U.S. DEPARTMENT OF ENERGY
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

NUCLEAR WASTE TECHNICAL REVIEW BOARD
JOINT PANELS ON HYDROGEOLOGY & GEOCHEMISTRY
AND STRUCTURAL GEOLOGY & GEOENGINEERING

SUBJECT: TOTAL SYSTEM PERFORMANCE ASSESSMENT UPDATES

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Outline

• Review key elements of isolation argument and potential effects of alternate thermal loads
• Summarize fundamental thermo-hydrologic assumptions affecting TSPA-1993 results
• Present additional sensitivity analyses of TSPA-1993 results
• Describe revisions to TSPA-1993 using preliminary drift-scale thermo-hydrologic analyses
• Present plans for TSPA-1995
Key Components of Waste Isolation Argument at Yucca Mountain

- Dry environment within engineered barriers
- Robust engineered materials for those packages contacted by liquid water/humid air
  - Waste package and zircaloy cladding
- Slow dissolution of waste matrix due to limited availability of water and low solubility of radionuclides
- Slow release of radionuclides through the engineered barrier due to limited water
- Slow release of radionuclides through the geosphere

[modified from NWTRB briefing by J. Younker October 12, 1994]
Potential Effects of Thermal Load on Key Components of Waste Isolation Argument

- Thermo-hydrologic regime within drifts
  - “Dryness” of environment around engineered barriers
- Initiation of aqueous corrosion
  - Dependent on temperature and humidity environment
- Rate of aqueous corrosion
  - Dependent on temperature and humidity environment
- Rate of waste-form dissolution
  - Dependent on temperature and liquid saturation
- Radionuclide solubilities in liquid water
  - [Depends more on geochemical environment]
- Adveective and diffusive flux rates
  - Dependent on temperature and liquid saturation
Fundamental Thermo-Hydrologic Assumptions Affecting Waste-Package Failures in TSPA-1993

- Near-field temperatures and saturations based on panel-scale T-H model
  - Represents “average” T-H response
  - Accounts for spatial variability in T-H response
  - Under-predicts expected waste-package temperature
  - Over-predicts expected drift-scale saturations

- Either temperature or liquid saturation criterion assumed to initiate corrosion
  - Neglects drift-scale T-H response
  - Initiates aqueous corrosion conservatively early

- Pitting corrosion rates considered to be temperature-dependent
  - Leads to very conservative (high) corrosion rates for saturation initiation
Other Fundamental Assumptions Affecting Waste Package Failures in TSPA-1993

- Pitting corrosion rate of mild steel evaluated with two different models:
  - One (Stahl) assumed rate increased with increasing temperature and decreased with time
  - Other (Lamont) assumed rate independent of time and was a maximum at about 70°C
  - For assumed saturation initiation, leads to very conservative (high) corrosion rates
Other Fundamental Assumptions Affecting Waste Package Failures in TSPA-1993

(continued)

- Pitting corrosion rate of corrosion-resistant material evaluated with two different models
  - Deterministic model (Stahl) assumed extremely high rates
  - Stochastic model (Lamont) assumed high rates at high temperatures (~96°C) and 100x decrease at 70°C
  - Stochastic model combined with very high corrosion rate of mild steel
  - Combined effects led to very conservative corrosion rates for most packages

- Degradation of cladding assumed to be congruent with corrosion-resistant material

- Waste package (+cladding) failure distribution
- **Entire** waste package surface assumed to be degraded at time of failure
  - Failure conservatively defined by first pit penetration
  - Increased surface area allows greater diffusive releases
- Thermally perturbed advective fluxes evaluated at panel scale
  - Considered spatial distribution
  - Neglects capillary barrier effect in the drift
- **Entire** waste-form surface assumed to be exposed and contacted by liquid water film at time of failure
  - Neglects capillary barrier effect in the drift
• Dissolution rates and solubility limits considered to be temperature-dependent
  – Based on laboratory observations at PNL/LLNL and LBL/LANL

