, events, and processes in the performance assessment. Specific features, events, and processes 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
- Provide the technical basis for either inclusion or exclusion of degradation, deterioration, or alteration processes of engineered barriers in the performance assessment, including those processes that would adversely affect the performance of natural barriers. Degradation, deterioration, or alteration processes of engineered barriers 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
- Provide the technical basis for models used in the performance assessment such as comparisons made with outputs of detailed process-level models and/or empirical observations (e.g., laboratory testing, field investigations, and natural analogs)

§63.114 Implications for DOE's Performance Assessments

- **DOE's performance assessments must:**
  - Provide basis for models selected and the features, events and processes evaluated and excluded
  - Provide basis for data used and for derived parameter ranges
  - Provide basis for judging adequacy of modeling

Yucca Mountain Review Plan Criteria

4.2.1 Performance Assessment Risk-Informed Review Process for Performance Assessment

- **Conservative approach can be used**
  - To decrease need to collect information
  - To justify simplified modeling approach
- **Conservative estimates for dose may be used to demonstrate compliance**
  - Caution: conservatism in one process may not mean conservatism in dose projection
  - Technical basis needed for claimed conservatism

Yucca Mountain Review Plan Criteria

4.2.1 Performance Assessment Risk-Informed Review Process for Performance Assessment

(Continued)

- **Use of conservatism to manage uncertainty has implications for risk-informed review**
  - Staff to evaluate assertions of conservatism from perspective of overall system performance
  - Staff will use any available information to risk-inform its review
- **The Yucca Mountain Review Plan's review methods and acceptance criteria emphasize staff intent to thoroughly review potential nonconservatisms at subsystem and system levels**

Realism Desirable, Not Required

- **DOE believes that adding in realism where practicable is a prudent approach because it allows:**
  - More meaningful safety-margin evaluations
  - Taking a more informed, less conservative approach to barrier design
  - More straightforward communication of the case for system safety
  - Improved understanding of system performance

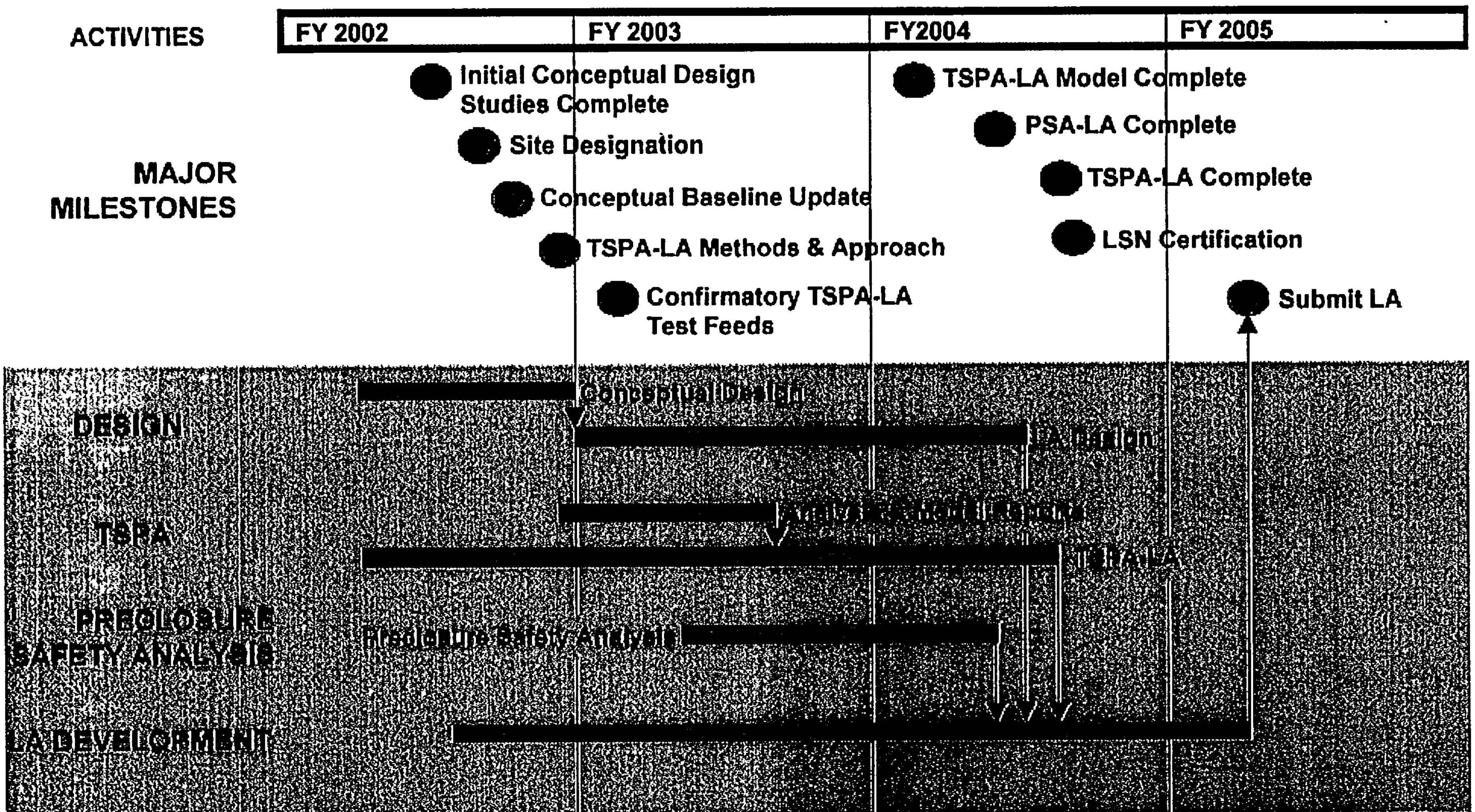
Conservatism Has Advantages, Disadvantages

- As recognized in the Yucca Mountain Review Plan, conservatism may allow assurance of safety with lesser time and other resource expenditures
- Pragmatically it can become a tradeoff issue between design and materials costs and research costs
- Conservatism tends to understate safety

Use of Pragmatic Realism

- Advisory Committee on Nuclear Waste and Nuclear Waste Technical Review Board comments–realism allows more meaningful uncertainty and safety-margin evaluations; DOE agrees
- Realism has improved as Total System Performance Assessment has evolved
  - As realism has been added, long-term safety estimates improved
  - Realism has improved understanding of system performance to the level needed to demonstrate safety in a regulatory context

Summary Schedule to License Application Submittal



NOTE: PSA-LA - Preclosure Safety Analysis - License Application
LSN - Licensing Support Network

Summary

- Total System Performance Assessment - License Application will have a mix of conservative and realistic models that meet 10 CFR Part 63 requirements
- Performance Confirmation Program to enhance confidence in key process models
- Long-Term Test and Evaluation Program to add understanding and realism for modeling
- Science and Technology Program to evaluate new science and technology for enhancing safety, efficiency and understanding

Realism in Simulating Long-Term Waste Package Corrosion and Radionuclide Source Term

Presented by

Dr. Joe H. Payer

Case Western Reserve University

Presented to

Advisory Committee on Nuclear Waste

140th ACNW Meeting

March 25, 2003

Rockville, MD

Outline

- Yucca Mountain Conditions
  - Background and Perspective
- Composition of Waters
  - Contacting Waste Package and Entering Waste Packages
- Corrosion
  - The Primary Determinant of Waste Package Lifetime
- Waste Form Degradation and Radionuclide Mobilization
  - The Source Term

Yucca Mountain Conditions: Background and Perspective

Perspective on Proposed Yucca Mountain Repository

- A geologic repository for the disposal of high-level radioactive waste and spent nuclear fuel
- Containment strategy for the disposal site is twofold
  - First and foremost, complete isolation of the waste
  - Subsequent retardation of the egress of radionuclides from the penetrated waste package

Repository Conditions: Overview of Time, Temperature, Environment

A particular challenge for the analysis is the extraordinarily long time period required for performance.

- **Operational phase of 50 years for emplacement of waste packages.**
- **Monitoring phase out to 300 years.**
- **Closure phase when the repository is closed. Regulatory period of 10,000 years. Projected performance to 100,000 yrs and more.**

In the analysis, it is important to consider not only the conditions that could initiate a process, but also the time period over which those conditions persist.

Consider conditions at 50, 500, 1000, 3000, 10,000, 50,000, 100,000

Localized Corrosion: Waste Package Materials and Water Chemistry Determine Performance

- **Long-lived Waste Packages** (WP) are essential for long-term isolation of radionuclides
- **Localized corrosion** is the greatest, realistic threat to WP performance, i.e. pitting, crevice corrosion and stress corrosion cracking
- **Materials selection and design** based on crevice corrosion resistance is prudent and sound engineering
- **General key issues and processes** are reasonably well understood in corrosion science and technology
- **Corrosion Performance at Yucca Mountain** is under active study and can benefit from further experiments and analysis

Waters on and in Waste Packages: Important water chemistry and properties

- Temperature & Time-of-Wetness
- Acidity-alkalinity (pH)
- Oxidizing-reducing (Eh)
  e.g. oxygen, ferric ion
- Detrimental ionic species, e.g. chloride, reduced sulfur
- Beneficial species, e.g. nitrate, silicate
- Complexing species

- Important to consider the ***mixed species*** effects and not species in isolation

Ambient waters innocuous for waste package corrosion

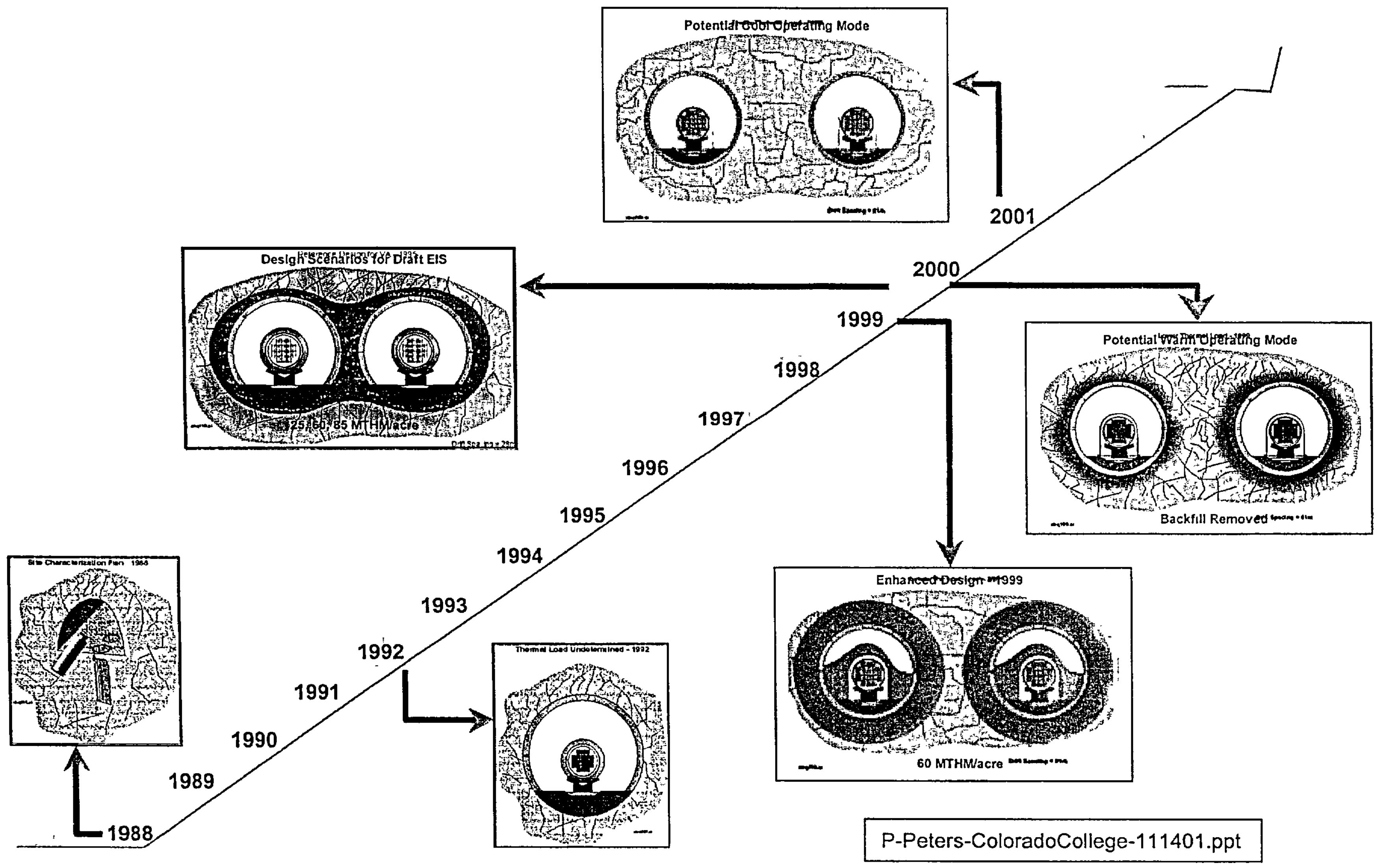
- Neutral, sodium bicarbonate water with low dissolved solids and mixed salts
  - (ppm): Si-30, Na-50, Ca-10, K-5, Mg-2, Li-0.1, Fe-0.1
  - (ppm): $HCO3^{-}$ 150, $SO4^{=}$ 20, $NO3^{-}$ 10, Cl^{-} 8, F^{-} 2
- Aerated and higher P_{CO2} than atmospheric
- Modulation processes during thermal period are evaporation, concentration, dissolution/precipitation of solids

- *Modulations to waters on metal and waste form surfaces are likely greater than those outside of drift*

Waste Form Degradation and Radionuclide Mobilization

- Oxidizing or reducing (Eh) is major effect for UO_2 corrosion
- Amount of waters and composition: into, in, and from
- Alteration of Spent Fuel and Incorporation Mechanisms
- Interaction with degraded waste form; alteration products; and corrosion products (internals and waste package)
- Interactions with invert and drift support
- Transport processes: into, in, and from

Evolution of Repository and Waste Package Design and Operating Mode

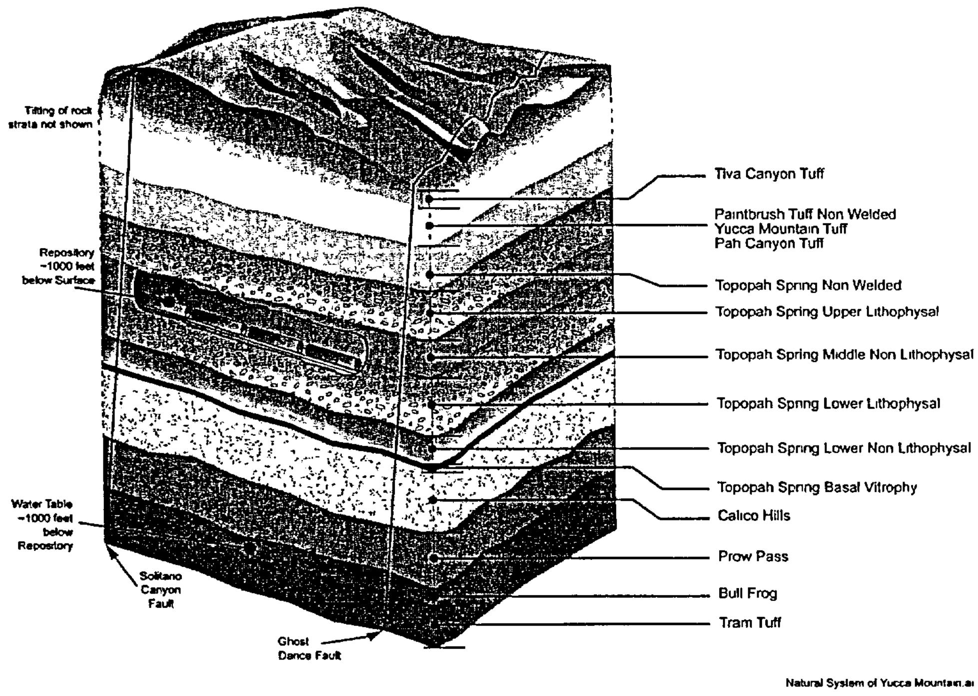


P-Peters-ColoradoCollege-111401.ppt

Evolution of Repository Design

- Design has evolved over last 15-20 years
- Will continue to evolve
  - Initial design must be safe, suitable and reasonable
  - Unrealistic to think that waste package #108, #1017 or #10,054 will be same as #1.
  - Better performance, more confidence, less expensive

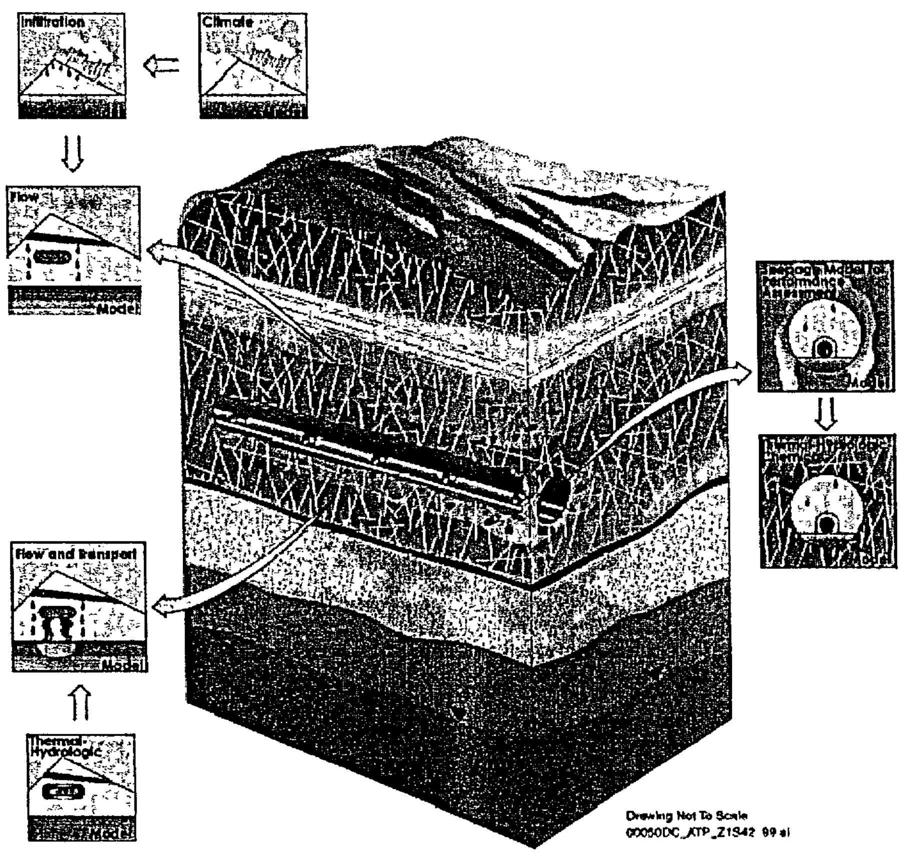
Natural System of Yucca Mountain



Important Factors

- Repository in Unsaturated Zone
  - Porous Rock
  - Pores partially filled with water
- Atmospheric pressure
- High Relative Humidity
- Ambient waters are dilute and near neutral

Water Flow through Yucca Mountain



Important Factors

Limited amount of water enters soil (mm's/year)

Water movement through fractures and matrix (pores)

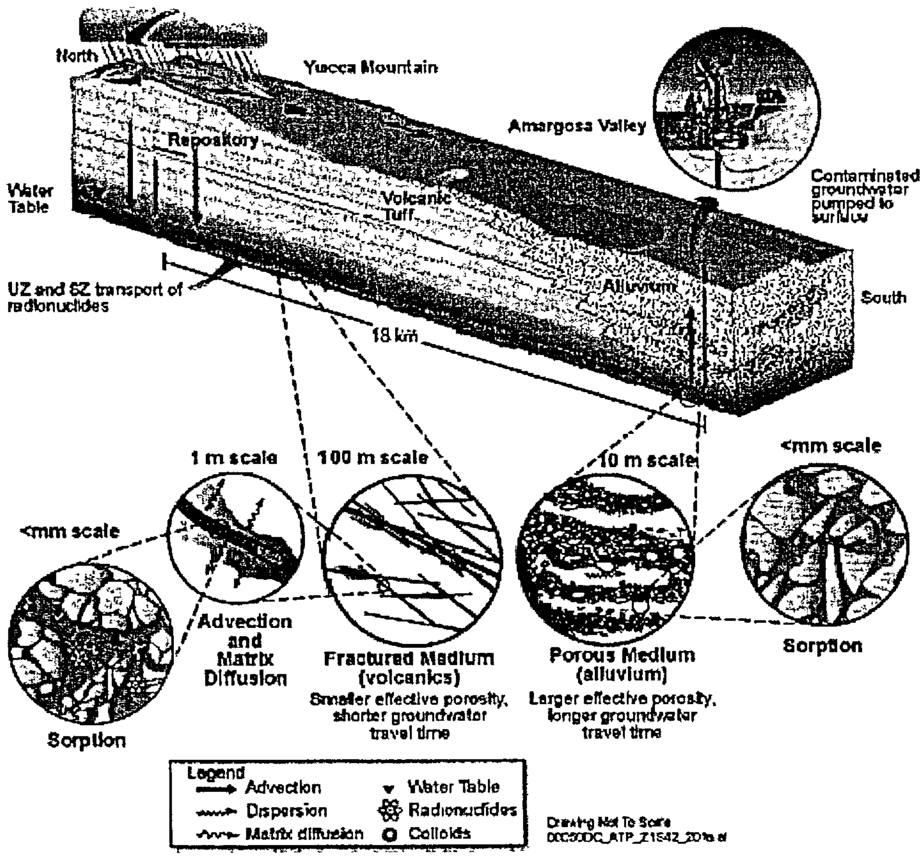
Limited and variable seepage and drips into drifts

Transport into, in and from waste packages is crucial

Large thermal effects

Episodic flow behavior

Processes Occur on Many Scales



Mountain scale (macro)

10's – 100's meter

Drift scale (meso)

cm – meter

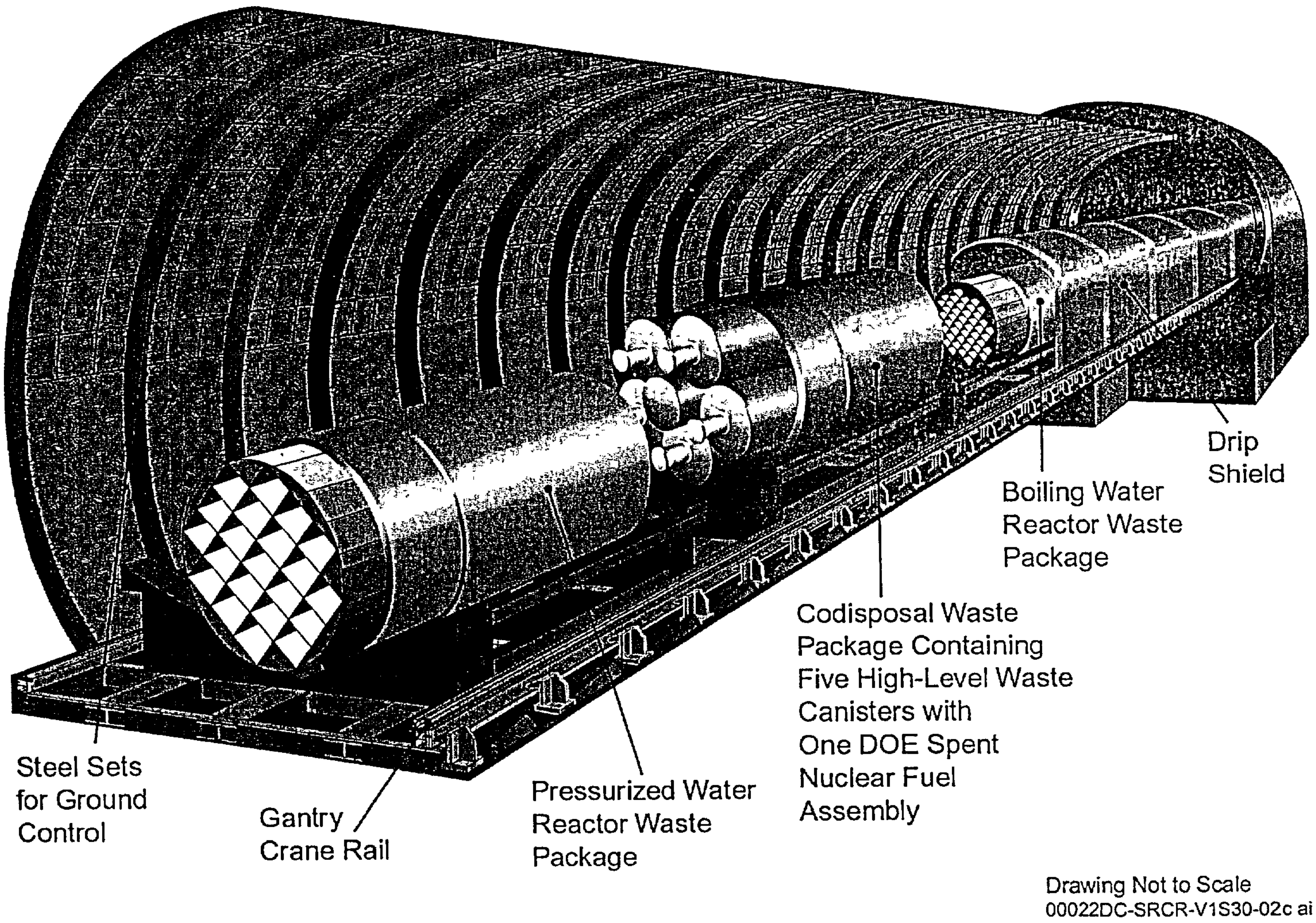
Particles and Droplets (micro)

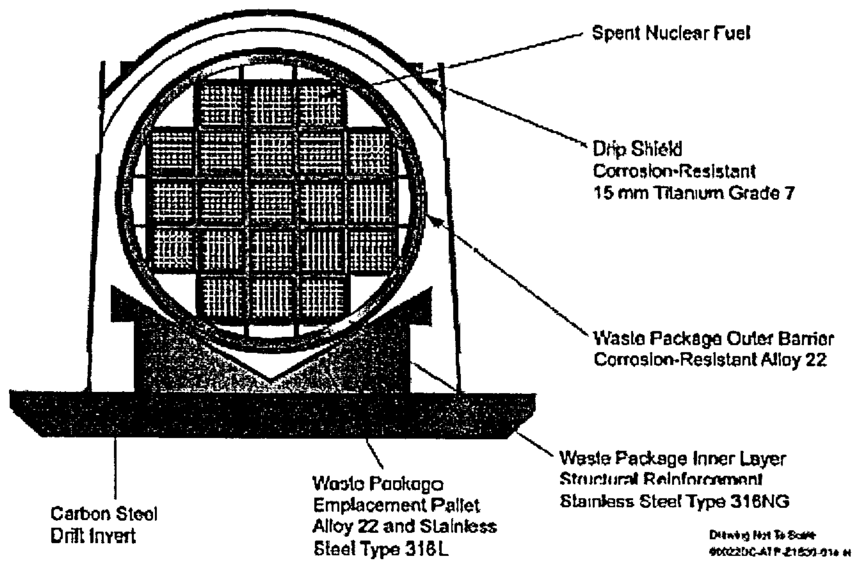
μm-mm

Films and molecules (nano)

nm-μm

Cutaway of a Drift with Three Types of Waste Packages





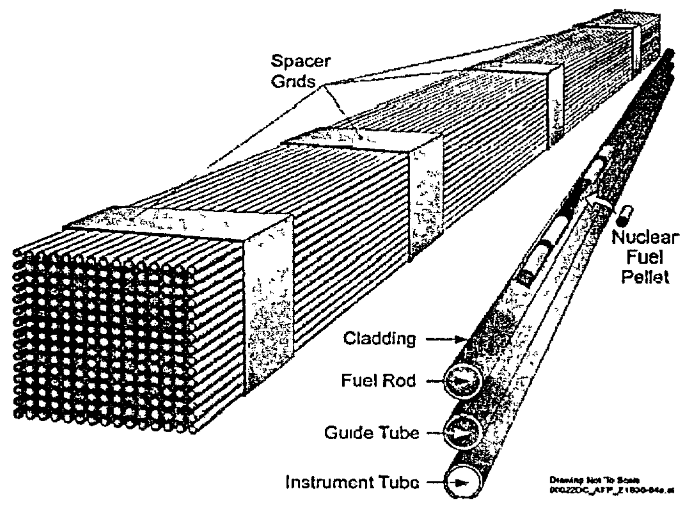


Figure 3-1. Cross-Sectional Illustration of an Alloy 22 and Stainless Steel Emplaced Dual-Metal Waste Package

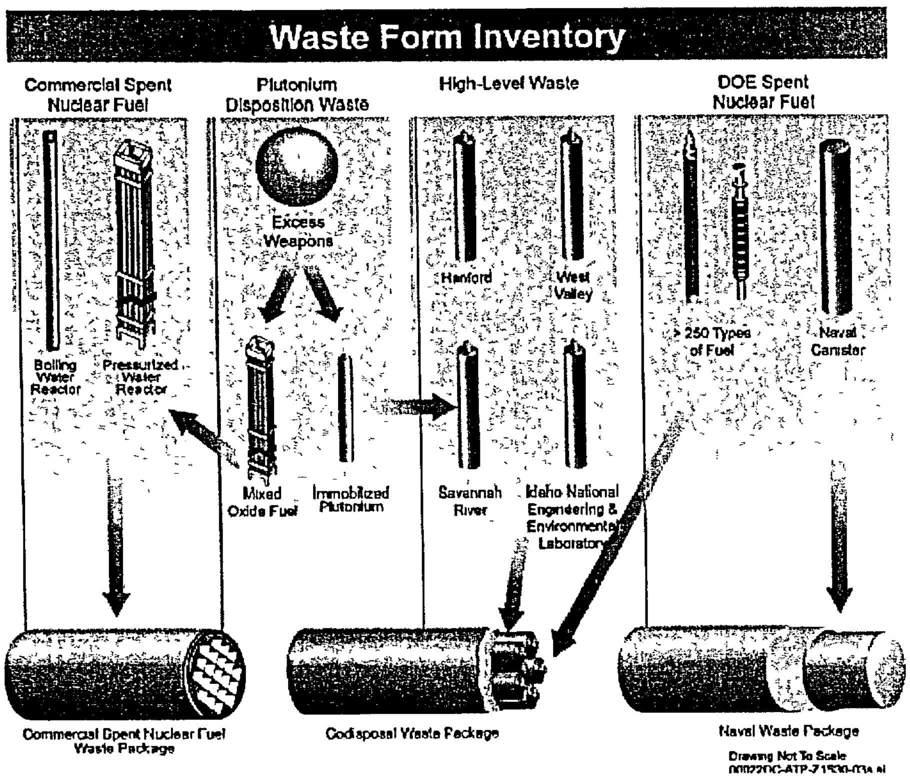
The figure illustrates a waste package supported on an emplacement pallet and covered by a titanium drip shield, showing multiple engineered barriers that provide defense in depth The use of engineered barriers of different materials protects against common mode failures

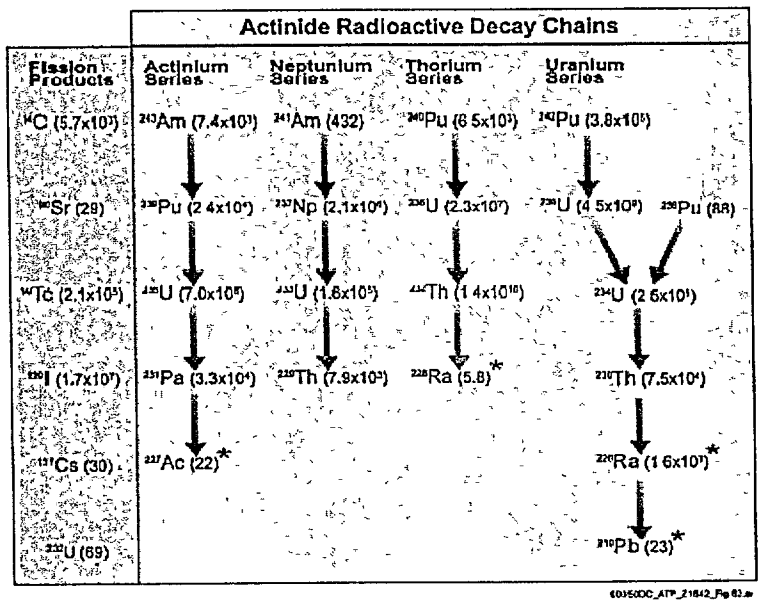
Table 3-9. Waste Package Design Component Materials

Component	Material
Dual-layer design:	
Inner structural shell	Stainless Steel Type 316NG
Outer corrosion-resistant barrier	Alloy 22 (SB 575 N06022)
WP fill gas	Helium
Fuel tubes for commercial SNF WP basket design	Carbon steel (SA 516 Grade 70)
Neutron absorber interlocking plates for commercial SNF WP	Neutronit A 978 (borated 316 stainless steel)
Interlocking plates for 21-PWR Control Rod design	Carbon steel (SA 516 Grade 70)
Structural guides for commercial SNF WP basket design	Carbon steel (SA 516 Grade 70)
Canister guide for 5-DHLW/DOE SNF designs	Carbon steel (SA 516 Grade 70)
Thermal shunts for commercial SNF WP basket design	Aluminum plate (SB 209 6061 T4)

NOTES: SNF = spent nuclear fuel; WP = waste package.

Waste Forms and Radionuclides



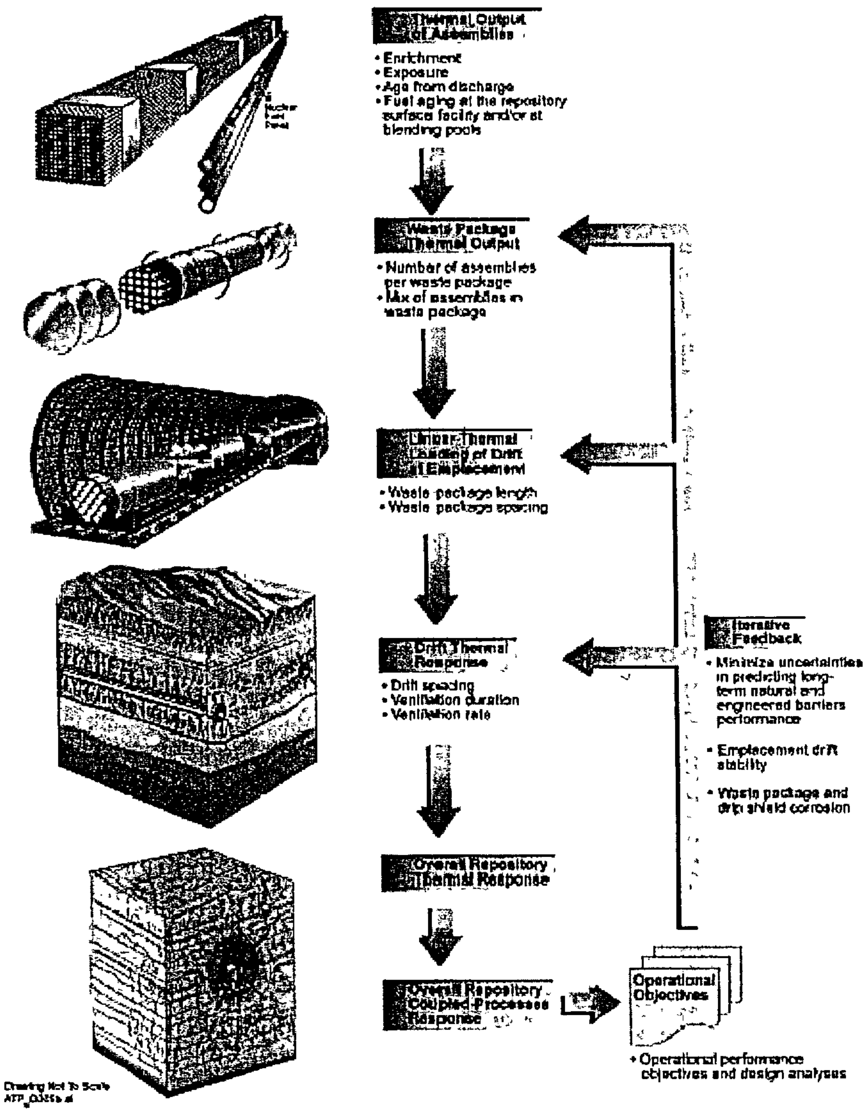


Important to peak-dose calculations only

* Calculated by assuming secular equilibrium

Figure 4-176 All Radionuclides Considered in the TSPA model, Showing Decay-Chain Relationships (with Half-Lives in Years)

Source Term: Thermal Performance of Repository

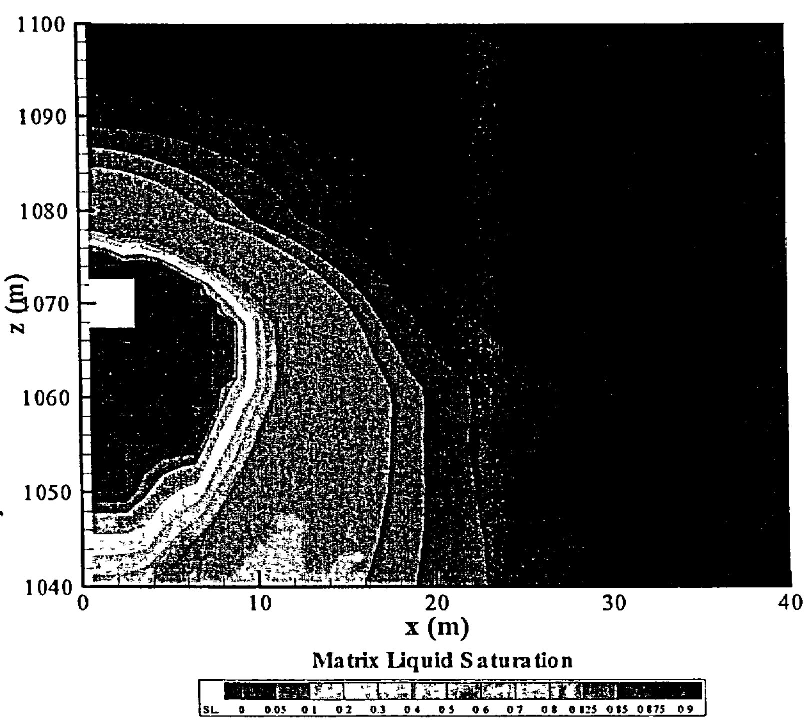


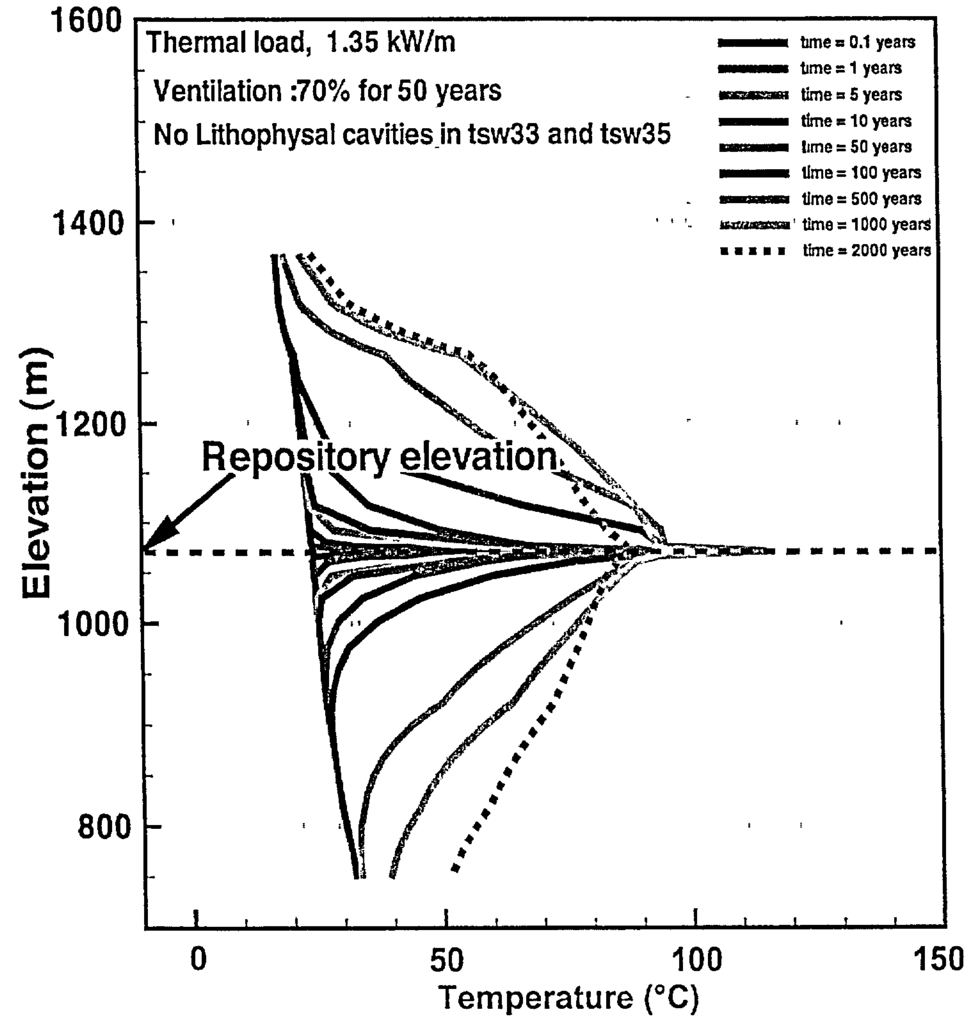
- Heat from spent fuel
- Heat transfer within and from waste package
- Heat transfer to drift walls and into rock

Design and Operation Factors

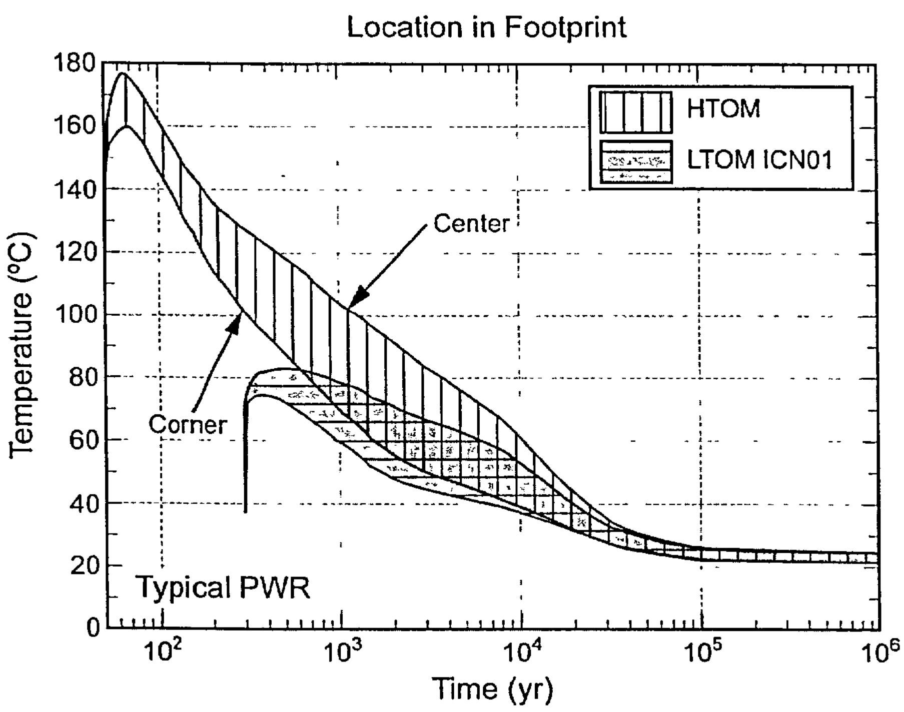
- Drift spacing
- Package spacing
- Package size/length
- Fuel type and age
- Package loading
- Ventilation

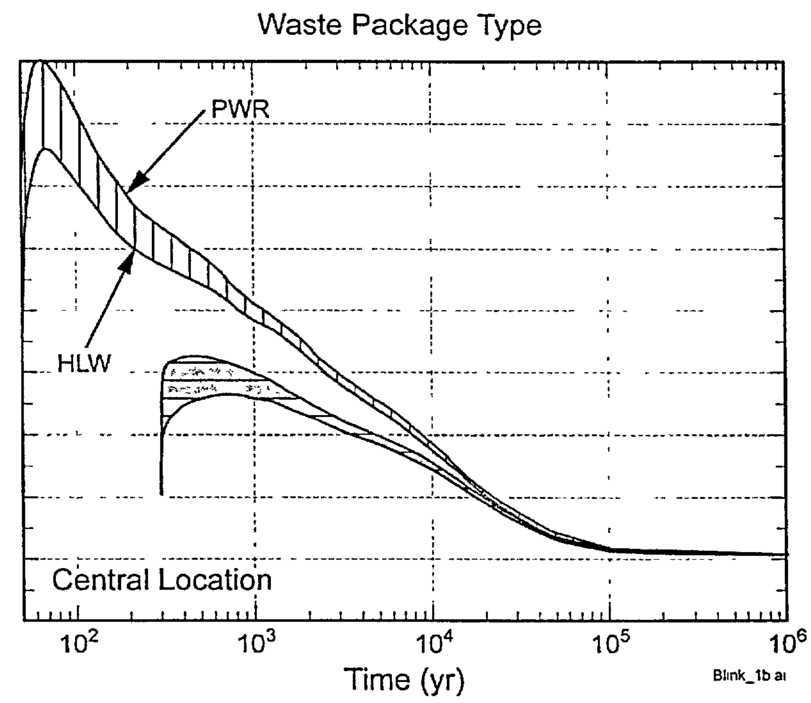
Dry Condition around Hot Waste Packages





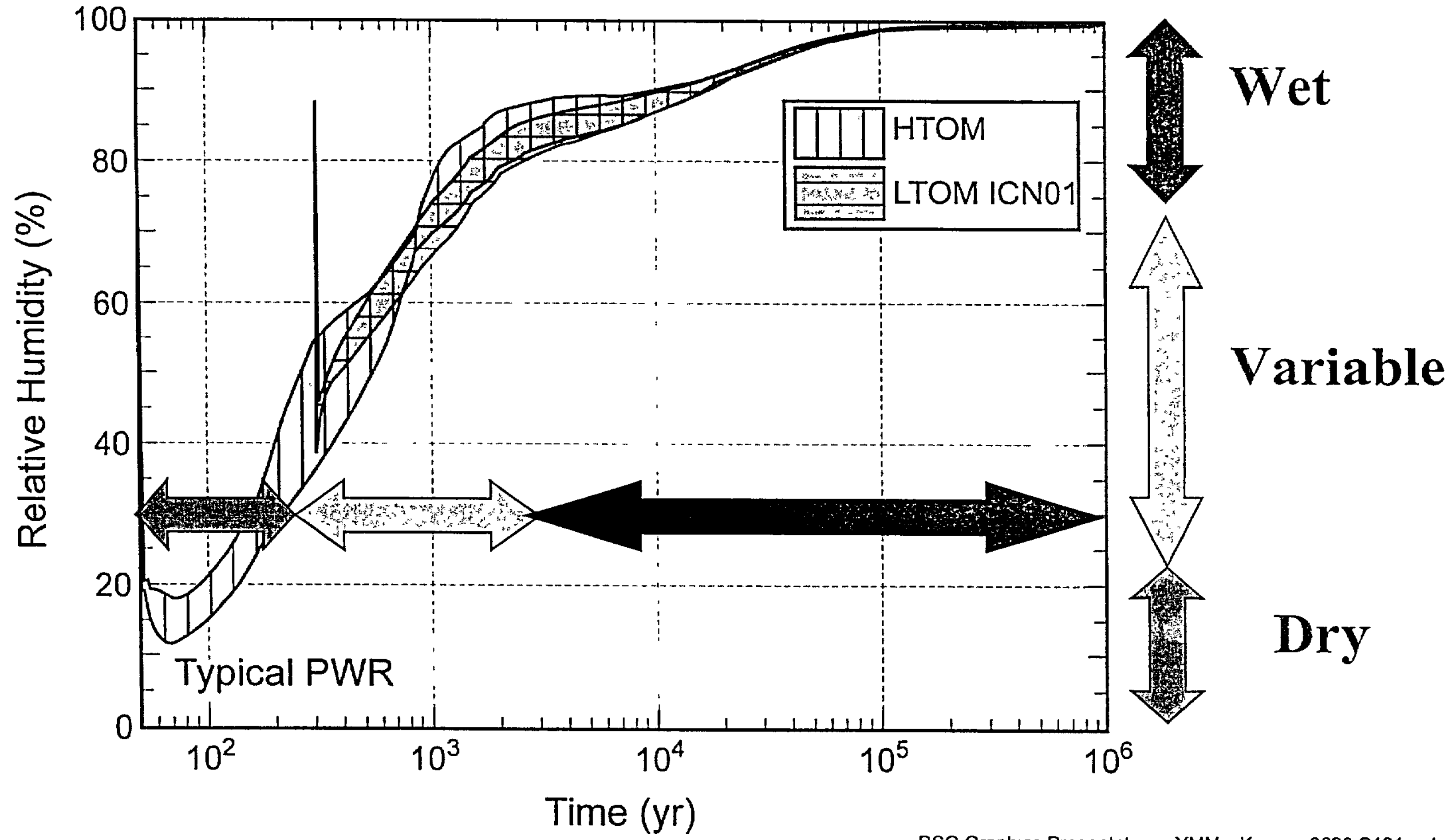
Example Thermal Load Time Profiles





BSC Graphics Presentations_YMBlink_08/02/01.ppt

Example of Equilibrium Humidity and Its Connection to Moisture on Surfaces



BSC Graphics Presentations_YMMacKinnon_0620-2101.ppt

Repository Conditions: Time-Temperature-Relative Humidity

Waste Package Temp, °C	Higher Temp Conditions	Lower Temp Conditions
120 C	At 500 yrs	Not applicable
100 C	At 1000 yrs	Not applicable
80 C	At 3000 yrs	At closure to 1000 yrs
60 C	At 10,000 yrs	At 5000 yrs
40 C	At 25,000 yrs	At 25,000 yrs
Ambient (~25 C)	At 100,000 yrs	At 100,000 yrs

- **Crucial to get the first several hundred to one thousand years correct, that is have high confidence that the waste packages are durable for this time period.**
- **Conditions become more benign during this period: gamma radiation level drops, temperature decreased**
- **Likelihood of localized corrosion and stress corrosion cracking decrease, and the uniform corrosion rates decrease.**