• Diffusion coefficients through waste package and backfill (invert) based on average rock water contents from panel-scale T-H model
  – Neglects capillary differences between rock and backfill
Objectives of Additional Sensitivity Analyses on TSPA-1993

- Complete sensitivity analyses of temperature-based corrosion initiation criterion
- Correct advective flux through waste package for 114 kW/acre case
- Evaluate effect of a different thermal load
  - 87 kW/acre
- Compare HLW versus spent fuel releases
- Compare alternate waste package designs
  - SCP, 6 PWR MPC, 21 PWR MPC
- Initiate sensitivity analyses of peak EBS release rates
- Initiate evaluation of drift-scale T-H analyses
- Prepare for TSPA-1995
Summary of TSPA-1993 Waste Package Failures*:
Sensitivity to Thermal Load, Waste Package Thickness,
and Corrosion Initiation Criterion

<table>
<thead>
<tr>
<th>Thermal Load (kW/Ac)</th>
<th>Outer Thickness (cm)</th>
<th>Corrosion Initiation Criterion</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.5</td>
<td>10</td>
<td>Sat</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>Temp</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>Sat</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>Temp</td>
</tr>
<tr>
<td>57</td>
<td>10</td>
<td>Sat</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>Temp</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>Sat</td>
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<tr>
<td></td>
<td>20</td>
<td>Temp</td>
</tr>
<tr>
<td>87</td>
<td>10</td>
<td>Sat</td>
</tr>
<tr>
<td></td>
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<tr>
<td></td>
<td>20</td>
<td>Sat</td>
</tr>
<tr>
<td>114</td>
<td>10</td>
<td>Sat</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>Temp</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>Sat</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>Temp</td>
</tr>
</tbody>
</table>

- □ Start of Corrosion Initiation
- ■ End of Corrosion Initiation
- △ Start of Waste Package Failures
- ▲ End of Waste Package Failures

*Correspond to failure of corrosion-allowance barrier
Based on panel-scale thermo-hydrology
## Summary of TSPA-1993 Cumulative Waste Package $^{237}$Np and $^{99}$Tc Releases Normalized to Table 1 of 40 CFR 191: 10,000 and 100,000 Years

<table>
<thead>
<tr>
<th>Thermal Load (kW/Ac)</th>
<th>Outer Thickness (cm)</th>
<th>Corrosion Initiation Criterion</th>
<th>10,000 Yr.</th>
<th>100,000 Yr.</th>
<th>Percent of Release from HLW</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$^{237}$Np</td>
<td>$^{99}$Tc</td>
<td>$^{237}$Np</td>
</tr>
<tr>
<td>28.5</td>
<td>10 cm</td>
<td>Sat.</td>
<td>1.2</td>
<td>0.14</td>
<td>11.7</td>
</tr>
<tr>
<td>28.5</td>
<td>10 cm</td>
<td>Temp.</td>
<td>1.2</td>
<td>0.14</td>
<td>11.7</td>
</tr>
<tr>
<td>28.5</td>
<td>20 cm</td>
<td>Sat.</td>
<td>0.0</td>
<td>0.0</td>
<td>8.4</td>
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<tr>
<td>28.5</td>
<td>20 cm</td>
<td>Temp.</td>
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<td>0.0</td>
<td>8.4</td>
</tr>
<tr>
<td>57</td>
<td>10 cm</td>
<td>Sat.</td>
<td>3.7</td>
<td>0.43</td>
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</tr>
<tr>
<td>57</td>
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<td>Temp.</td>
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<td>0.33</td>
<td>13.3</td>
</tr>
<tr>
<td>57</td>
<td>20 cm</td>
<td>Sat.</td>
<td>1.9</td>
<td>0.21</td>
<td>13.1</td>
</tr>
<tr>
<td>57</td>
<td>20 cm</td>
<td>Temp.</td>
<td>0.35</td>
<td>0.04</td>
<td>12.7</td>
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<tr>
<td>87</td>
<td>10 cm</td>
<td>Sat.</td>
<td>1.3</td>
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<td>13.9</td>
</tr>
<tr>
<td>87</td>
<td>10 cm</td>
<td>Temp.</td>
<td>1.1</td>
<td>0.25</td>
<td>13.7</td>
</tr>
<tr>
<td>87</td>
<td>20 cm</td>
<td>Sat.</td>
<td>1.2</td>
<td>0.31</td>
<td>13.8</td>
</tr>
<tr>
<td>87</td>
<td>20 cm</td>
<td>Temp.</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>114</td>
<td>10 cm</td>
<td>Sat.</td>
<td>0.1</td>
<td>0.31</td>
<td>14.2</td>
</tr>
<tr>
<td>114</td>
<td>10 cm</td>
<td>Temp.</td>
<td>0.03</td>
<td>0.02</td>
<td>14.0</td>
</tr>
<tr>
<td>114</td>
<td>20 cm</td>
<td>Sat.</td>
<td>0.06</td>
<td>0.06</td>
<td>14.0</td>
</tr>
<tr>
<td>114</td>
<td>20 cm</td>
<td>Temp.</td>
<td>0.0</td>
<td>0.0</td>
<td>14.0</td>
</tr>
</tbody>
</table>
Summary of Relevant TSPA-1993 Conclusions