Thermal-Hydrological-Chemical Processes

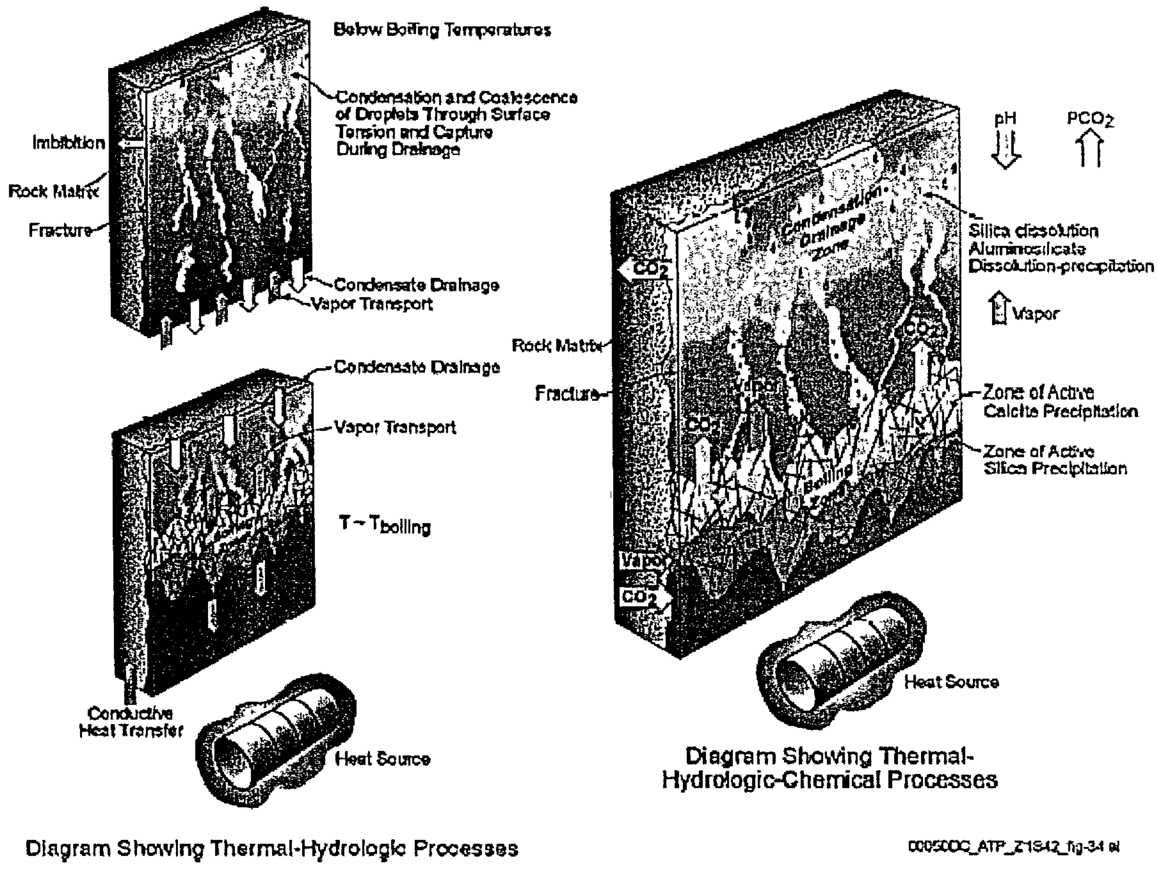
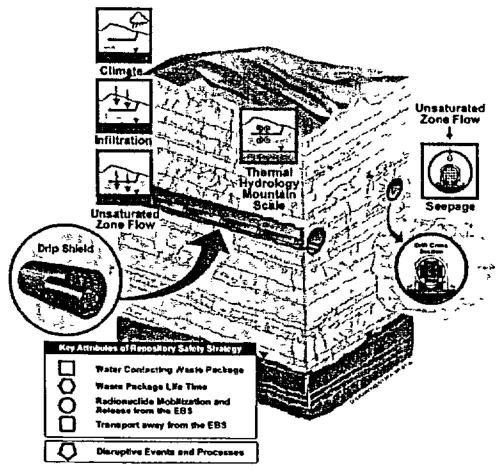


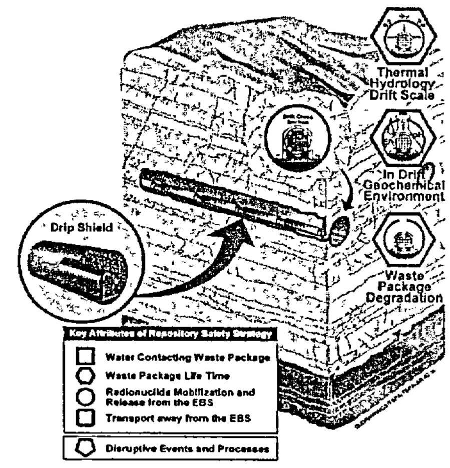
Figure 4-40. Schematic Diagram Showing Relation between Thermal-Hydrologic Processes and Geochemical Processes
Source: CRWMS M&O 2000c, Figure 3.10-2.

Sequence of Events (*from TSPA Model Components*)

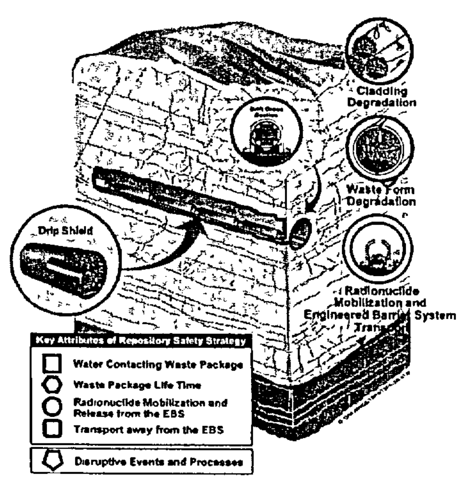
Water Contacting Waste Package



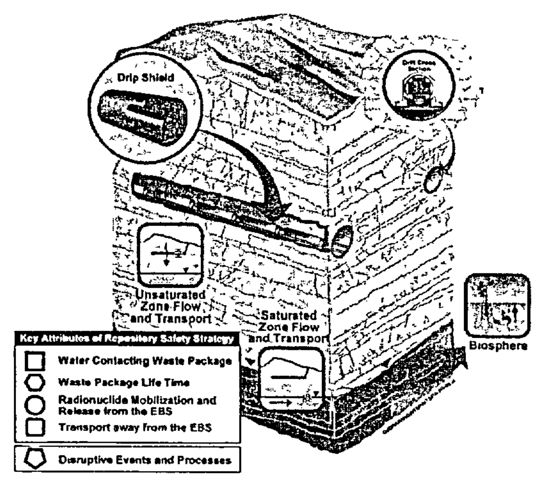
Waste Package Lifetime



Releases from Waste Package



Radionuclide Concentration in Groundwater



Key Components of Models of Source Term

Water is the primary accesser, mobilizer and transporter

Waters on waste package surface (access)

-when, how much, chemistry

-determines corrosion behavior

Waters into waste package (access/mobilize)

-when, how much, chemistry

-form, frequency and distribution of penetrations

Waters in waste package (mobilize)

-on clad, waste form and internals

-determines radionuclide mobilization

Waters from waste package and drift (transport)

-when, how much, chemistry

-determines radionuclide transport

Characteristics of Reality for Source Term

Composition (corrosivity) of waters on waste package surface

When penetrations of waste packages occur

Form, number and distribution of any penetrations

Amount of water entering packages through penetrations

Waste form degradation and radionuclides mobilization

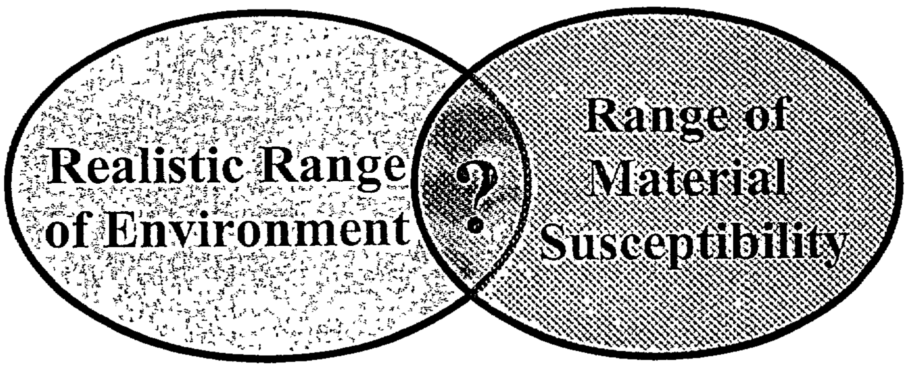
Interaction (retardation) of radionuclides with corrosion products, waste form alterations, invert

Transport of radionuclides from drift

Water Contacting Waste Package and Entering Waste Packages

Necessary Conditions for Significant Corrosion to Occur on Waste Packages

- Water must contact WP
- Water must remain on WP
- Corrosive species must be present to form electrolyte
- Material must be susceptible to corrosion under these conditions
- Conditions must persist over sufficiently long time



After Kelly 3-25-2002

Composition of Waters

Primary Controlling Factors

ON- Waste Package Surface

ON-Waste Form

From-Waste Package/Drift

Three Important Conditions

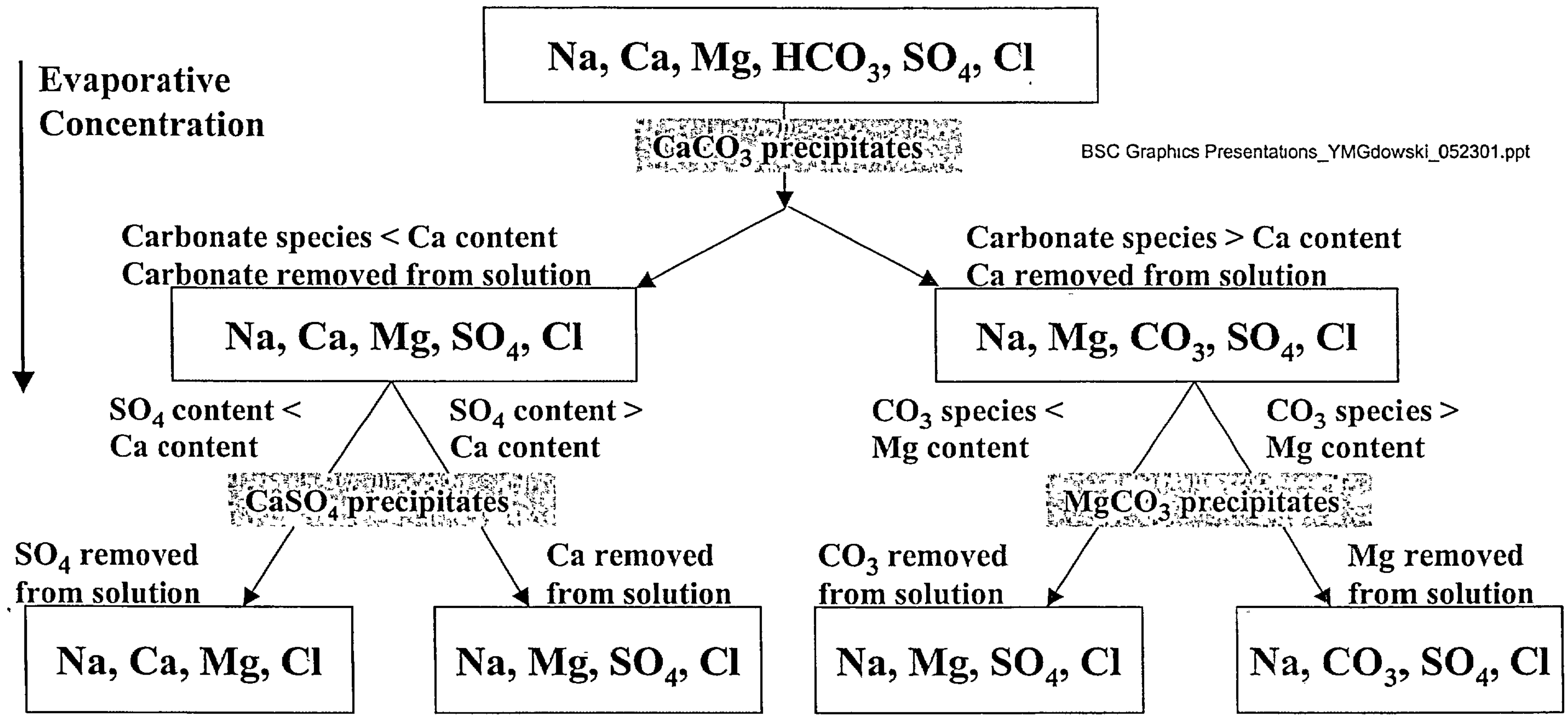
➢**Condensation leads to moist dust**

➢**Dripping seepage water forms mineral scale**

➢**Crevice areas entrap environments**

- **Ambient Waters:**
  Dilute solutions
  Na-Ca-Mg-HCO_3-CO_3-Cl-NO_3-SO_4
  pH 5.6-7.4
- **Waters can be concentrated**
  modified during movement
  thermal-chemical processes
- **Modifications on waste package and waste form**
  Can be greater effect than in rock
  Chemical and electrochemical processes

The Chemical Divide Principle for Brine Evolution from Dilute Natural Waters



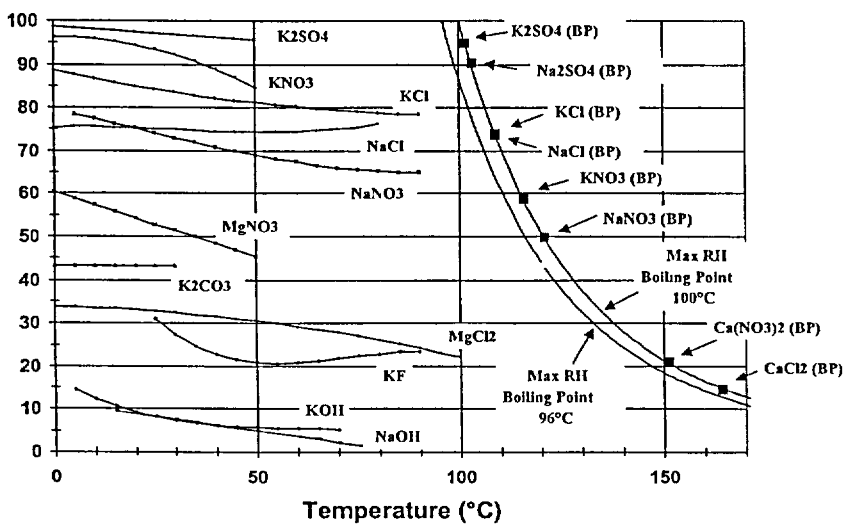
Death Valley, CA	(Na)*
Bristol Dry Lake, CA	(Na, Ca)
Cadiz Lake, CA	(Na, Ca)
Carson Sink, NV	(Na)

Saline Valley, CA	(Na)*
Danby Lake, CA	(Na)
Salton Sea, CA	(Na)

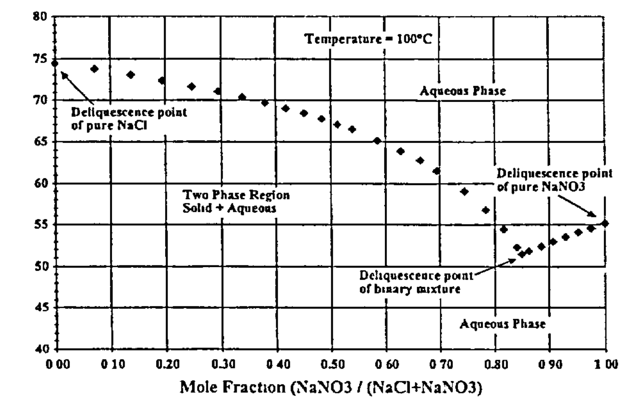
Surprise Valley, CA
Mono Lake, CA
Owens Lake, CA
Soda Lake, CA
Pyramid Lake, NV
Winnemucca Lake, NV

* dominant cation(s) in brine

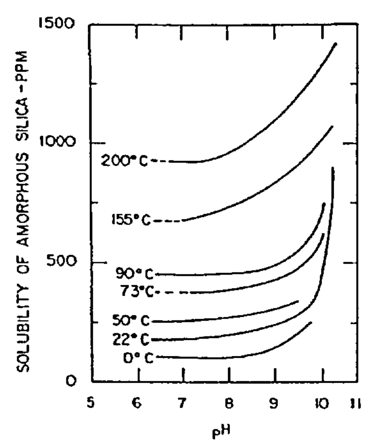
Deliquescence Points for Salts



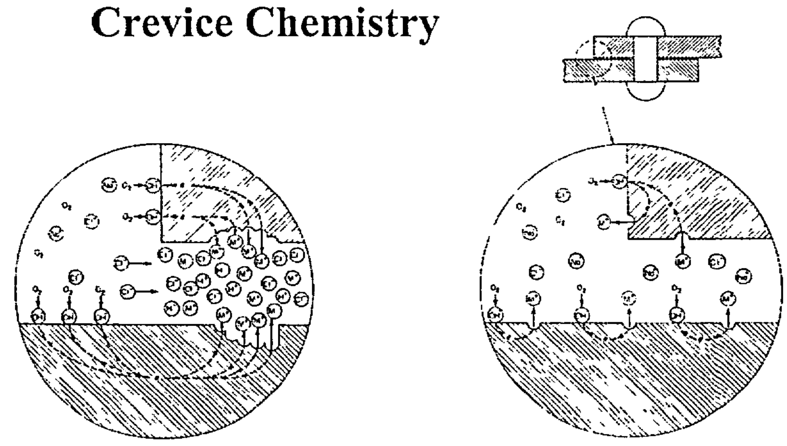
Phase Diagram for Mixture of NaCl + $NaNO_3$



Silica Solubility vs. pH



Crevice Chemistry



Corrosion the Primary Determinant of Waste Package Lifetime

Waters at Yucca Mountain

Water composition <u>in</u> Yucca Mountain

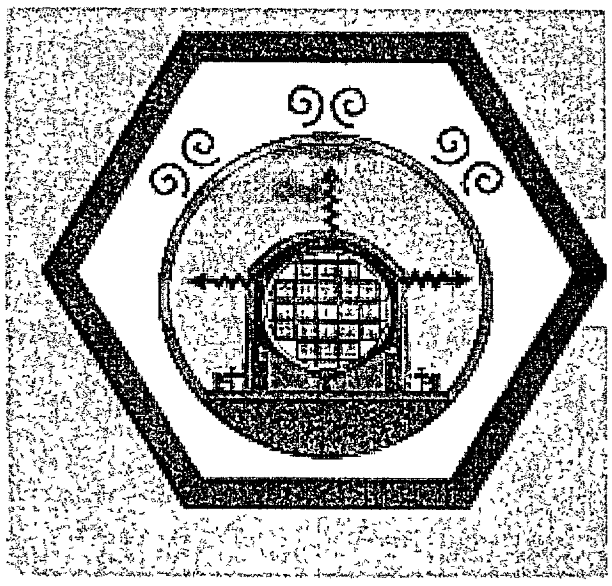
–naturally occurring

–major source of water and ionic species

Aqueous environments <u>on</u> metal surfaces and <u>on</u> spent fuel

–alteration of waters due to thermal and chemical conditions

- Full immersion of metal surfaces highly unlikely condition
- Two sources of water:
  Condensation from the air
  Seepage from the rock

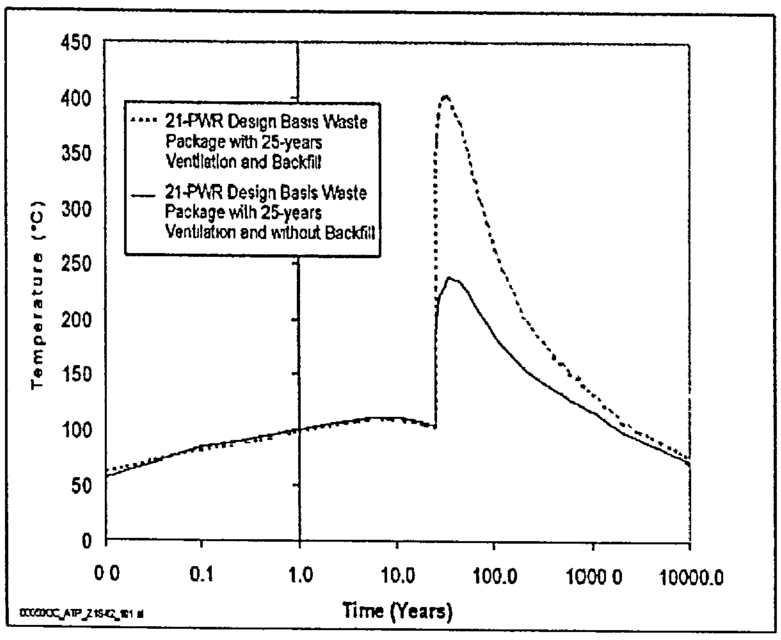


BSC Graphics Presentations_YMMacKinnon_0620-2101.ppt

Corrosion: Long-Term Materials Performance

- Nickel-base Alloy 22 and Titanium Grade 7
  - Principal alloys of interest for waste package and drip shield
  - Excellent corrosion resistance over a wide range of aqueous solution compositions and temperatures
- Nickel-base Alloy 22 and titanium Grade 7 are extremely resistant to localized corrosion
  - Nevertheless, these alloys are susceptible to crevice corrosion under extreme conditions of environment and potential
  - It is necessary to perform experiments under conditions beyond those thought to be relevant to Yucca Mountain in order to examine the margins of corrosion resistance.
- Two major considerations
  - Fabrication processes, particularly welding, can have a major impact on corrosion resistance and performance
  - Temperature has major effects on the composition of the environment and the behavior of materials.

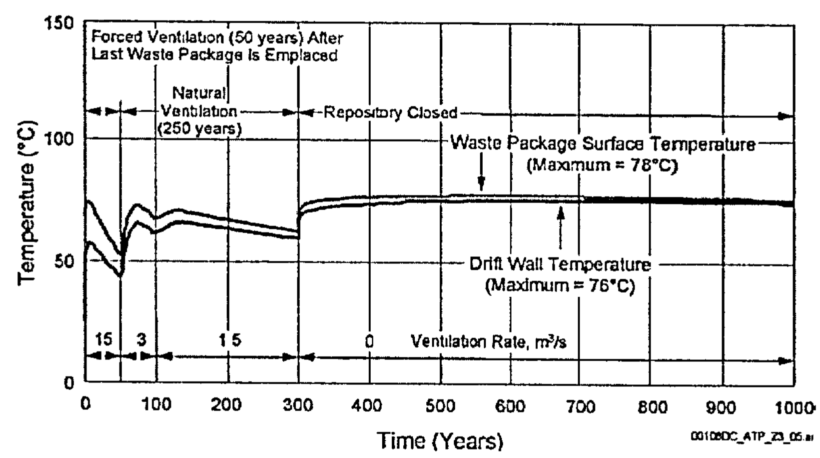
Repository Heat-up and Cool-down Cycle



One long and slow thermal cycle

Rise in temperature at end of ventilation period

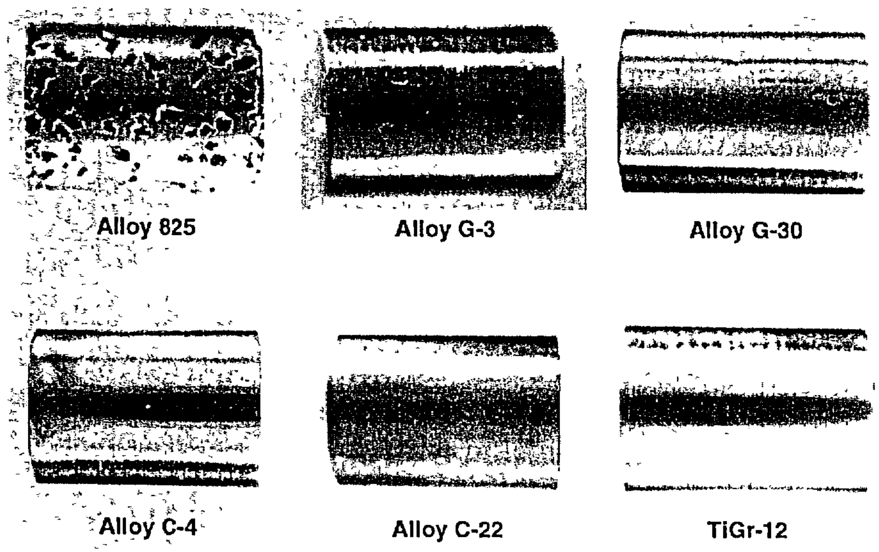
Long, slow cooling period

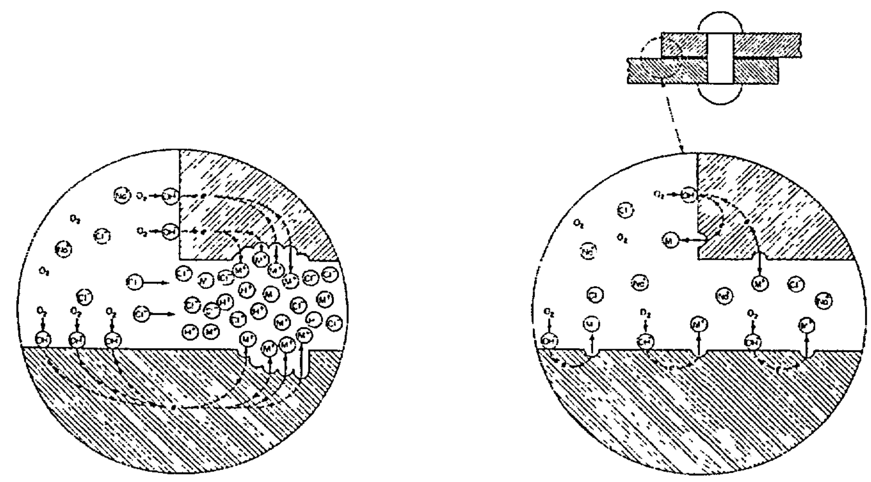


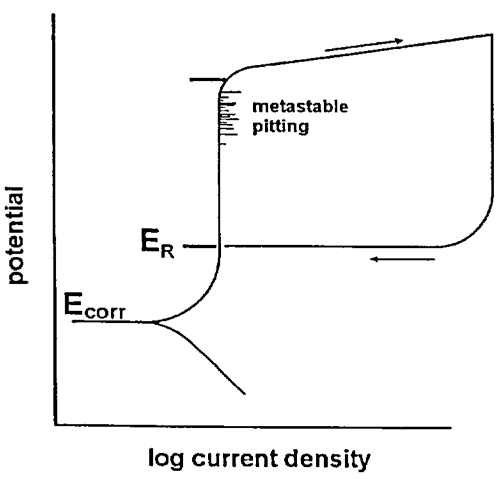
Important Performance Factors

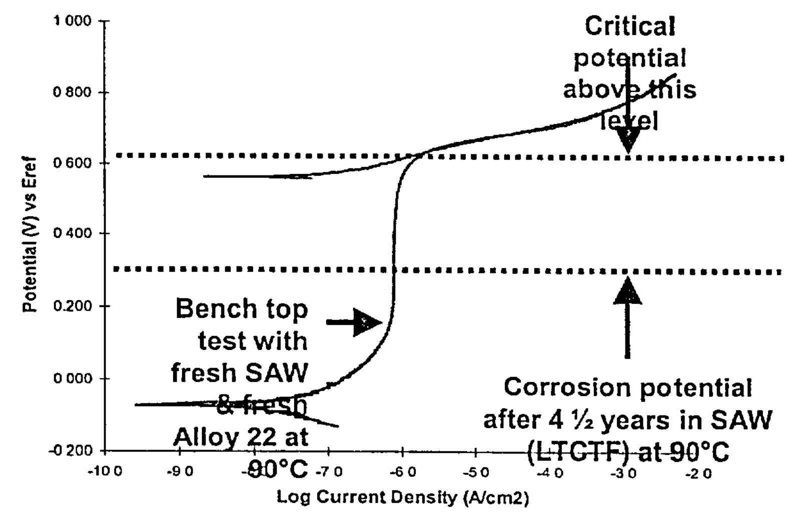
- Waste package surface temperature
- Form and amount of water
- Clad and internal temperature

Localized Corrosion









Vulnerable Temperature Range for Corrosion of Corrosion Resistant Metal (CRM)

Alternative perspective on crevice corrosion

CRM (C-22, Ti, ...) vulnerable to crevice corrosion

Vulnerable temp range, below which no crevice corrosion

$\Delta T_{VULN} = T_{AQS} - T_{CREV}$

T_{AQS} : highest temp for aqueous solution

Eqm boiling or droplet on hot surface

T_{CREV} : lowest temp to sustain crevice corrosion

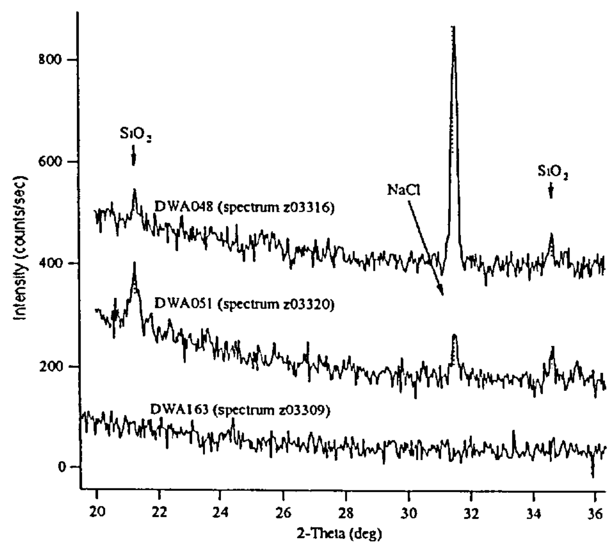
For given alloy is function of pH, Eh, X^{-n}, Y^{+m},

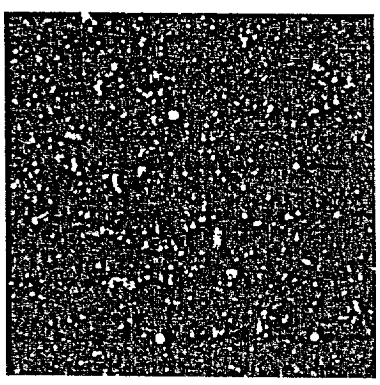
Where $T_{AQS} < T_{CREV}$ $\Delta T_{VULN} = 0$

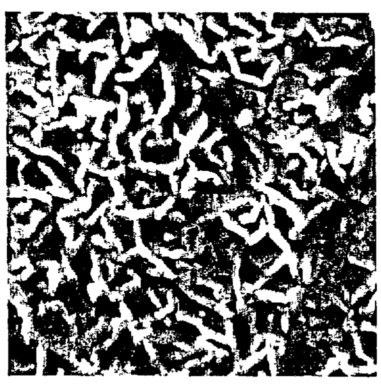
Where $T_{AQS} > T_{CREV}$ $\Delta T_{VULN} = T_{AQS} - T_{CREV}$

Vulnerable time: $\Delta t_{VULN} = t_{AQS} - t_{CREV}$

Passive Film: Formation and Stability







Important Factors

Stability of passive film is crucial to performance

Long lives (10,000's) of waste packages with stable films

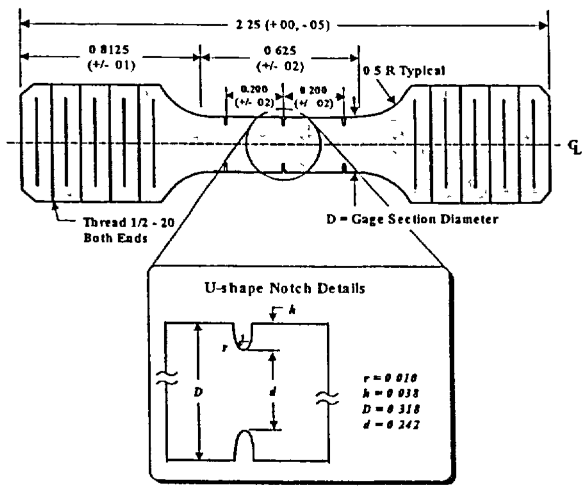
Boundaries of performance defined by localized corrosion processes

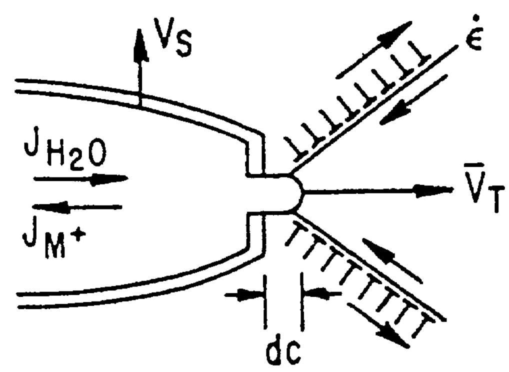
Thin films (nm's) examined for composition and structure

Models for passivity current area of corrosion research

Stress Corrosion Cracking

Notched Keno Specimen Geometry





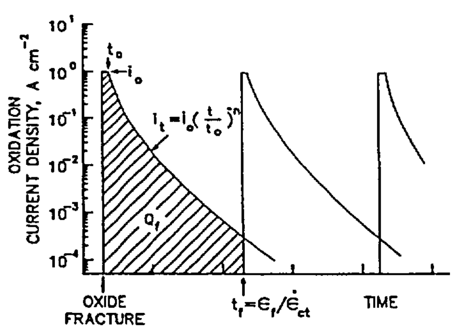
Important Factors

Residual stresses

Corrosive environment

Alloy stability: aging

Welds of particular interest



$V = \frac{da}{dt}$, $\bar V_{av} = \frac{M}{zF\rho}\cdot\frac{Q_f}{t_f}$

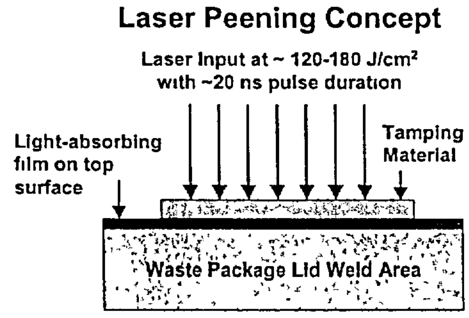
FOR HIGH $\dot\epsilon_{ct}$ AND/OR LONG t_o :

$\bar V_{av} = \frac{M}{zF\rho}\cdot i_o$

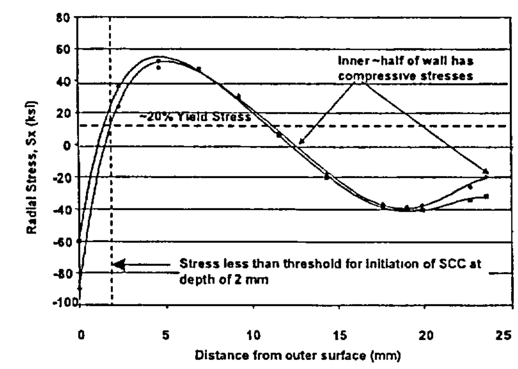
FOR LOW $\dot\epsilon_{ct}$ AND/OR SHORT t_o :

$\bar V_{av} = \frac{M}{zF\rho}\,\frac{i_o t_o^n}{(1-n)\epsilon_f^n}\,\dot\epsilon_{ct}^n = f(n)\,\dot\epsilon_{ct}^n$

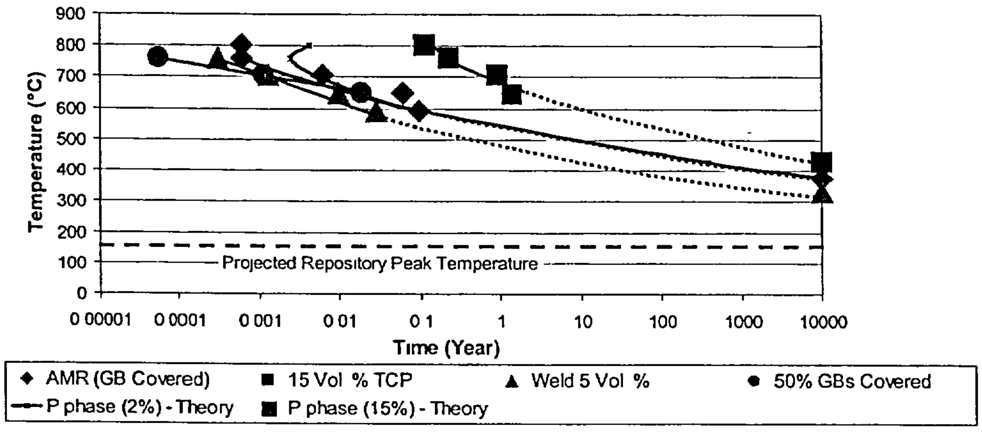
Laser Peening Concept



Through-Wall Stress in Laser Peened Areas



Long Term Stability of Alloys

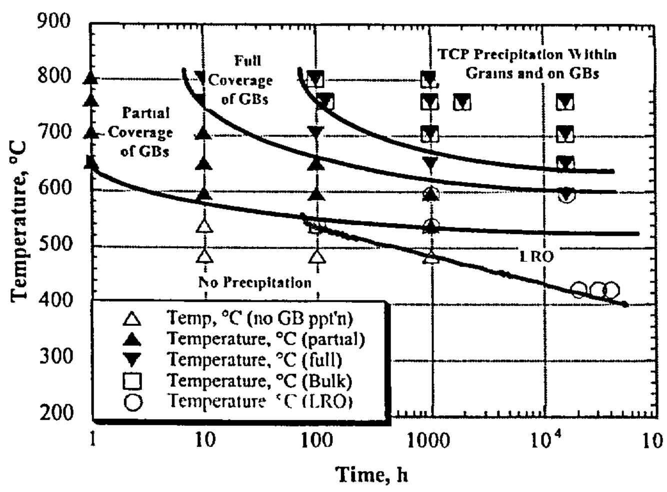


Important Factors

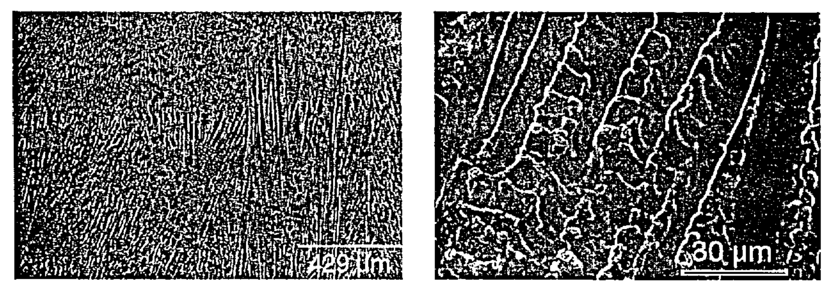
Aging and long range ordering can affect corrosion resistance

Time-temperature-composition

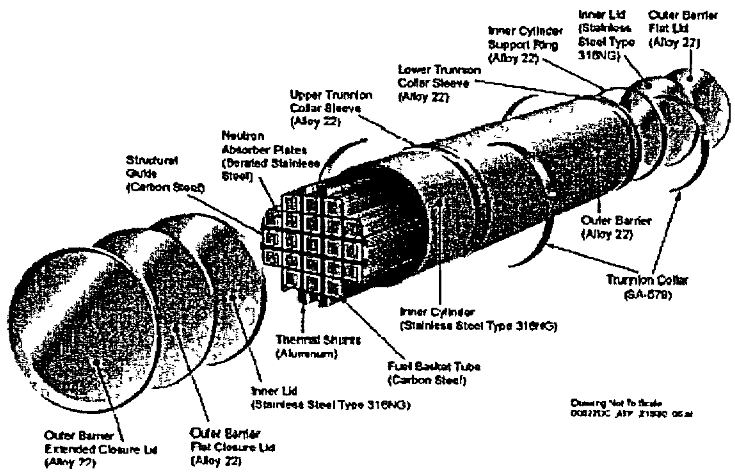
Bulk alloy and welds



As-welded Alloy 22 (Gas-Tungsten-Arc-Weld, GTAW)

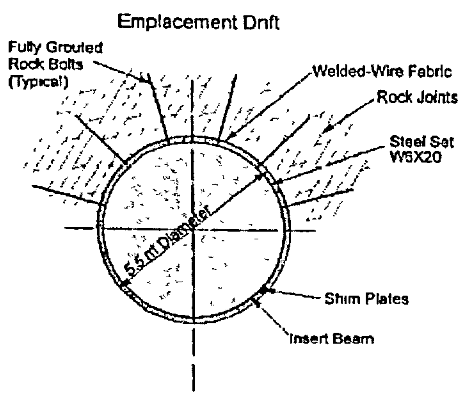


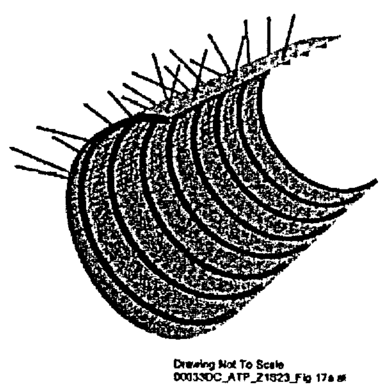
Design and Fabrication Processes

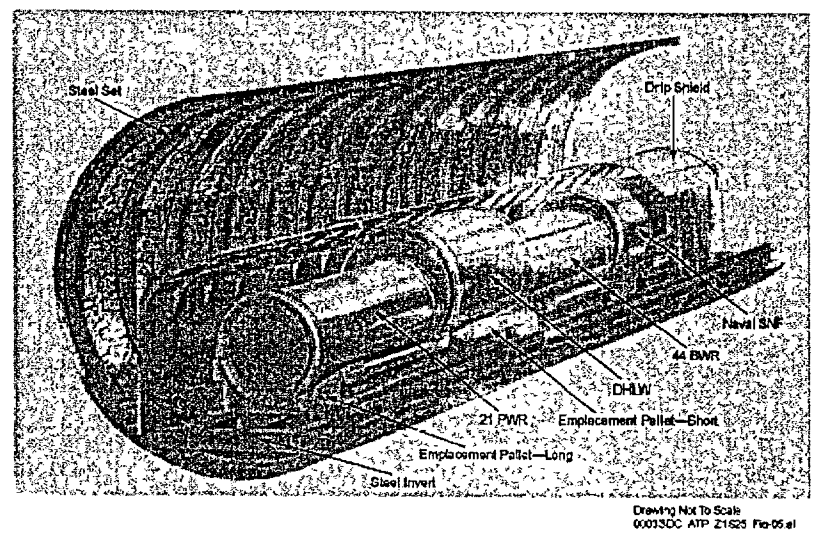


Some Important Factors

- Materials of construction
- Metallurgical structure
- Residual stresses
- Welds-Welds-Welds







Repository Conditions: Relevant to Waste Packages

- Several important aspects of the long-term storage.
  - Waste packages are exposed to one, long and slow, temperature cycle.
  - No moving parts.
  - Static exposure does not subject the waste packages to potentially detrimental, cyclic loads.
  - Low heat fluxes and extremely slow heating and cooling do not expose the waste packages to large thermal gradients or rapid thermal expansion and contraction.
  - In a higher temperature operating mode, the waste packages are exposed to dry conditions for long times (several hundred years) before the surfaces are wetted.

Repository Conditions: Relevant to Waste Packages

- The waste material gives off heat and radiation at rates that decrease with time.
  - Thermal effects diminish over several thousands of years
  - Radiation effects diminish over a few hundred years.
- At the repository level, the waste packages are isolated beneath 300 meters of rock and are a few hundred meters above the water table.
- The waste packages sit in air on support pallets.
  - Ambient air is saturated with water equivalent to 100% relative humidity.
  - While the amounts of moisture will be small, there is sufficient water for corrosion, therefore corrosion resistant metals are required.

Waste Form Degradation and Radionuclide Mobilization

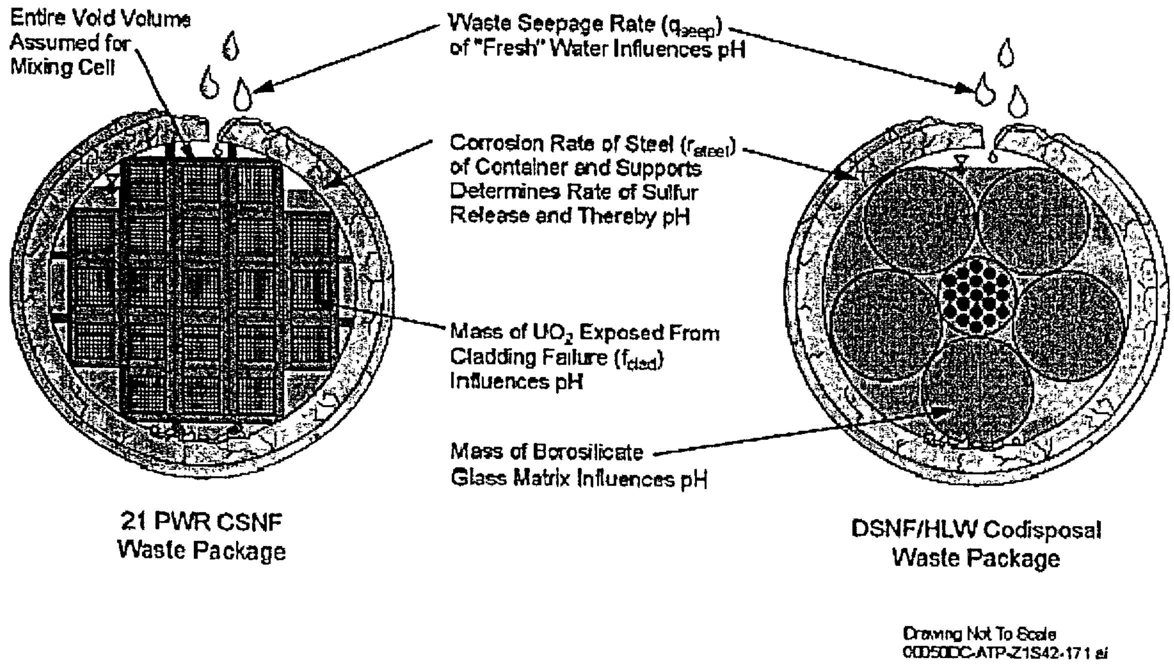


Figure 4-98. Conceptual Model of In-Package Chemistry
DSNF = DOE spent nuclear fuel; HLW = high-level radioactive waste; CSNF = commercial spent nuclear fuel
Source: CRWMS M&O 2000bm, Figure 3 2-1.

Bath-tub mode

Flow-through mode

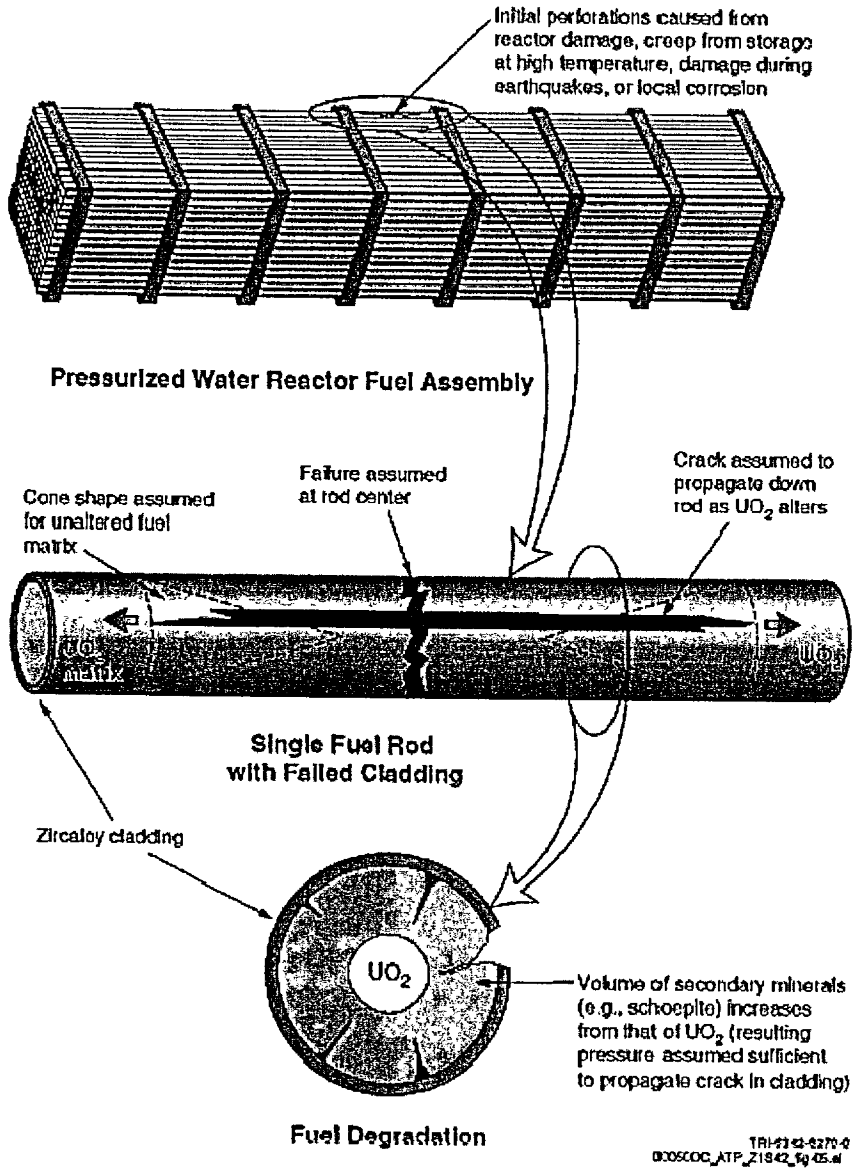


Figure 4-102. Conceptual Model of Commercial Spent Nuclear Fuel Cladding Degradation
Source CRWMS M&O 2000bm, Figure 3 6-2.

Important Factors

Water transport into waste package

Water composition: pH, Eh, chemistry

Degradation of Zr clad

UO_2 corrosion and alteration

Radionuclide mobilization

Corrosion of UO_2 Spent Fuel Matrix

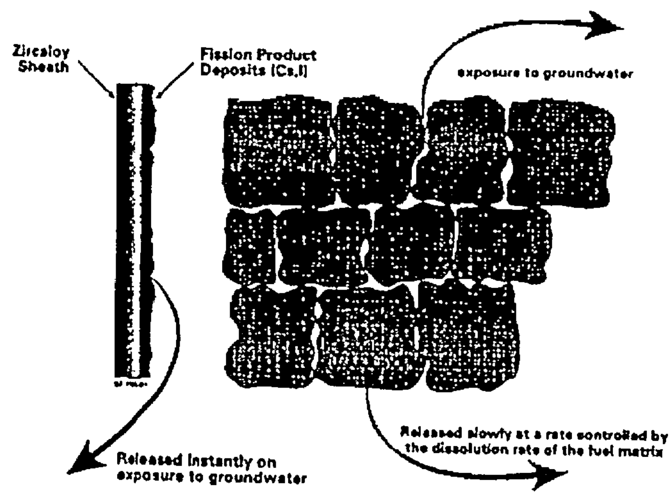
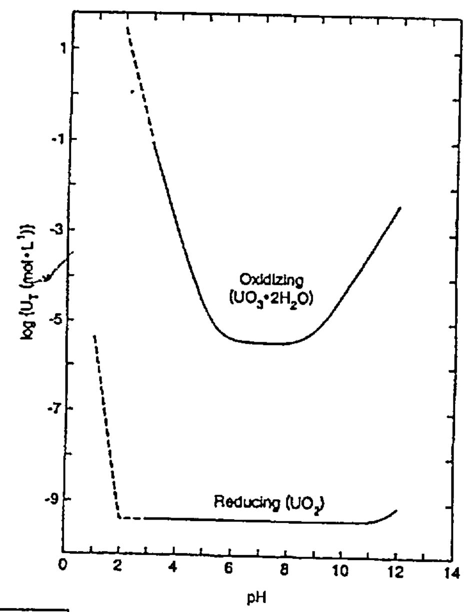


Fig. 1. Schematic diagram showing the distribution of radionuclides in used fuel. Radionuclides located at the fuel–Zircaloy cladding gap and at grain boundaries within the fuel are assumed to be instantly released.