- Waste-package failures dependent on model for corrosion initiation
  - Saturation-dependent occur earlier
- Spatial variability (due to edge effects) in corrosion initiation and rates affects distribution of failures
- Assumed corrosion model affects distribution of failures
- Diffusive releases from waste package/engineered barrier system generally dominate advective releases
- No significant waste-package cumulative release differences occur during 100,000 years
Preliminary TSPA Analyses Using Drift-Scale Thermo-Hydrologic Model:
Objectives

- Directly evaluate T-H response at drift scale
  - Temperature, liquid saturation and flux, relative humidity

- Evaluate range of designs for Systems Study
  - Two thermal loads: 25 and 87 kW/acre
  - Two backfill alternatives: none and gravel
  - Two waste package spacings: 39 x 39 m and 16 x 93 m
  - Three corrosion-allowance thicknesses: 10, 20 and 45 cm

- Evaluate sensitivity (waste-package failures) to corrosion initiation criterion
  - Relative humidity > 70% or temperature < 96°C

- Evaluate sensitivity (waste-package release) to release initiation criterion
  - Saturation > residual saturation of backfill

- Evaluate sensitivity (AE release and dose) to limited range of designs
Preliminary TSPA Analyses Using Drift-Scale Thermo-Hydrologic Model: Approach/Assumptions

- Analyze drift-scale T-H response
  - 2-D vertical section: surface to 1000 m below water table
  - Refined mesh in vicinity of drift
  - TOUGH2 and FEHM compared
  - Calculate temperature, saturation, flux, and humidity
  - Humidity determined from Kelvin relationship
  - Evaluate sensitivity to ambient percolation flux
    » 0.0, 0.1 and 0.2 mm/yr
  - Sensitivity to rock and backfill properties not evaluated

- Determine corrosion initiation
  - Humidity > 70% or temperature < 96°C
• Corrosion rates assuming Stahl (1993) with pitting
  – Not spatially variable
  – Spread of failures using two alternate models
    » +/- 25% of mean failure time
    » +/- 25% of time exponent
• Corrosion-resistant barriers (including cladding) fail congruently with corrosion allowance
• Entire waste-form surface exposed to water
  – Evaluate sensitivity to wetting criteria
• Dissolution rates and solubilities from TSPA-1993
• Diffusion coefficient from Conca
  – Minimum of 1.0E-06 m²/yr
Preliminary TSPA Analyses Using Drift-Scale Thermo-Hydrolgic Model Principal Results