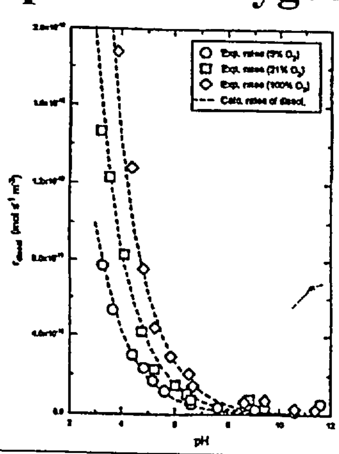
Oxidizing vs. Reducing

Eh and pH



after Shoesmith, J Nucl Matls, 282 (2000)

pH and Oxygen



Complexes/Alteration

$UO_2^{2+} + 2CO_3^{2-} \Longleftrightarrow UO_2CO_3(aq)$

$\log K_1 = 9.5 \pm 0.4$

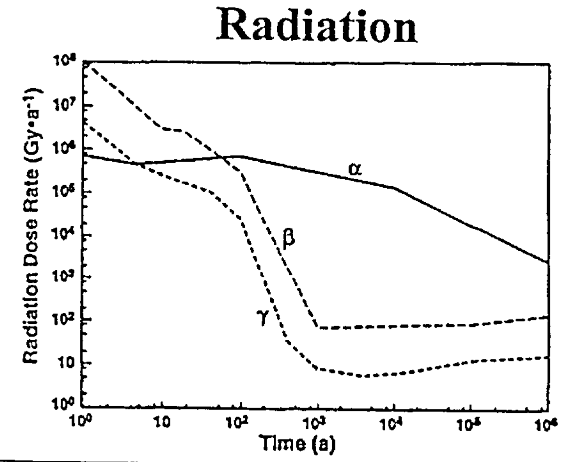
$UO_2^{2+} + 2CO_3^{2-} \Longleftrightarrow UO_2(CO_3)_2^{2-}$

$\log \beta_2 = 16.6 \pm 0.3$

$UO_2^{2+} + 3CO_3^{2-} \Longleftrightarrow UO_2(CO_3)_3^{4-}$

$\log \beta_3 = 21.6 \pm 0.6$

Radiation



140th ACNW Meeting March 25, 2003

Realism in Long Term Corrosion and Source Term; J.H. Payer

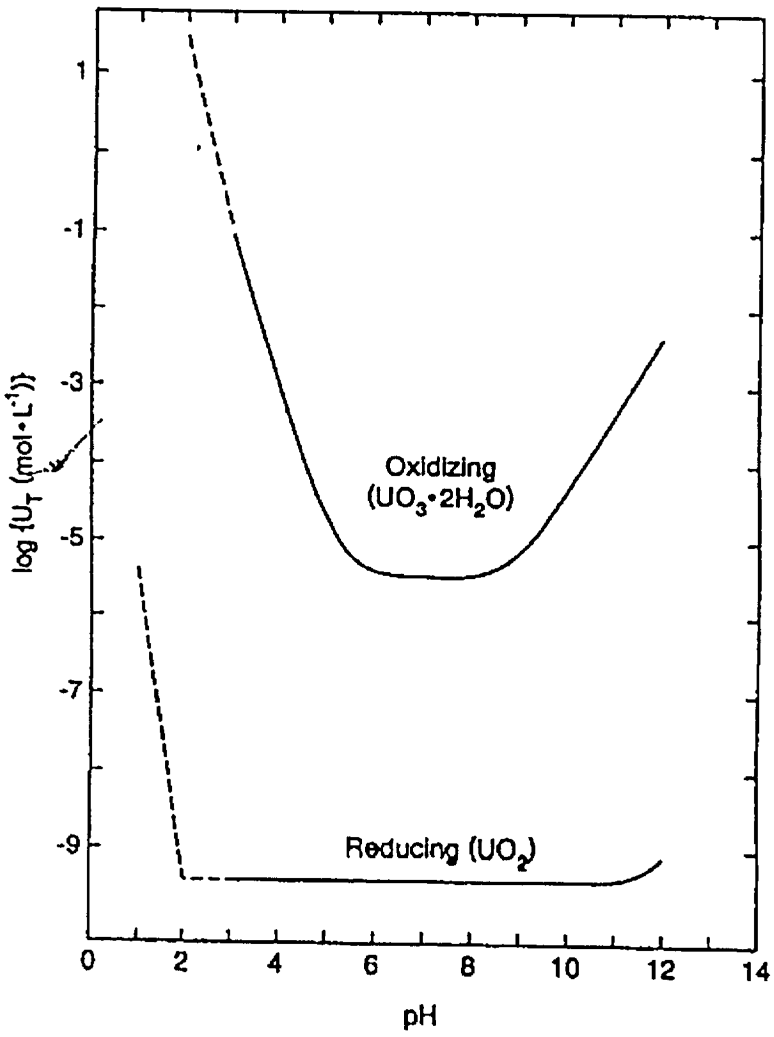
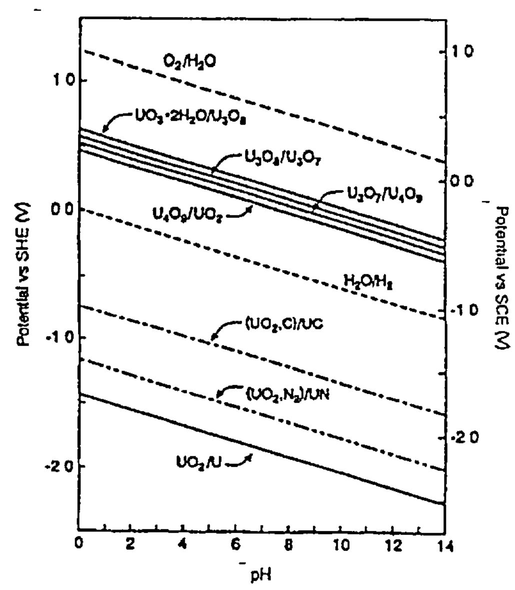
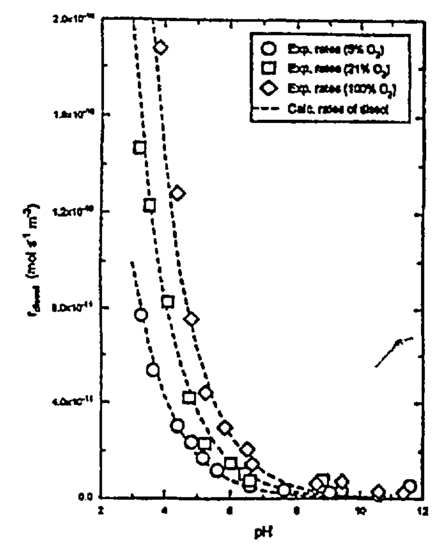


Fig. 3. Solubilities of uranium dioxide (UO_2) and schoepite ($UO_3 \cdot 2H_2O$) as a function of pH at 25°C [4].





Important Factors

Oxidizing vs. Reducing

Oxidizing potential (Eh)

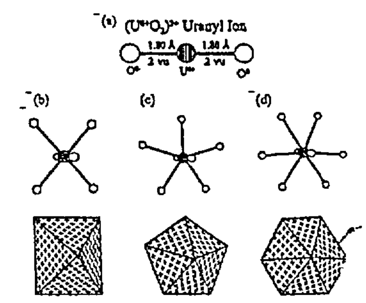
Acidity (pH)

after Shoesmith, J Nucl Matls, 282 (2000)

Alteration of Spent Fuel and Incorporation Mechanisms

Table 1
Uranyl phases found as alteration products of UO_2

Structure known	
schoepite	$[(UO_2)_8O_2(OH)_{12}](H_2O)_{12}$
becquerelite	$Ca[(UO_2)_3O_2(OH)_3]_2(H_2O)_8$
compreignacite	$K_2[(UO_2)_3O_2(OH)_3]_2(H_2O)_8$
billietite	$Ba[(UO_2)_3O_2(OH)_3]_2(H_2O)_4$
soddyite	$(UO_2)_2(SiO_4)(H_2O)_2$
Na–boltwoodite	$(Na,K)(H_3O)[(UO_2)(SiO_4)]$
sklodowskite	$Mg[(UO_2)(SiO_3OH)]_2(H_2O)_6$
uranophane	$Ca[(UO_2)(SiO_3OH)]_2(H_2O)_5$
haiweeite	$Ca(UO_2)_2Si_6O_{15}(H_2O)_5$
Structure not known	
Dehydrated schoepite	$UO_3(H_2O)_{0.8-1.0}$



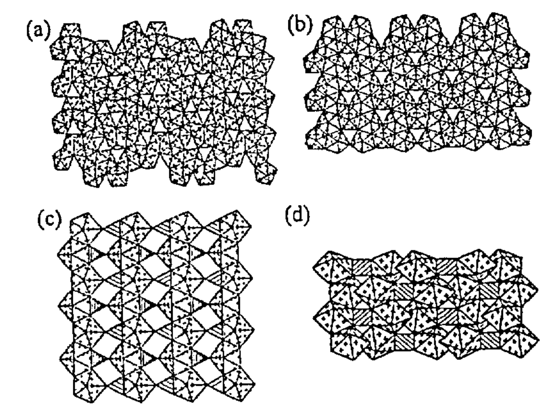


Fig 6 Sheets occurring in the uranyl phases that were found as alteration products of UO_2 (a) schoepite (b) becquerelite compreignacite (c) α-uranophane and boltwoodite (d) soddyite.

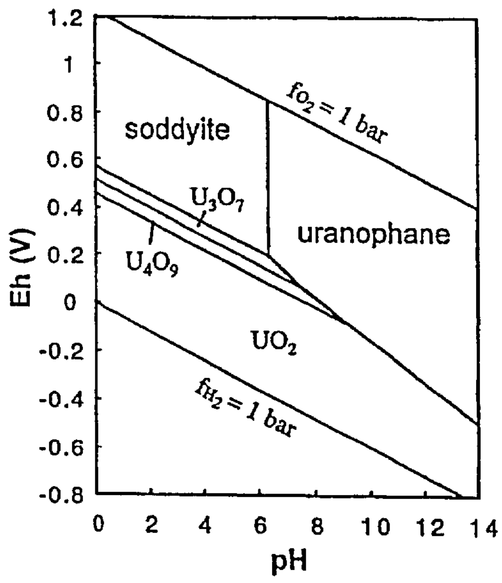


Fig 2 Eh–pH diagram showing the stability relations among uranium phases equilibrated with Yucca mountain J-13 groundwater The thermodynamic data for the uranyl phases are from [17], those for the uranium oxides are from [18]

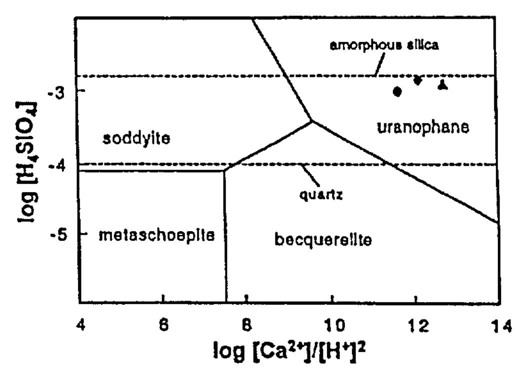


Fig 1 Activity-activity diagram for SiO_2–CaO–UO_3–H_2O

after Burns, Ewing, Miller, J Nucl Matls, 245, 1997

Important Factors

Crystal chemistry

Chemical analysis

Thermodynamics

Fission product and actinide incorporation??

Radionuclide Transport

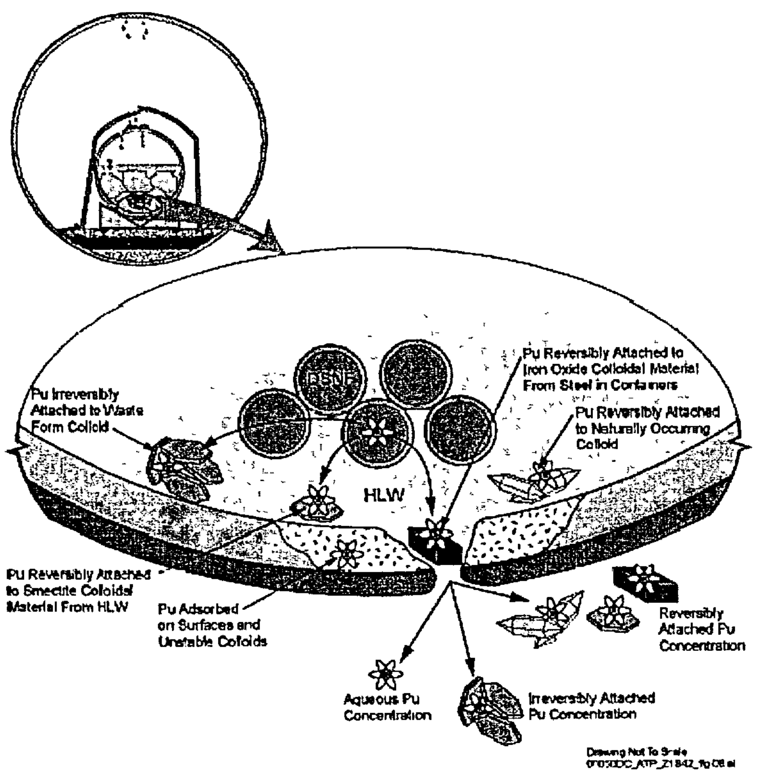


Figure 4-99 Conceptual Model of the Formation of Reversibly and Irreversibly Attached Radionuclides on Colloids
DSNF = DOE spent nuclear fuel, HLW = high-level radioactive waste Source CRWMS M&O 2000bm, Figure 3 8-1

Important Factors

Interaction with degraded waste form-alteration products

Interaction with corrosion products: internals and waste package

Interactions with invert and drift support

Transport processes

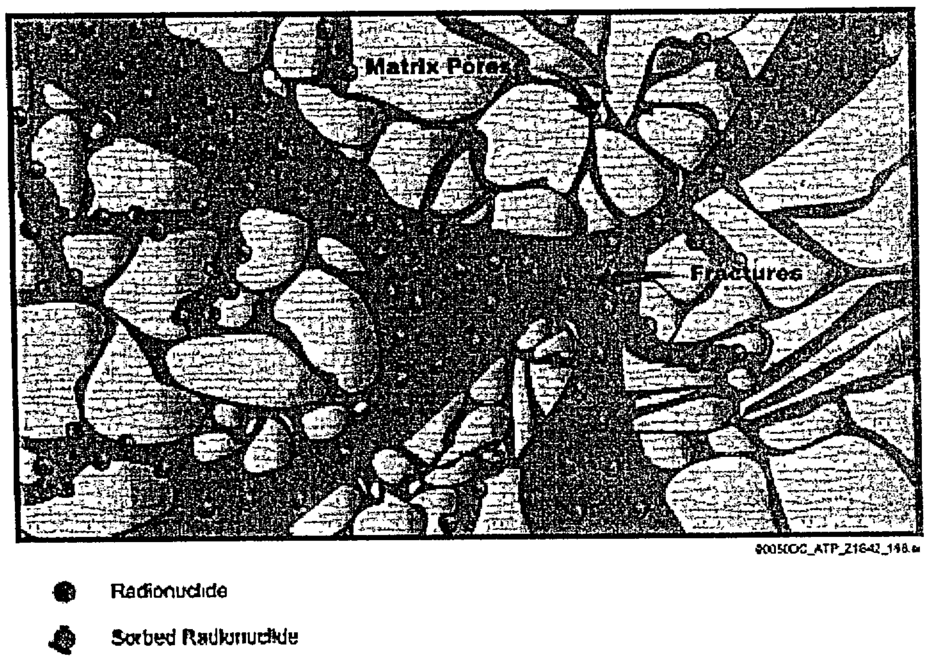


Figure 4-134. Conceptualization of Solute and Colloid Transport in a Fracture with Sorption in the Rock Matrix
Sorption in the fracture rock is conservatively ignored in TSPA-SR calculations. After diffusing into the matrix, solutes are sorbed into the rock matrix Source CRWMS M&O 2000a, Figure 3 7-4.

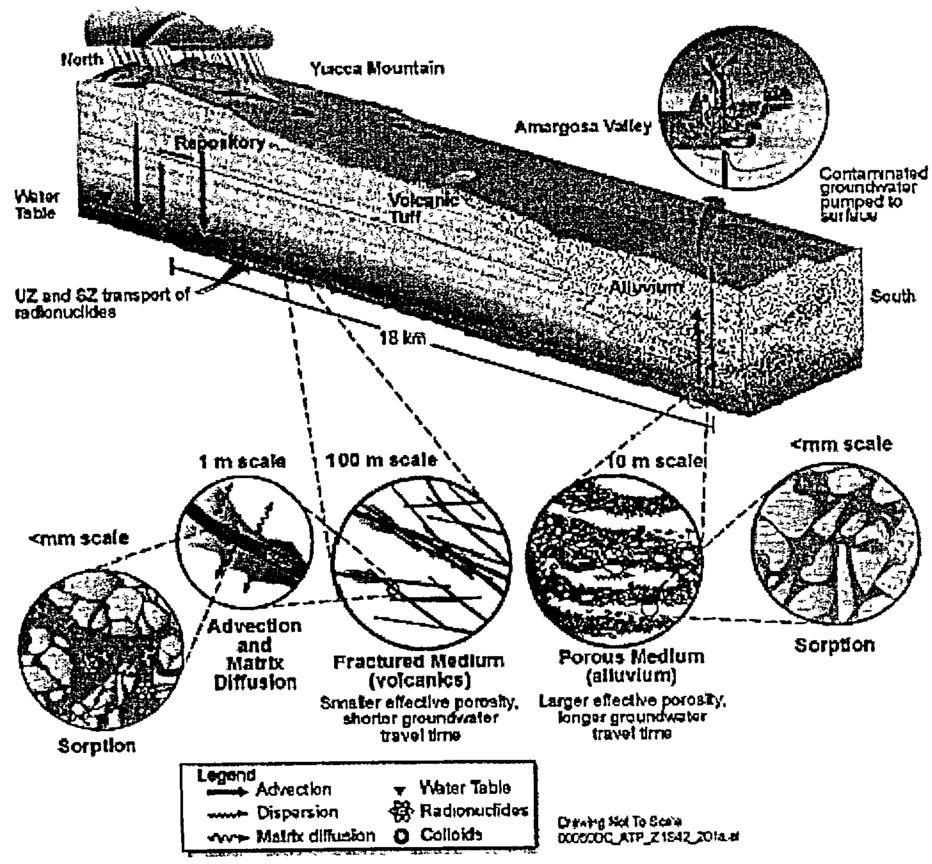


Figure 4-128. Conceptualization of Features and Processes Important to Saturated Zone Transport
This schematic illustration presents transport processes in fractured and porous media flow at Yucca Mountain, providing a conceptualization of transport through the saturated zone to the location of the reasonably maximally exposed individual in the Amargosa Valley. Moving groundwater carries (advects) dissolved or suspended radionuclides in fractures in the volcanic rocks and in pores between individual rock grains in the alluvium. The processes of diffusion and sorption slow the transport of radionuclides to the accessible environment. Radionuclides diffuse into and out of the unfractured portion (matrix) of the volcanic rocks. In the alluvium, radionuclides diffuse into and out of regions where water is stagnant or flows very slowly. UZ = unsaturated zone, SZ = saturated zone.

Summary

Goal is for a set of models that capture reality—important processes, controlling factors and performance relevant to conditions at Yucca Mountain.

Water Contacting Waste Package

Waste Package Lifetime

Releases from Waste Form and Alteration

Mobilization and transport of Radionuclides

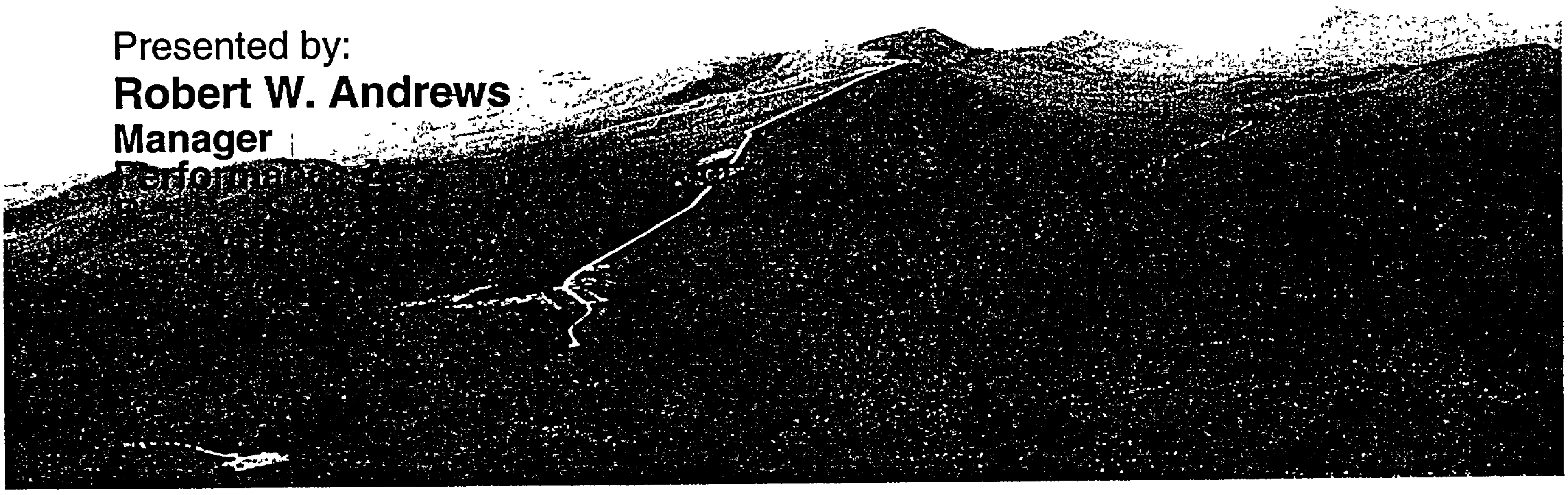
U.S. Department of Energy
Office of Civilian Radioactive Waste Management

YUCCA MOUNTAIN PROJECT

Elements of the U.S. Department of Energy Source Term Model for Total System Performance Assessment

Presented to:
Advisory Committee on Nuclear Waste

Presented by:
Robert W. Andrews
Manager

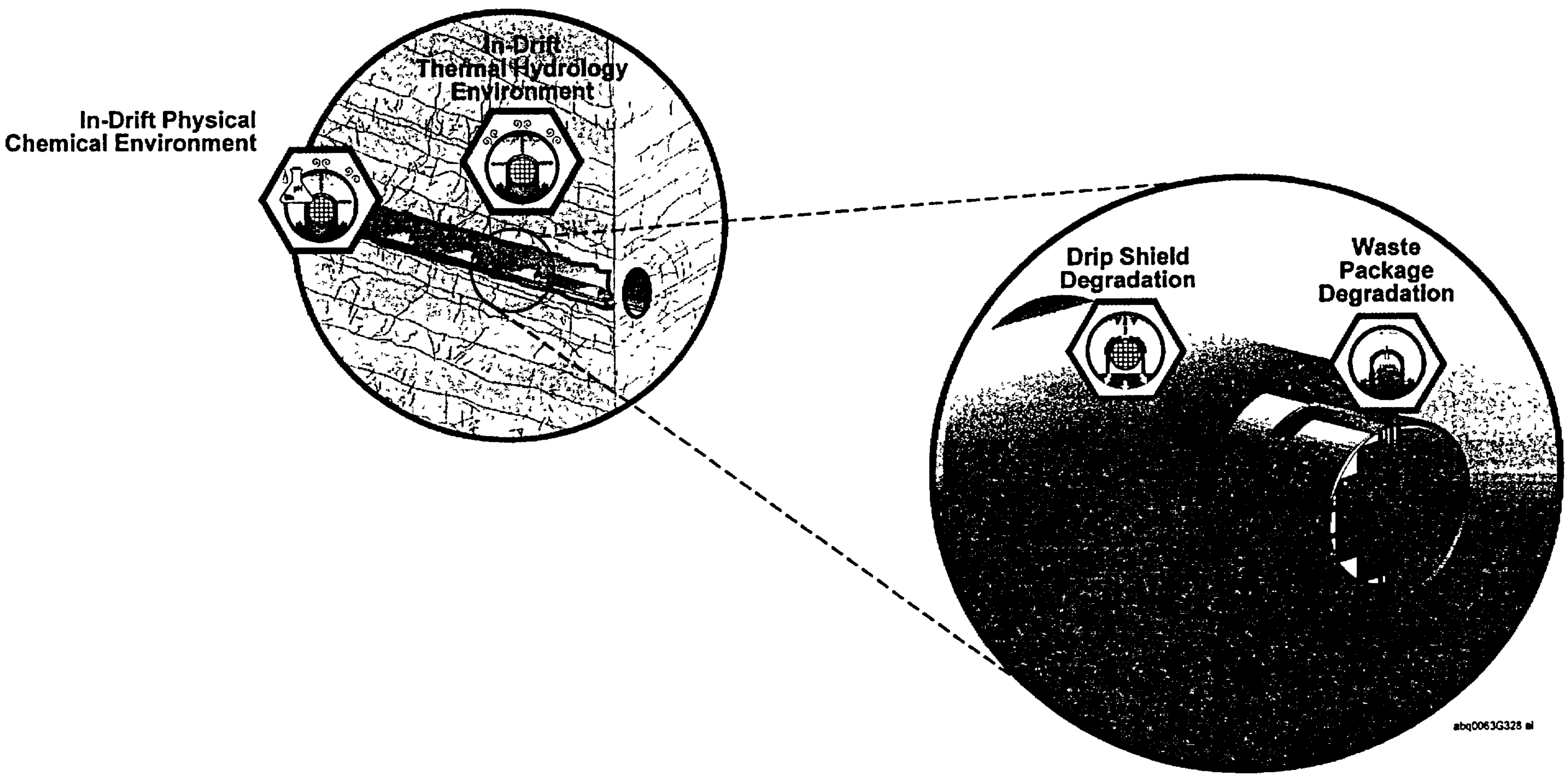


Outline

Factors Potentially Affecting the Total System Performance Assessment Source Term