- Representative drift-scale T-H responses
- Waste package failure distributions
- Waste package cumulative releases
  - 10,000 year
  - 100,000 year
In-Drift Distribution of Temperature, Saturation and Humidity:
25 kW/Acre; gravel backfill; rectangular spacing

![Graph showing temperature, saturation, and humidity over time.](image)
In-Drift Distribution of Temperature, Saturation and Humidity:
25 kW/Acre; no backfill; rectangular spacing

![Graph showing temperature, saturation, and humidity distribution over time.](image-url)
In-Drift Distribution of Temperature, Saturation and Humidity: 87 kW/Acre; gravel backfill; rectangular spacing
Summary of Waste Package Failures Using Drift-Scale Thermo-Hydrology: Sensitivity to Thermal Load; Backfill; Spacing; Corrosion Initiation--10cm Outer Barrier; 0.1 mm/yr Percolation Flux

<table>
<thead>
<tr>
<th>Thermal Load (kW/Ac)</th>
<th>Backfill</th>
<th>Spacing</th>
<th>Corrosion Initiation Criterion</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>none</td>
<td>rect.</td>
<td>r.h. temp.</td>
</tr>
<tr>
<td>25</td>
<td>none</td>
<td>sq.</td>
<td>r.h. temp.</td>
</tr>
<tr>
<td>25</td>
<td>gravel</td>
<td>rect.</td>
<td>r.h. temp.</td>
</tr>
<tr>
<td>25</td>
<td>gravel</td>
<td>sq.</td>
<td>r.h. temp.</td>
</tr>
<tr>
<td>87</td>
<td>none</td>
<td>rect.</td>
<td>r.h. temp.</td>
</tr>
<tr>
<td>87</td>
<td>gravel</td>
<td>sq.</td>
<td>r.h. temp.</td>
</tr>
</tbody>
</table>

- □ Start of Corrosion Initiation
- △ Start of Waste Package Failures
- ▲ End of Waste Package Failures
- • Time: Sat > Sres

1) rect. = rectangular: 92.7 m spacing between drifts, 16m opening along drift
   sq. = square: 38.5m spacing between drifts, 38.5m opening along drift
2) r.h. = relative humidity > 70%
   temp. = temperature < 96° C
Summary of Waste Package Failures Using Drift-Scale Thermo-Hydrology: Sensitivity to Thermal Load; Backfill; Spacing; Corrosion Initiation--20cm Outer Barrier; 0.1 mm/yr Percolation Flux

<table>
<thead>
<tr>
<th>Thermal Load (kW/Ac)</th>
<th>Backfill</th>
<th>Spacing</th>
<th>Corrosion Initiation Criterion</th>
<th>Start of Corrosion Initiation</th>
<th>Start of Waste Package Failures</th>
<th>End of Waste Package Failures</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>none</td>
<td>rect.</td>
<td>r.h. temp.</td>
<td>□</td>
<td>▲</td>
<td>▲</td>
</tr>
<tr>
<td>25</td>
<td>none</td>
<td>sq.</td>
<td>r.h. temp.</td>
<td>□</td>
<td>▲</td>
<td>▲</td>
</tr>
<tr>
<td>25</td>
<td>gravel</td>
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<td>r.h. temp.</td>
<td>□</td>
<td>▲</td>
<td>▲</td>
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<tr>
<td>25</td>
<td>gravel</td>
<td>sq.</td>
<td>r.h. temp.</td>
<td>□</td>
<td>▲</td>
<td>▲</td>
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<tr>
<td>87</td>
<td>none</td>
<td>rect.</td>
<td>r.h. temp.</td>
<td>□</td>
<td>▲</td>
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<tr>
<td>87</td>
<td>gravel</td>
<td>rect.</td>
<td>r.h. temp.</td>
<td>□</td>
<td>▲</td>
<td>▲</td>
</tr>
</tbody>
</table>