- In-Drift Environment
  - Chemical, mechanical, thermal, hydrologic
- Drip Shield and Waste Package Degradation
  - General corrosion
  - Stress corrosion cracking
  - Improper heat treatment
- In-Package Environment
- Waste Form Degradation
- Waste Form and Engineered Barrier Radionuclide Release
- Summary and Conclusion

Components Related to the Source Term, Waste Package, and Drip Shield Degradation



Coupled Thermal Chemical Effects on Water Composition

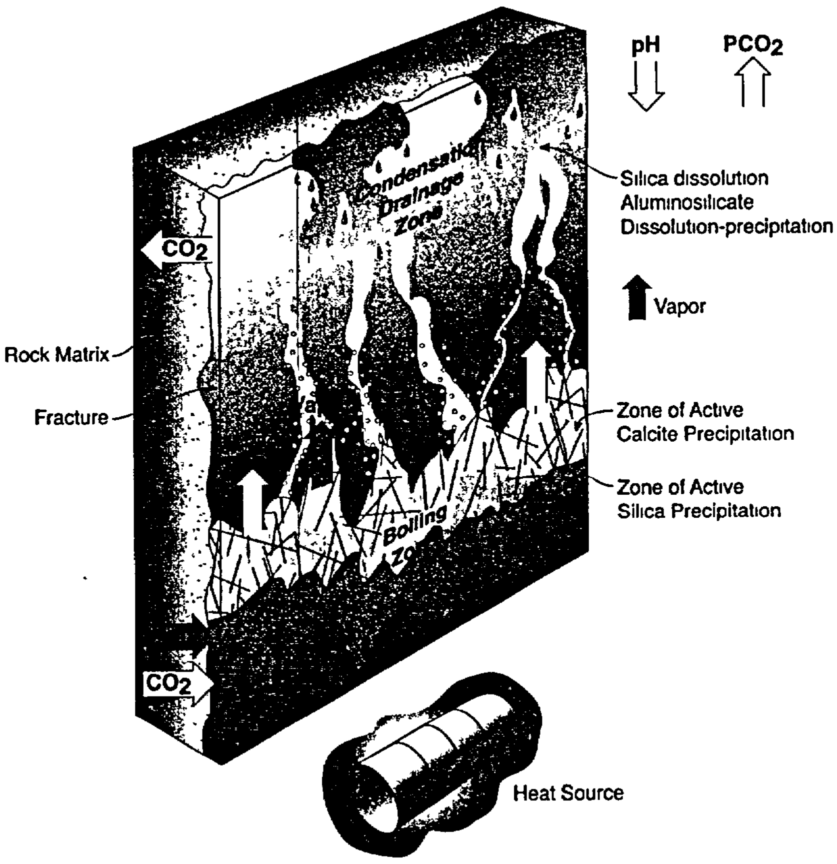
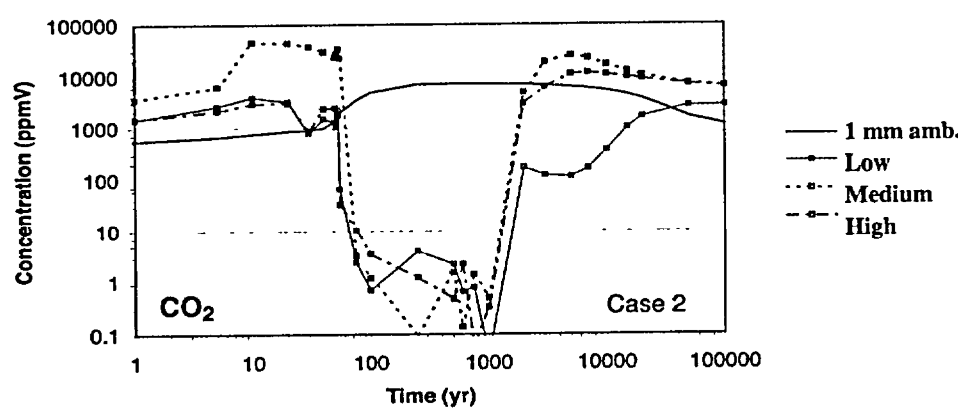


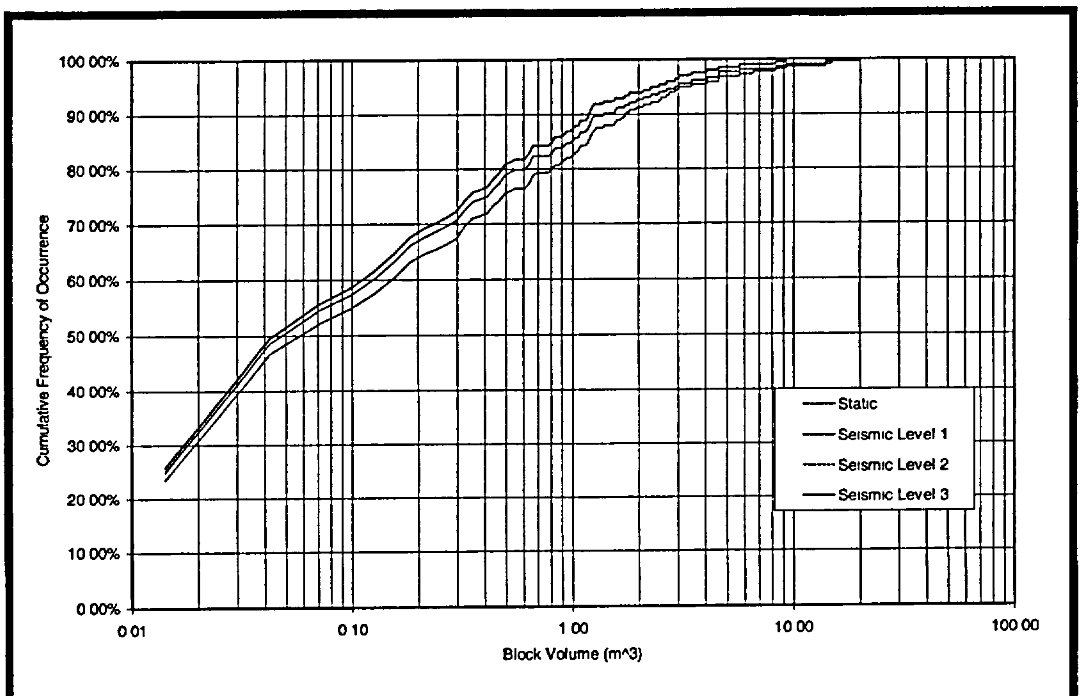
Diagram Showing THC Processes

- Incoming water and gas composition derived from coupled thermal-hydro-chemical model for a range of infiltration rates
- Model validated based on drift-scale heater test results
- Aqueous chemical constituents include CO_3^{-2}, pH, HCO_3^-, F^-, and Cl^-
- Gas composition considers CO_2 evolution over a range of infiltration rates



In-Drift Physical Environment
Mechanical Degradation by Rock Fall

- **Key-block analysis defines rock-fall size and frequency, which are a function of**
  - **Lithology**
  - **Joint strength**
  - **Drift orientation**
  - **Seismic level**
    - **1 (1,000 yr recurrence)**
    - **2 (5,000 yr recurrence)**
    - **3 (10,000 yr recurrence)**

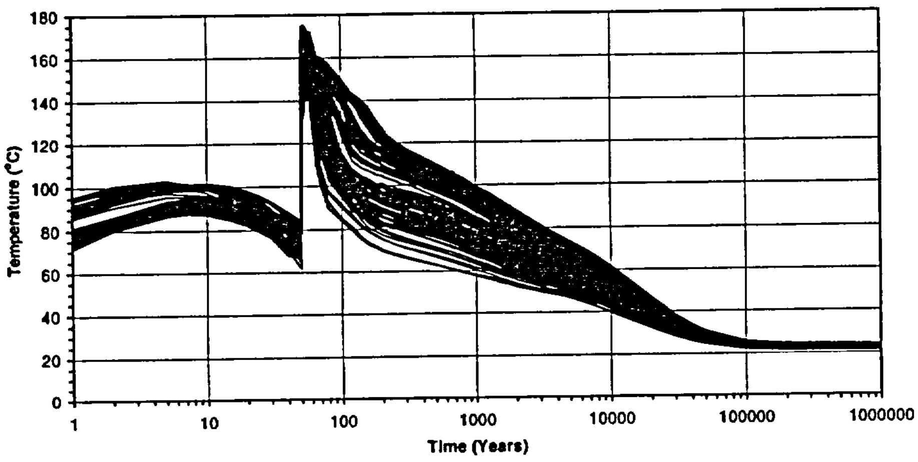


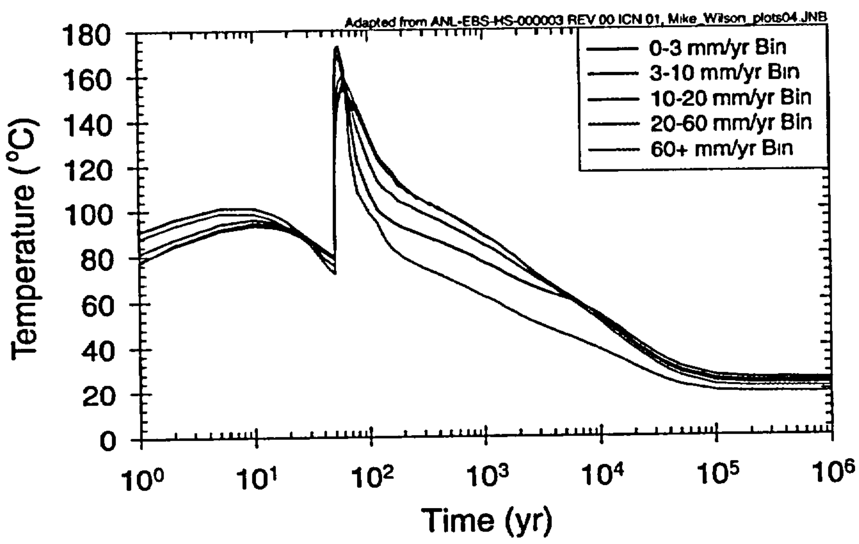
NOTE The seismic level 2 and seismic level 3 distribution curves are identical

- **Rock falls induce mechanical stress on drip shield but are insufficient to induce stress corrosion cracking of drip shield**
- **Rock fall assumed to occur after design life of drift support system**
- **Rock-fall model compared to analog information**

In-Drift Physical Environment

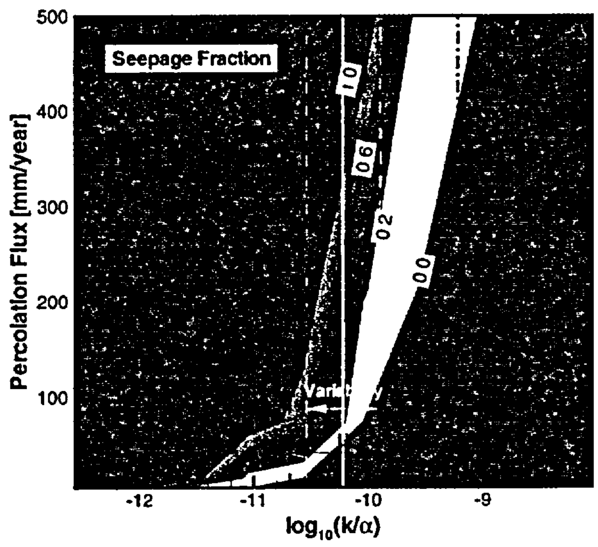
Temperature and Humidity

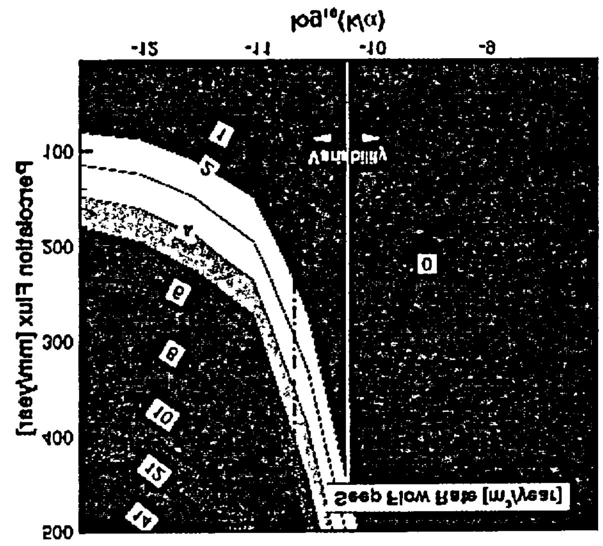




- Temperature and relative humidity on drip shield and waste package determined by repository design
  - Thermal load (areal and line)
  - Ventilation (rate and duration)
- Initiation of corrosion is a function of water composition, critical relative humidity, and deliquescent salts
- Model compared with drift scale test results

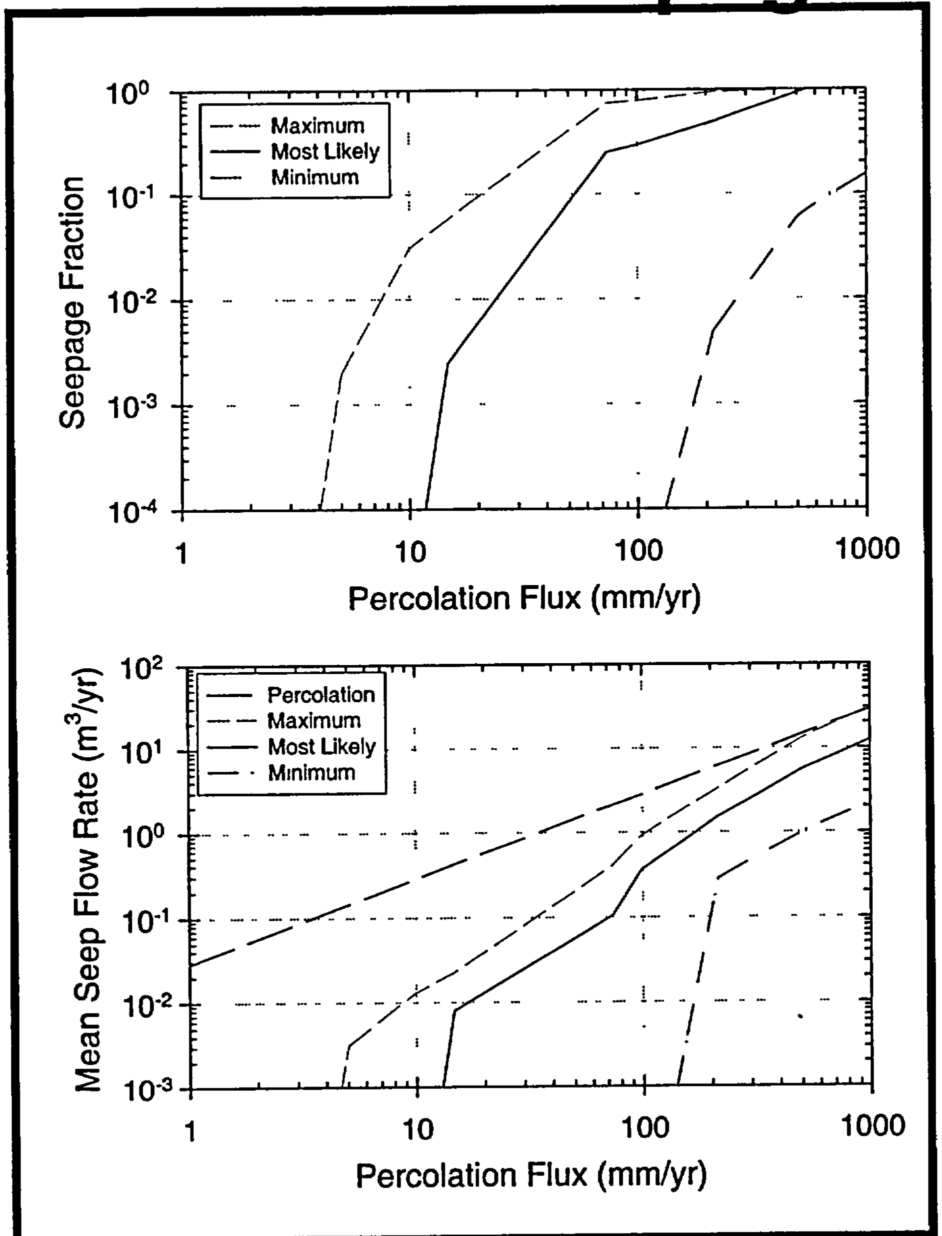
Seepage into Emplacement Drifts





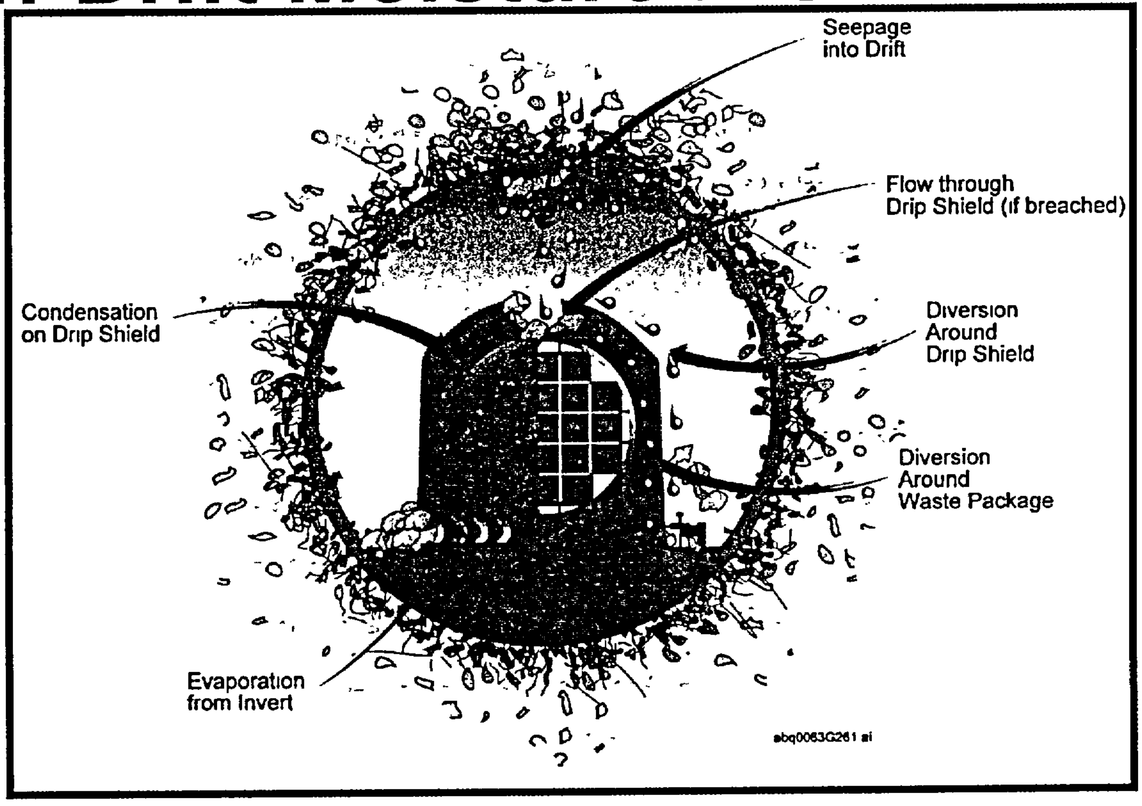
- Seepage model applied over range of fracture characteristics, drift shapes, flow focusing, and episodicity
- Seepage model validated using niche experiments in Exploratory Studies Facility
- Fracture characteristics (especially permeability (k) and capillarity ($^1/_\alpha$)) are uncertain and variable based on Exploratory Studies Facility tests
- Percolation flux from thermo-hydrologic model modified to account for flow focusing and episodicity

Seepage Abstraction



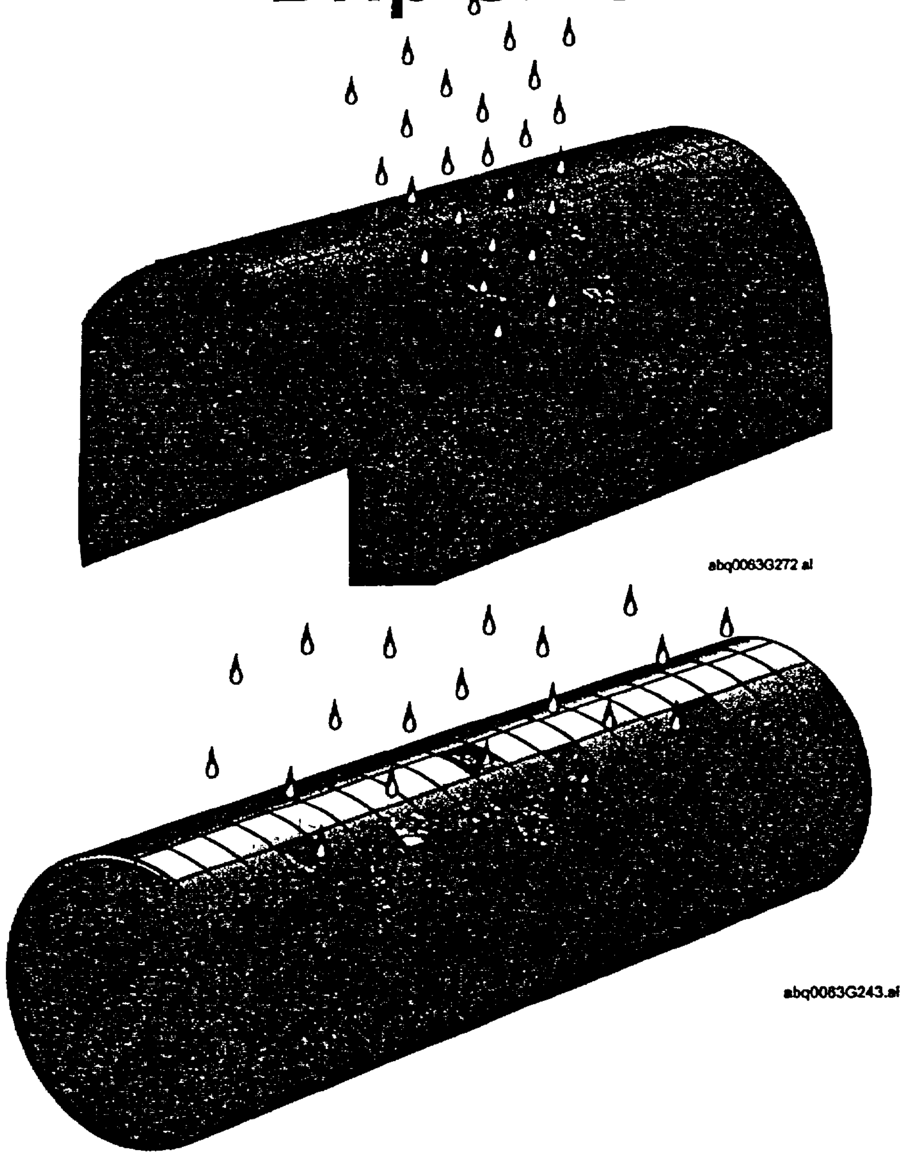
- Seepage fraction and seep flow rate are sampled from triangular distributions
- Seepage is calculated for 610 spatial locations and then averaged over five discrete infiltration bins
- Seepage fraction and seepage flow rate vary with climate state, which affects percolation flux

In-Drift Moisture Distribution



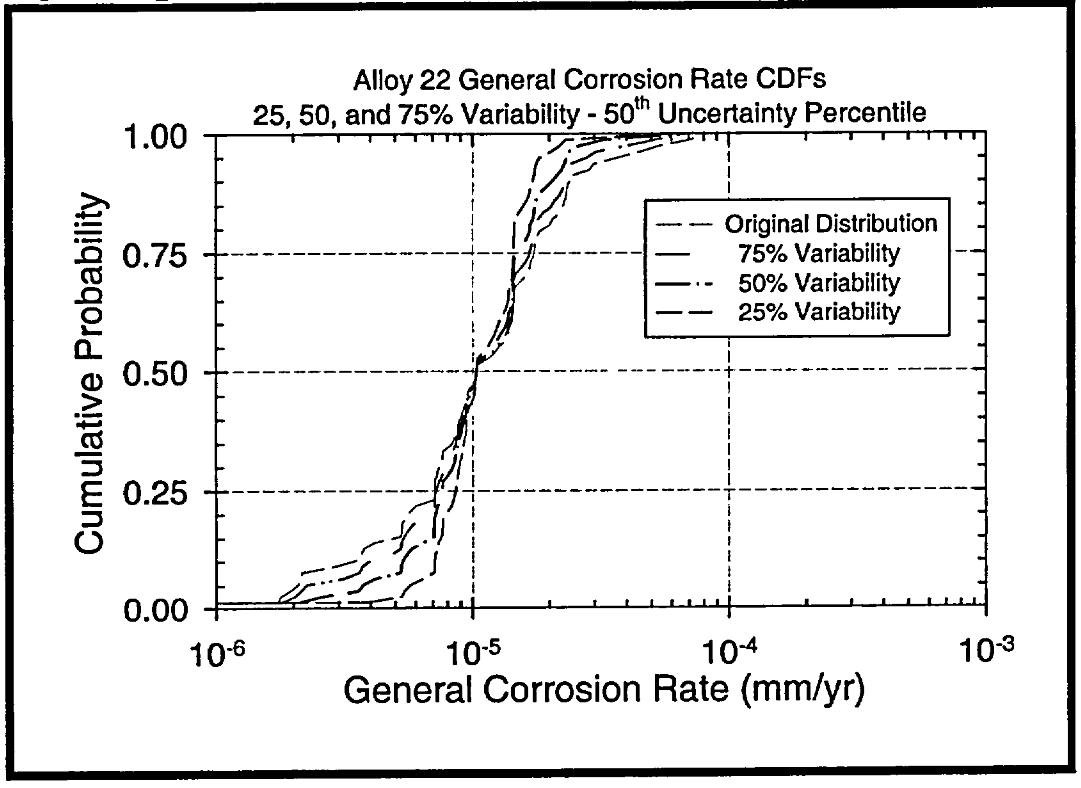
- **All seepage flux into drift assumed to contact drip shield**
- **Seepage flux through drip shield depends on area of drip shield degraded**
- **No credit taken for thermal gradient between commercial spent nuclear fuel, waste package and drip shield**

Implementation of Degradation Models for the Drip Shield and Waste Package



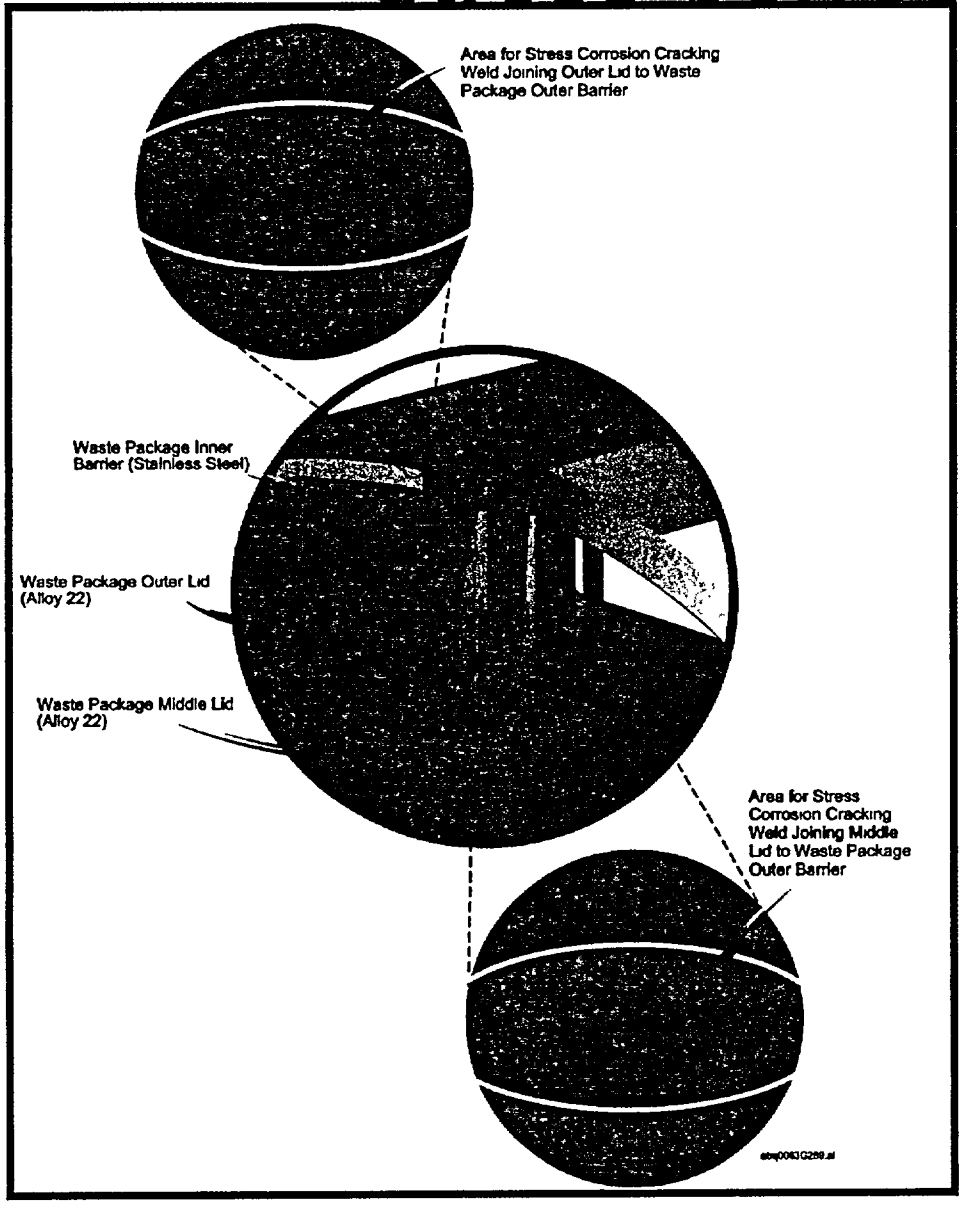
- Divide drip shield and waste package surface into patches
- General corrosion occurs dependent on relative humidity of deliquescent $NaHCO_3$
- Local corrosion model included but never invoked because critical potential > corrosion potential for expected environments based on cyclic polarization tests
- Stress corrosion cracking model dependent on stress state following stress mitigation at welds and failure criterion (% of yield)
- Early failures considered derived from possible improper heat treatment

General Corrosion of Waste Package



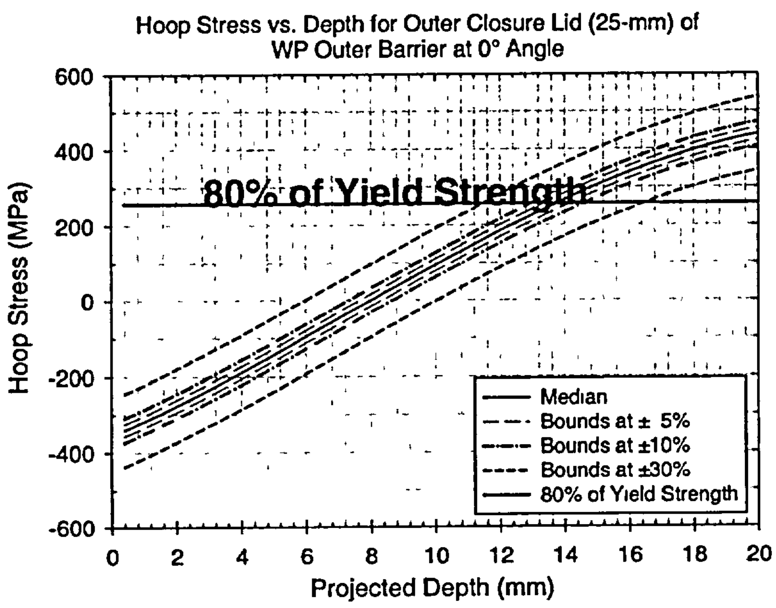
- Uncertainty and variability in rates considered based on 2-year data from long-term corrosion test facility
- Corrosion rates increased by up to 2x for microbiologically influenced corrosion effects and up to 2.5x for aging effects based on data from laboratory tests

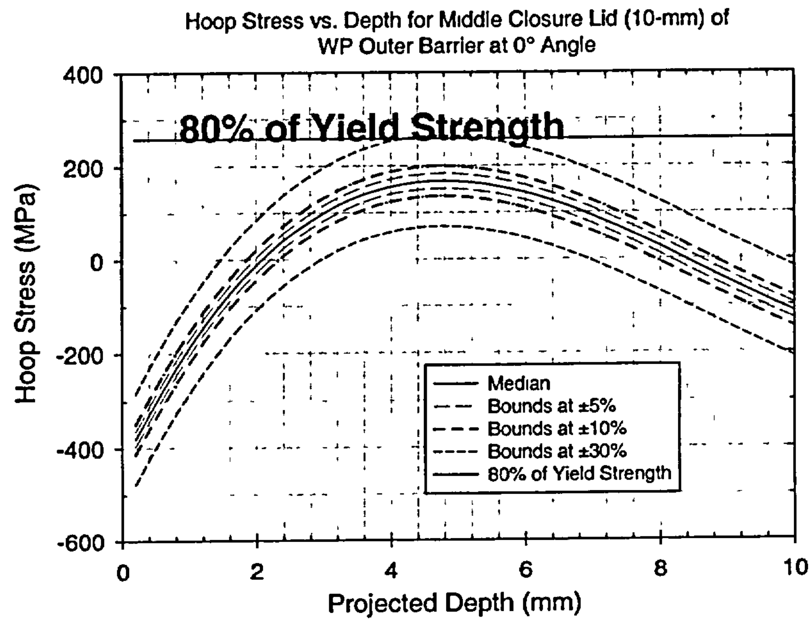
Stress Corrosion Cracking



- Occurs only in weld-region patches for outer and middle closure lids
- Stress corrosion cracking modeled using slip dissolution model
  - Rate of crack growth a function of
    - Stress intensity factor
    - Crack growth rate parameter
- Stress corrosion cracking requires stress at crack tip to be greater than stress threshold
  - Uncertainty in stress state (following stress mitigation) and yield stress evaluated
- Stress mitigation method was solution annealing for outer lid and laser peening for middle closure lid

Uncertainties Affecting Stress Corrosion Cracking Initiation





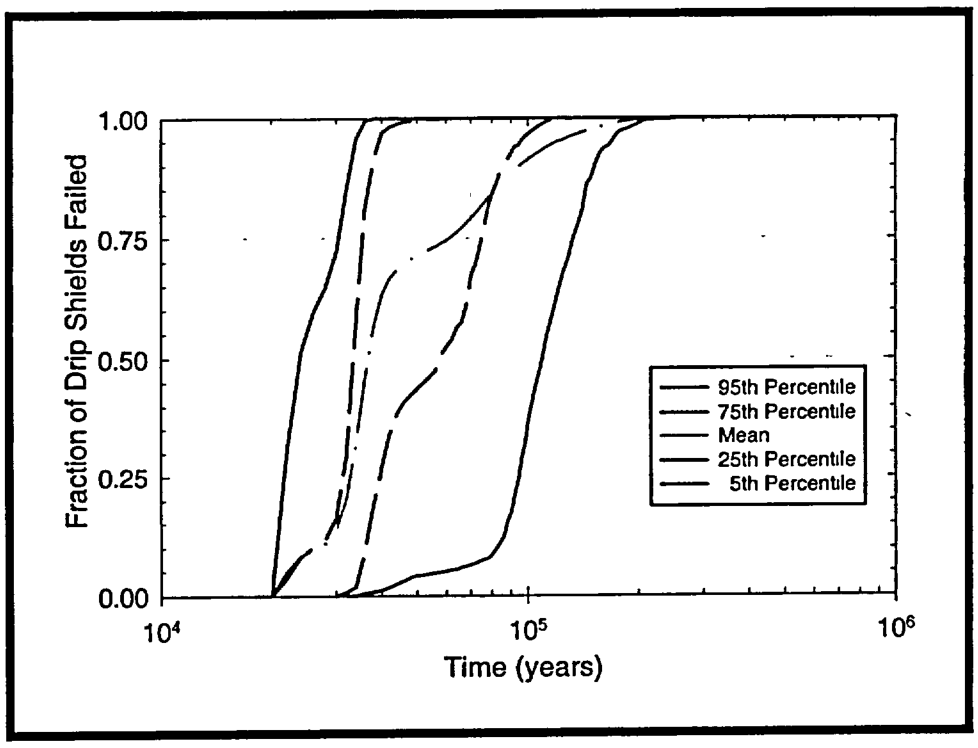
- **Total System Performance Assessment - Final Environmental Impact Statement model used stress value of 80% of yield as point where stress corrosion cracking could initiate based on laboratory testing**
- **Total System Performance Assessment - Final Environmental Impact Statement model included very small probability of stress corrosion cracking initiation of the inner closure-lid weld region**
- **Total System Performance Assessment - Site Recommendation used 20 to 30% of yield strength as the stress threshold (therefore stress corrosion cracking was initiated earlier in the Total System Performance Assessment - Site Recommendation model)**

Early Waste Package Failure Representation in Total System Performance Assessment - Final Environmental Impact Statement – Improper Heat Treatment

- Probability of undetected improper heat treatment (solution annealing) estimated to be ~ 2×10^{-5}
- For ~ 12,000 waste packages, expected number of improperly heat treated waste packages is ~ 0.26
- 20 out of 100 realizations have at least one waste package failed early, and 3 realizations have two waste packages failed early
- Assume affected waste package(s) fail immediately when corrosion initiates
  - Assume conservatively weld regions of both the outer and inner closure-lids of the outer barrier fail immediately
- Current approach will use laser peening instead of solution annealing

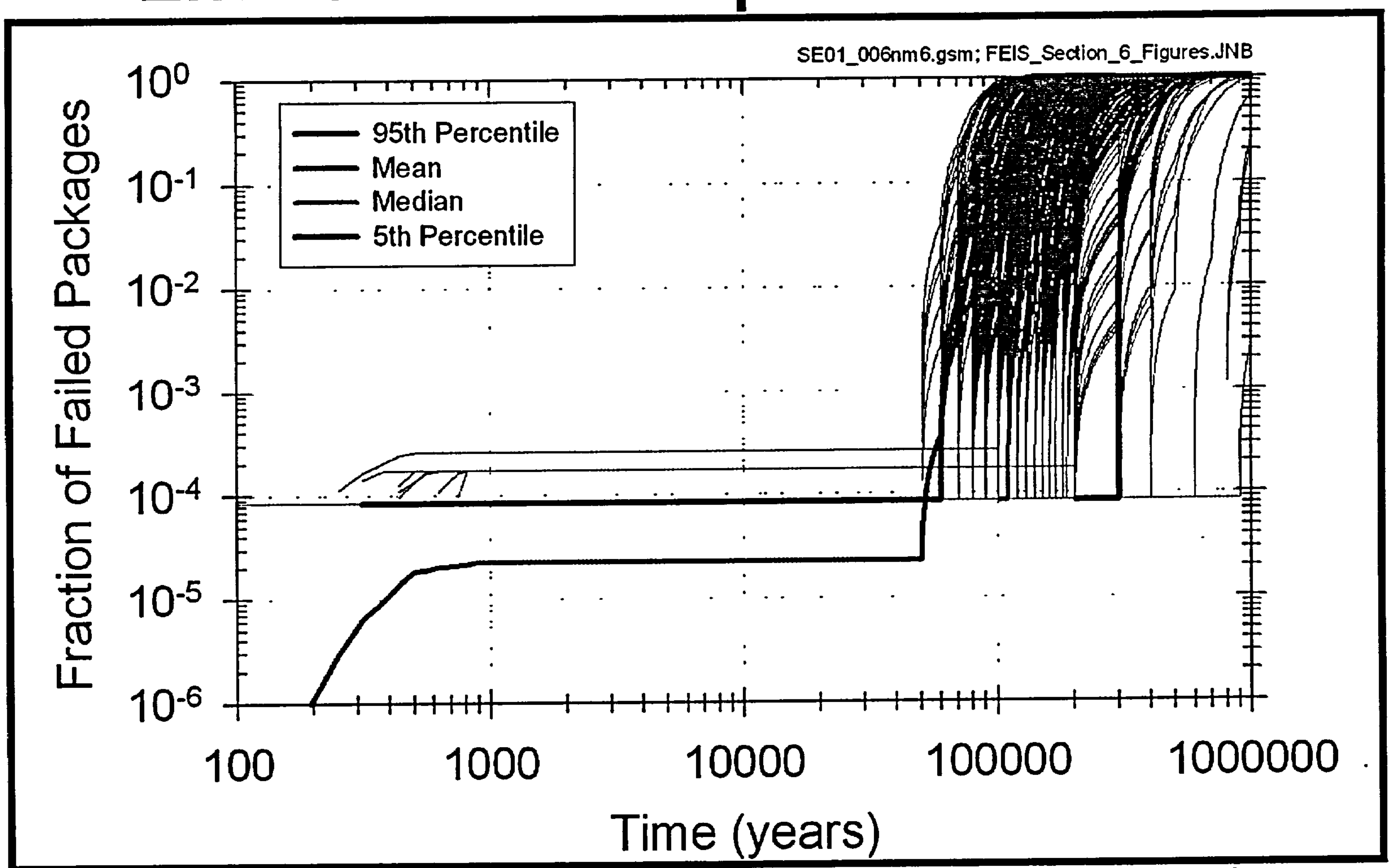
Calculated Cumulative Drip-Shield Failures

- The first drip-shield failures occur at about 20,000 years
- General corrosion only
- On average, most of the drip shields fail within 40,000 years and almost all fail within 100,000 years
- At the 95% probability level, almost all drip shields fail within 30,000 years

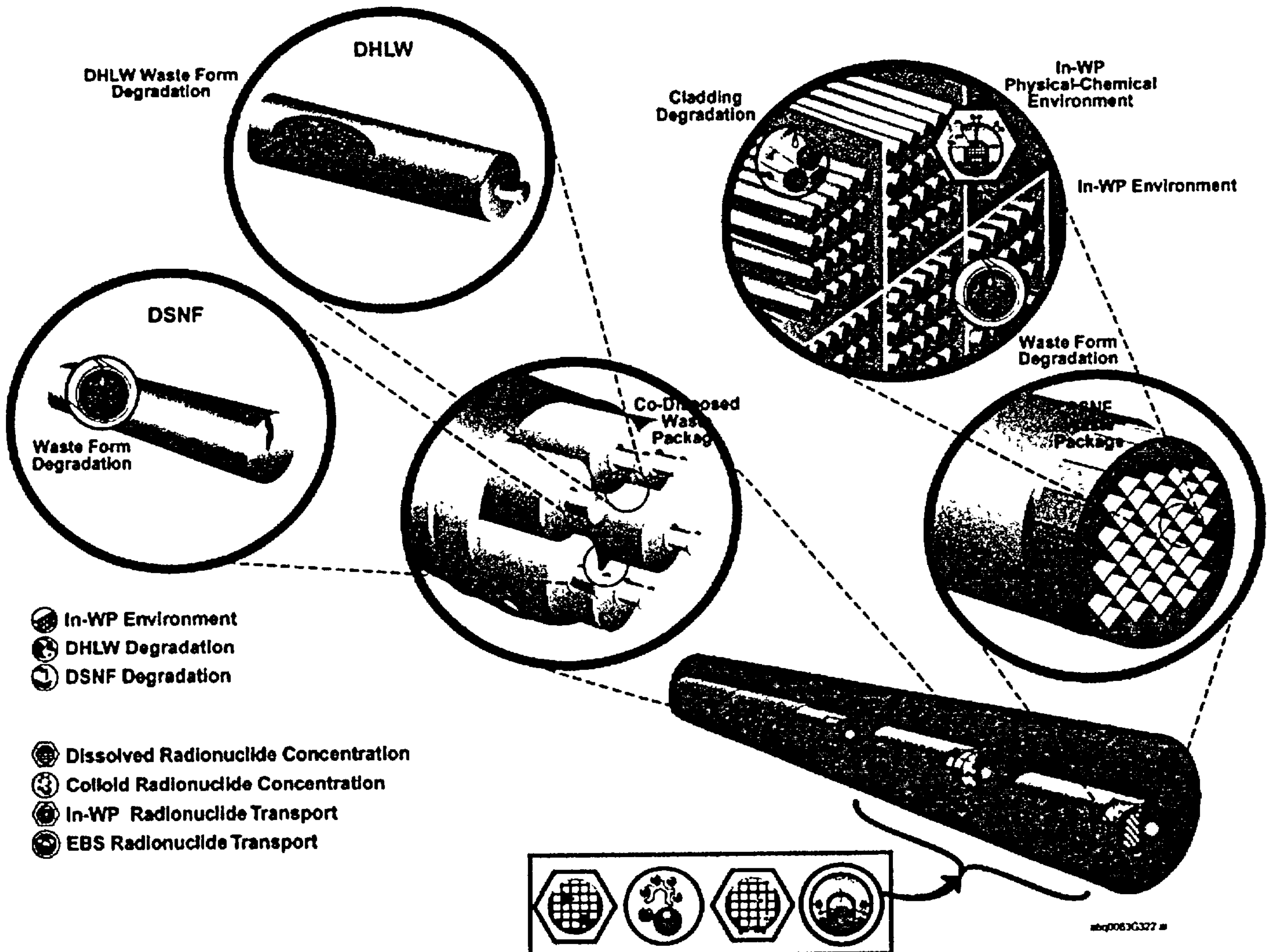


Total System Performance Assessment - Site Recommendation Nominal Performance

Fraction of Failed Waste Package for the Total System Performance Assessment - Final Environmental Impact Statement

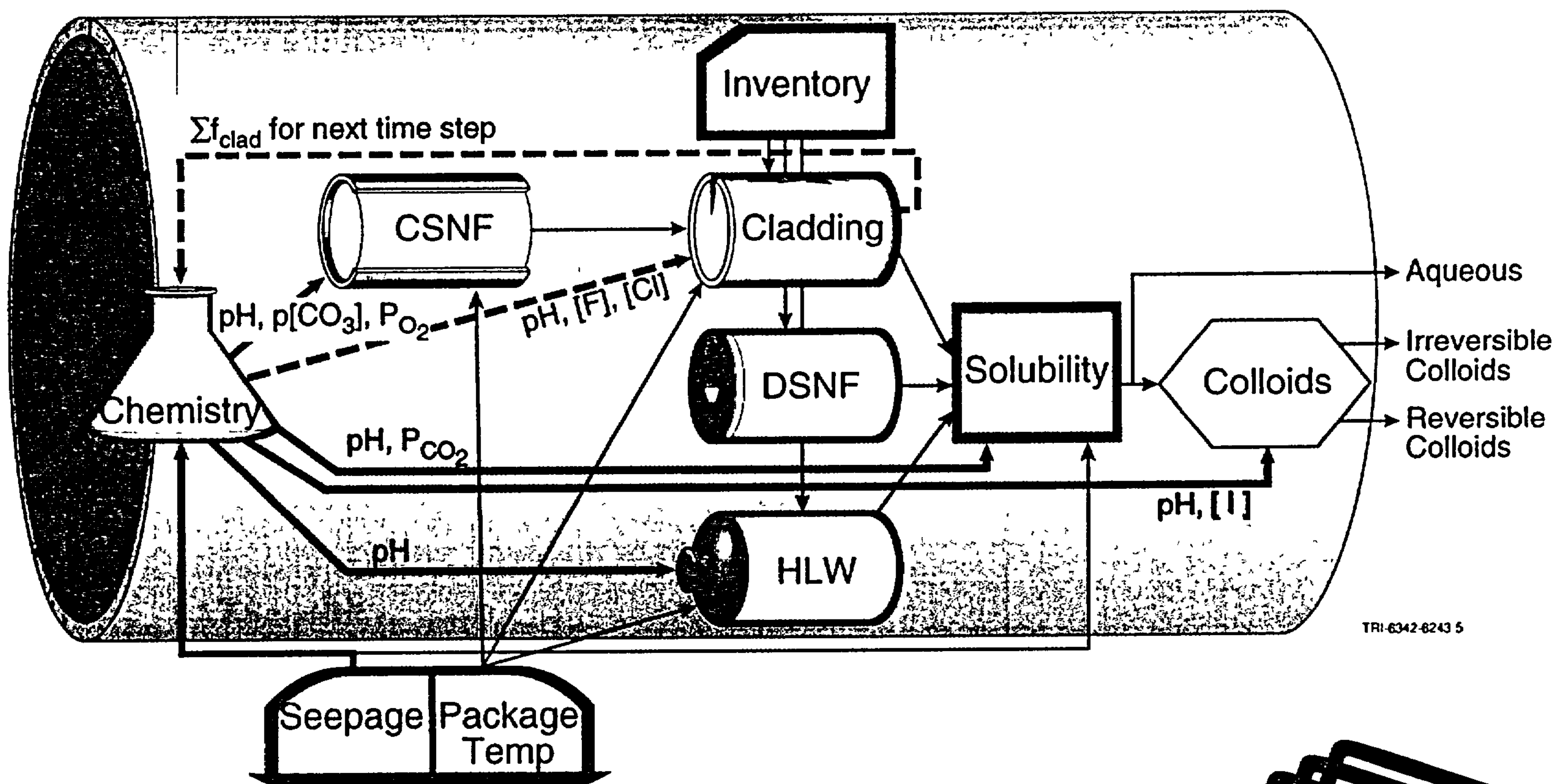


Components Related to the Source Term Radionuclide Release from the Waste Form



Waste Form Degradation Model in Total System Performance Assessment-Site Recommendation Consists of Eight Components

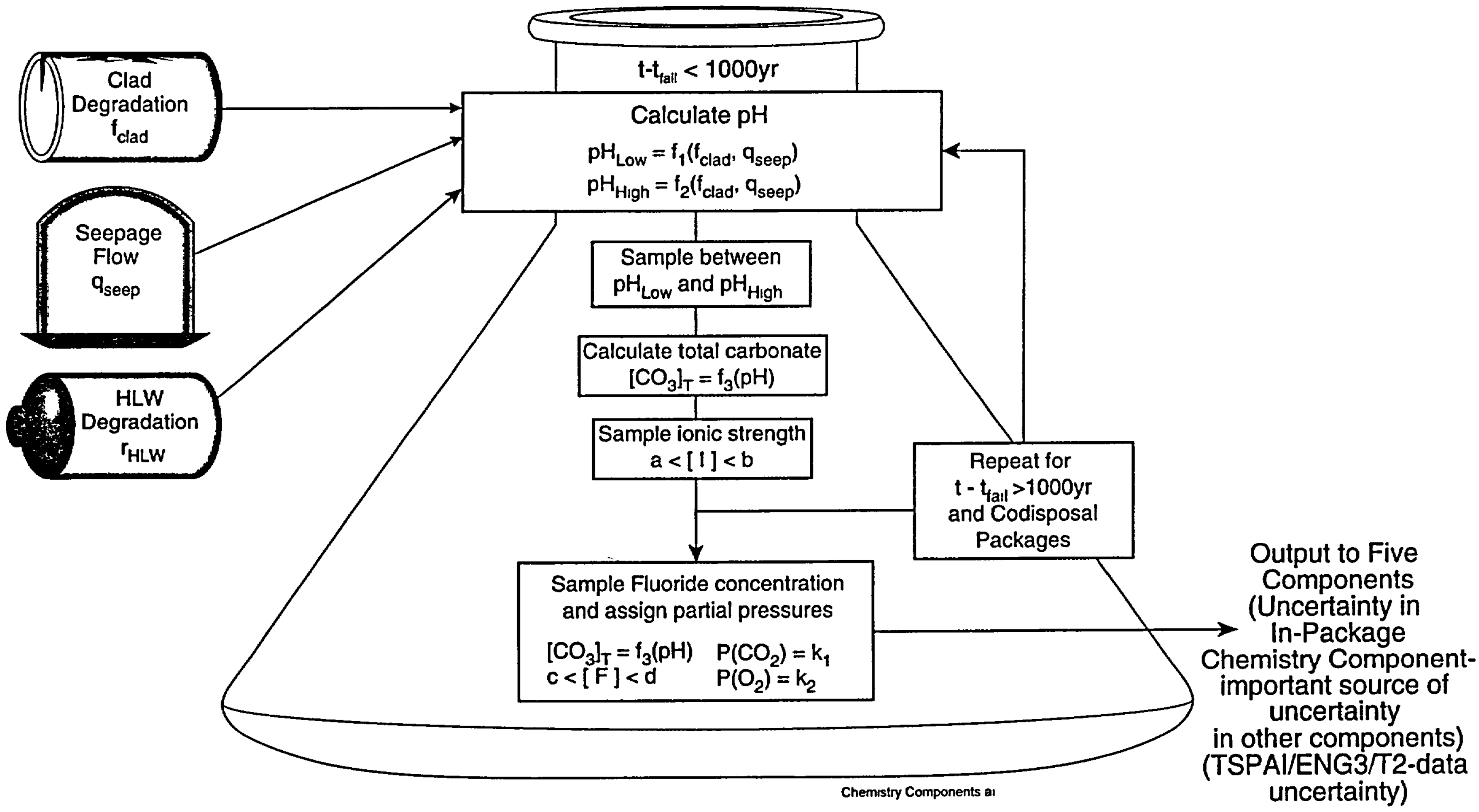
Chemistry component coordinates conditions for other components



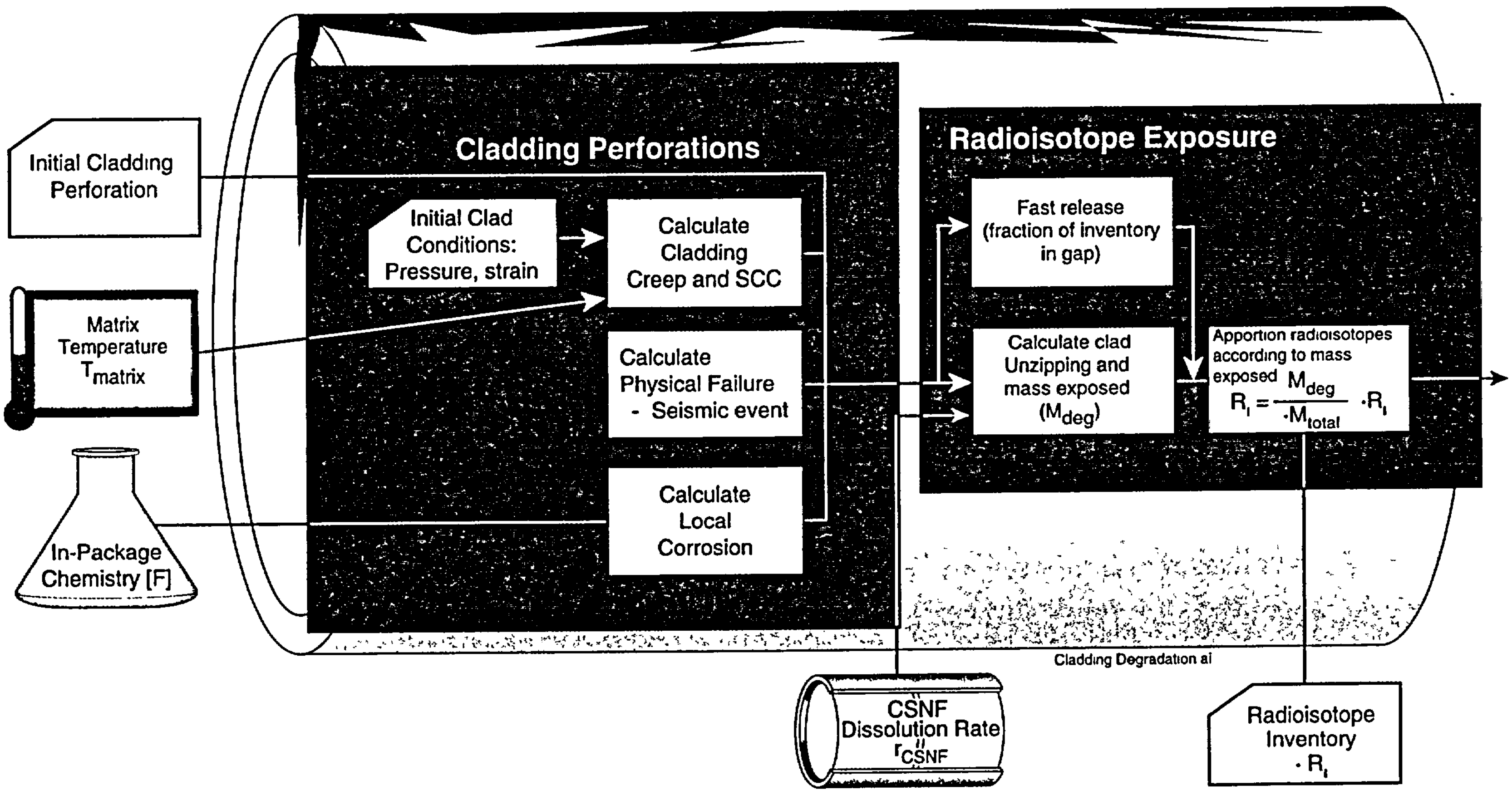
Technical Bases of In-Package Chemistry Component

- Cladding, high-level waste, and basket (e.g., stainless steel) degradation rates, and fixed gas pressures (CO_2 and O_2) control bulk chemistry (pH, $[CO_3^{-2}]_T$, [I], $[Cl^-]$,and $[F^-]$)
  - Degradation rates of basket and high-level waste evaluated in uncertainty
- Bulk chemistry approximated by well mixed, oxidizing conditions
  - Localized chemistry effects on cladding degradation (including the effects of radiolysis) not included, except for F^- flux
- Chemical condition in waste package dominates effect of incoming chemistry
  - Influence of evaporation evaluated
  - Influence of cement evaluated in features, events, and processes analysis

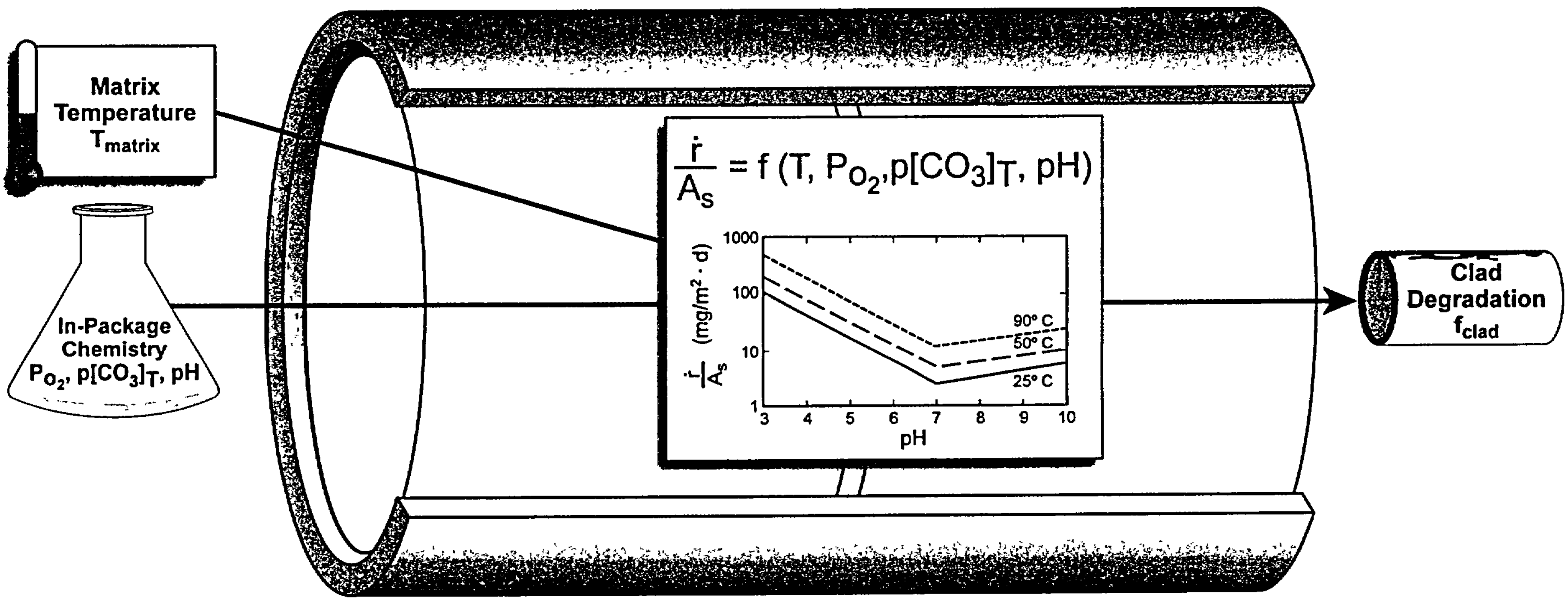
In-Package Chemistry Component Estimates pH, Calculates $[CO_3^{-2}]_T$, and Samples [I] and $[F^-]$



Cladding Degradation Consists of Two Steps Perforation and Unzipping



Commercial Spent Nuclear Fuel Matrix Degradation Component Based on Regression of Laboratory Experiments

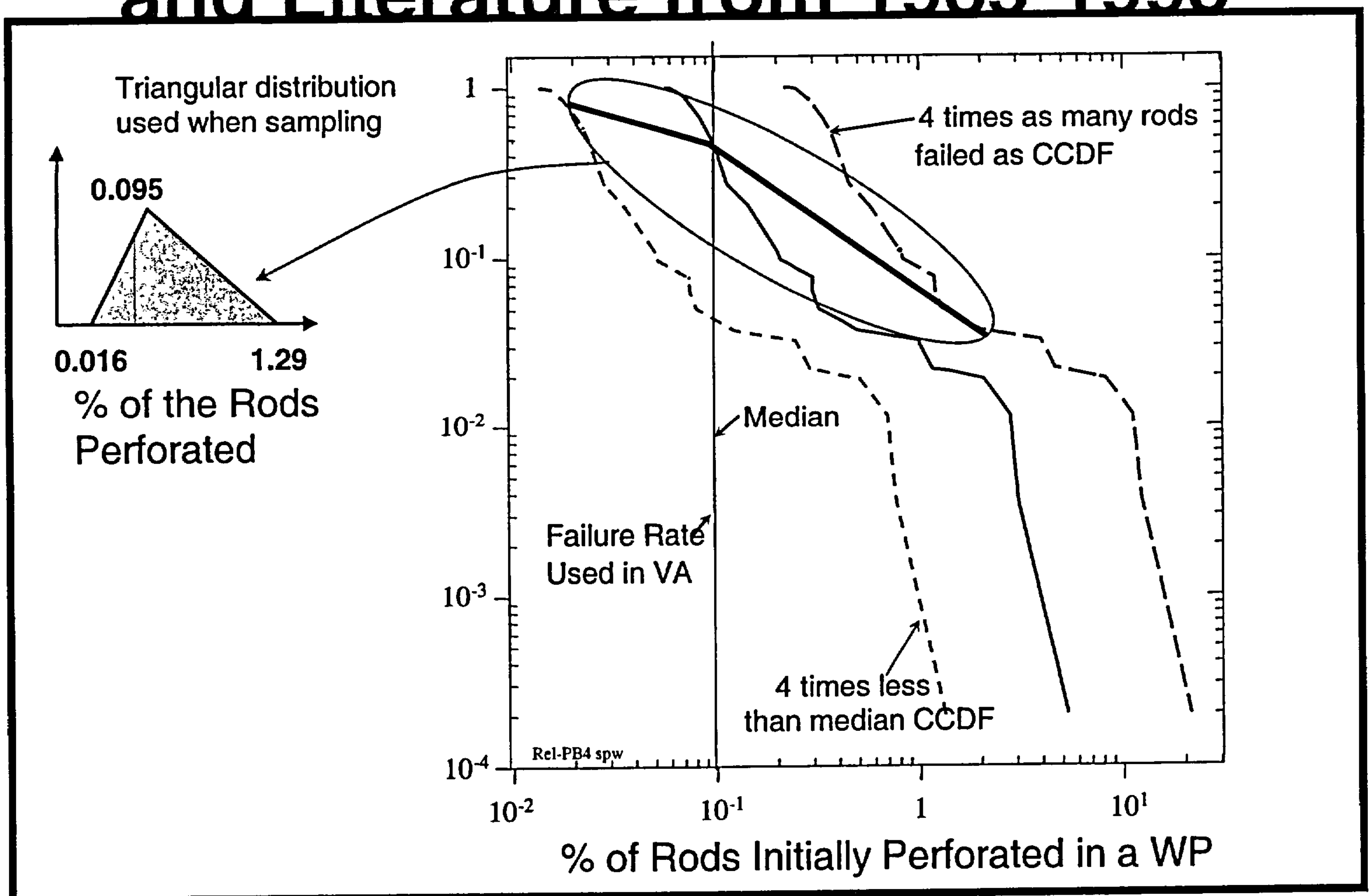


00185DR_Figure 4 ai

Figure Modified From
000200C-WFD-PMR-18-M&O Graphics/LV.ai

Drawing Not To Scale
CSNF Degradation Model.ai

Cladding Perforations before Receipt based on NRC Contractor Report (1969-1985) and Literature from 1985-1995



YUCCA MOUNTAIN PROJECT

Radionuclide Inventory

Nominal Performance

^{14}C, ^{99}Tc, ^{129}I, ^{227}Ac, ^{229}Th, ^{230}Th, ^{231}Pa, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{210}Pb, ^{226}Ra

Direct Release (volcanic eruption)

Above, plus ^{90}Sr, ^{137}Cs, ^{232}U

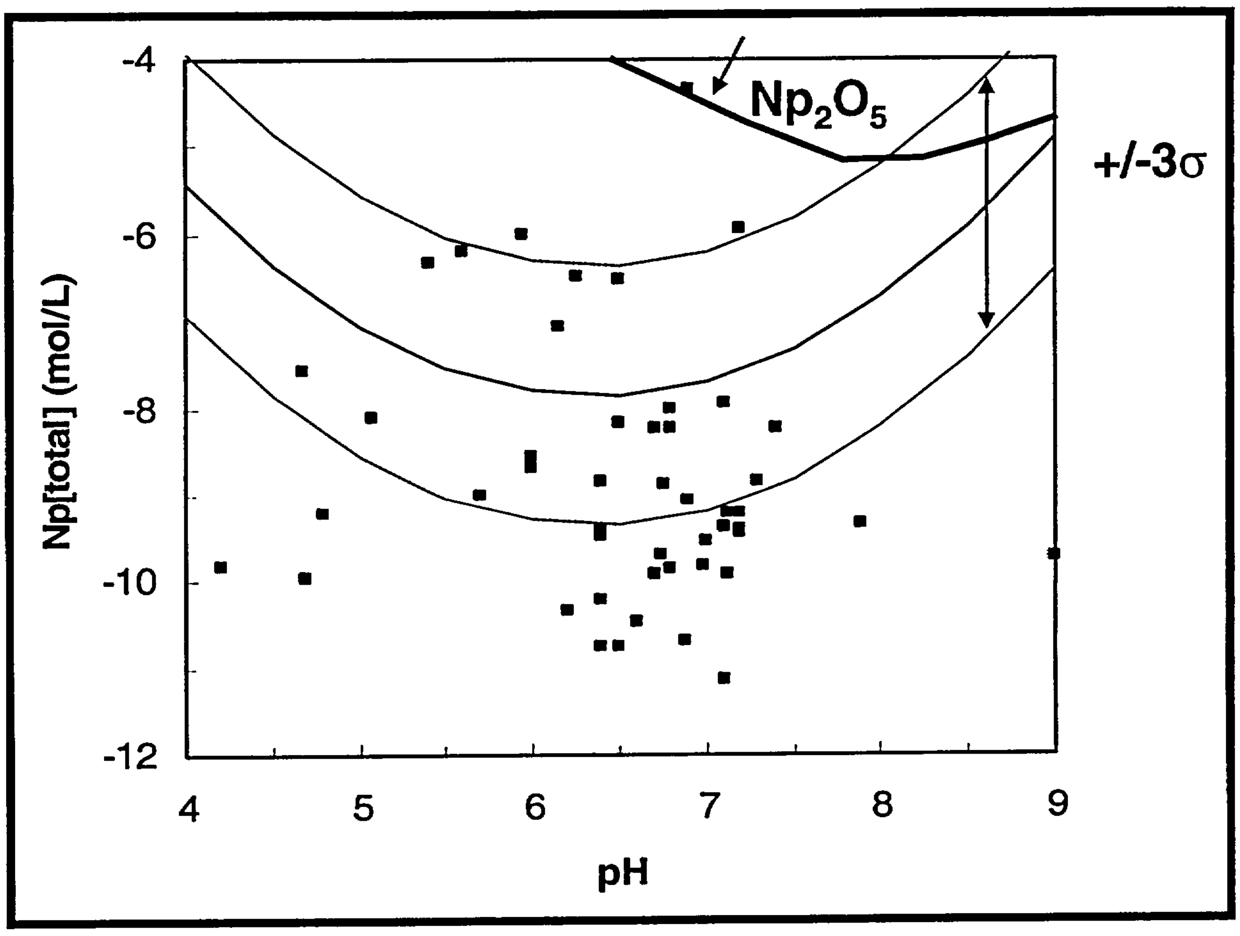
Human Intrusion

Above, plus ^{90}Sr, ^{137}Cs

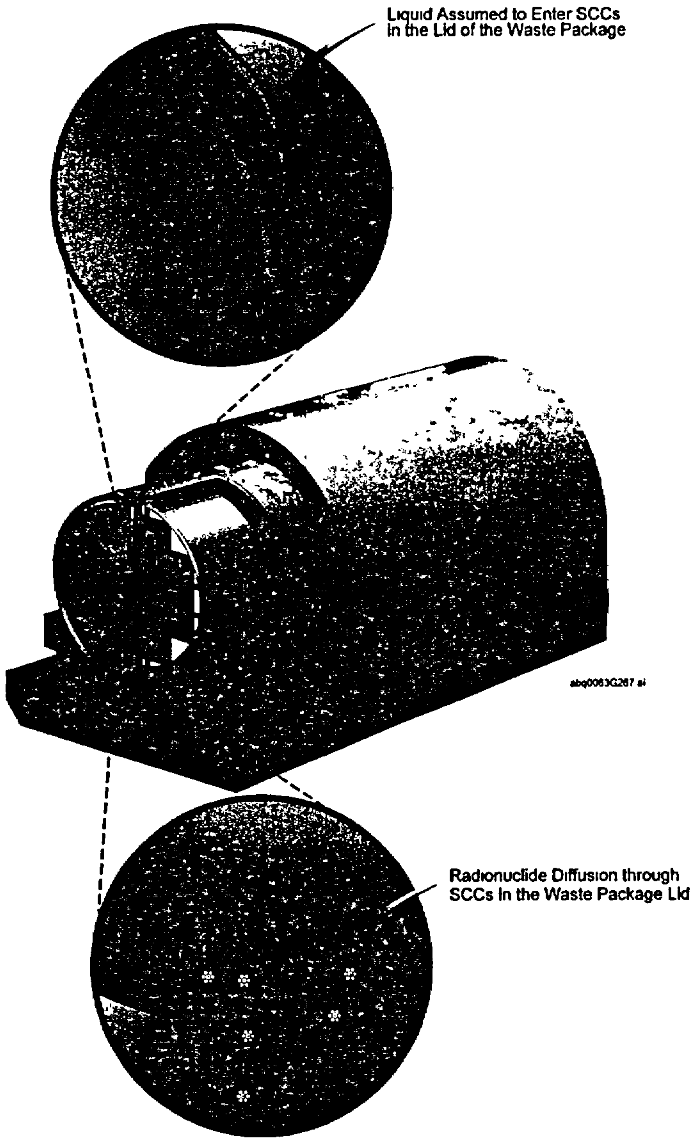
- Radionuclide suite depends on scenario
  - Parents and intermediate daughters of chains are included
  - Human intrusion and volcanic eruption scenarios require additional nuclides be included
- Radionuclide suite also depends on performance measure
  - Ground-water protection requires some additional nuclides, e.g., ^{228}Ra and ^{232}Th

Np Dissolved Concentrations

- Distribution based on laboratory data
- Conservatively selected pure phases to control solubility
- Conservatively fixed gas pressures CO_2, O_2 at atmospheric conditions
- Conservatively neglect sorption or coprecipitation of radionuclides



Engineered Barrier System Radionuclide Transport



- **Releases for most locations will occur by diffusion only, if**
  - **Little or no water seeps into drift**
  - **Little or no water seeps through drip shield**
  - **Little or no water condenses under drip shield**
  - **Only small cracks (stress corrosion cracking) in waste package**
- **Advective releases require flux to seep into drift, through degraded drip shield and degraded waste package**
- **Possible in-package evaporation of seepage into waste package for commercial spent nuclear fuel waste packages conservatively ignored**

Summary of Potential Differences Between the DOE and NRC Source Term Models

- **In-Drift Environment**
  - Fraction of repository with seeps
- **Drip Shield and Waste Package Degradation**
  - Fraction of degraded drip shields and waste packages due to improper placement, rock fall, seismic events
  - Degradation rate of Titanium and Alloy 22
  - Treatment of uncertainty and variability in degradation rates
  - Treatment of conditions potentially initiating localized corrosion of drip shield (F^-) and Alloy 22

Summary of Potential Differences Between the DOE and NRC Source Term Models

(Continued)

- **In-Package Environment**
  - Cladding degradation rates
  - Fraction of exposed waste that is contacted by moisture (available for diffusive transport) versus contacted by seepage flux (available for advective transport)
  - Chemical environment
- **Waste Form and Engineered Barrier System Mobilization and Transport**
  - Alteration rate of various waste forms
  - Solubility of radionuclides
  - Advective versus diffusive transport

Backup

Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Backup - Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Engineered Barrier System Environments

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

Backup - Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Drip Shield and Waste Package Degradation

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Waste Package Lifetime	Drip Shield Degradation and Performance	• Probability of material and manufacturing defect flaws in drip shield • Size of material and manufacturing defect flaws in drip shield • Probability and size of rockfall induced by seismic activity • Threshold for general corrosion initiation • General corrosion rate under drip and no-drip conditions • Crevice corrosion initiation threshold • Probability (or area) of crevice formation on drip shield • Stress and stress intensity factor profile in drip shield • SCC initiation threshold • SCC crack growth rate • Effect of material and manufacturing defects on SCC initiation and crack growth rate • Effect of rockfall damage on SCC initiation and crack growth rate • Hydrogen concentration profile in drip shield • HIC initiation threshold • Penetration opening size by general corrosion, localized corrosion and SC
	Waste Package Degradation and Performance	• Probability of material and manufacturing defect flaws in waste package • Size of material and manufacturing defect flaws in waste package • Threshold RH for general corrosion initiation under drip and no-drip conditions • General corrosion rate under drip and no-drip conditions • Crevice corrosion initiation threshold of WP outer barrier • Penetration opening size by general corrosion, localized corrosion and SCC • Stress and stress intensity factor profile at closure welds • SCC initiation threshold • SCC crack growth rate • Effect of material and manufacturing defect on SCC initial and crack growth rate • MIC factor on corrosion rate • Kinetics phase instability processes in base metal and weld • Aging factor on corrosion rate

NOTE: HIC - Hydrogen-Induced Cracking
MIC - Microbiologically Influenced Corrosion
SCC - Stress Corrosion Cracking
SC - Stress Corrosion
WP - Waste Package

Backup - Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Radionuclide Release From the Engineered Barriers

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

NOTE:
CSNF - Commercial Spent Nuclear Fuel
DSNF - Defense Spent Nuclear Fuel
EBS - Engineered Barrier System
HLW - High Level Waste