- □ Start of Corrosion Initiation
- ▲ Start of Waste Package Failures
- ▲ End of Waste Package Failures
Summary of Revised Thermo-Hydrologic Analyses on Cumulative Waste Package $^{237}$Np and $^{99}$Tc Releases Normalized to Table 1 of 40 CFR 191 (Temperature Corrosion Initiation Criterion, 10 cm Outer Barrier)

<table>
<thead>
<tr>
<th>Thermal Load (kW/Ac)</th>
<th>Backfill</th>
<th>Spacing</th>
<th>Release Dependent**</th>
<th>10,000 Yr.</th>
<th>100,000 Yr.</th>
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</thead>
<tbody>
<tr>
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<td></td>
<td></td>
<td>Np</td>
<td>Tc</td>
</tr>
<tr>
<td>25</td>
<td>None</td>
<td>Rect.</td>
<td>Sat.</td>
<td>3.5 E-5</td>
<td>1.3 E-4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Temp.</td>
<td>4.9 E-3</td>
<td>4.9 E-2</td>
</tr>
<tr>
<td>25</td>
<td>None</td>
<td>Sq.</td>
<td>Sat.</td>
<td>5.2 E-3</td>
<td>5.2 E-2</td>
</tr>
<tr>
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<td>Temp.</td>
<td>5.2 E-3</td>
<td>5.2 E-2</td>
</tr>
<tr>
<td>25</td>
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<td>Rect.</td>
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<td>Sat.</td>
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<td>1.3 E-4</td>
</tr>
<tr>
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<td>Temp.</td>
<td>4.9 E-3</td>
<td>5.0 E-2</td>
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<td>Temp.</td>
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<td>0.0*</td>
</tr>
<tr>
<td>87</td>
<td>Gravel</td>
<td>Rect.</td>
<td>Sat.</td>
<td>0.0*</td>
<td>0.0*</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Temp.</td>
<td>0.0*</td>
<td>0.0*</td>
</tr>
</tbody>
</table>

* No Failures for 87 kW/Ac for 10,000 years assuming temperature corrosion initiation.

** Sat. = Saturation in drift > residual saturation of gravel (0.01) before waste is wet.
Temp. = Temperature in drift < 96°C before waste is wet.
CCDF of Total Normalized Waste Package Release for 10,000 Years: Effect of Spacing and Release Initiation

- 25 kw / rect / sat dep.
- 25 kw / sq / sat dep.
- 25 kw / rect / temp dep.
- 25 kw / sq / temp dep.
CCDF of Total Normalized Waste Package Release for 10,000 Years: Effect of Thermal Load, Spacing, and Outer Barrier Thickness
Summary of Initial TSPA Results Based on Preliminary Drift-Scale Thermo-Hydrologic Model

- Humidity-initiated corrosion can lead to earlier failures at higher thermal loads
  - [Not accounting for humidity effects on corrosion rates]
- Backfill leads to slightly higher failure times
  - Depends on corrosion initiation criterion
- Rectangular spacing leads to slightly higher failure times
- 20 cm outer barrier leads to increased failure times
  - [Conservative treatment of inner barrier and cladding]
- Although differences occur in waste package and AE release, their significance is strongly affected by assumptions in waste package/engineered barrier system model
Thermally Related Issues to be Addressed in TSPA-1995

- Revised drift-scale thermo-hydrologic model
  - Alternate backfill characteristics
  - Alternate thermal loads
  - Evaluate effect of rock property uncertainty
  - Direct prediction of humidity
  - Indirect prediction of spatial variability

- Revised model(s) for initiation of aqueous corrosion

- Drift-scale liquid saturations used to define
  - Percent of waste-form surface exposed to water
  - Percent of waste package and EBS with diffusive pathway
Other Issues to be Addressed in TSPA-1995

- Revised unsaturated zone hydrologic model
  - Spatially variable infiltration
  - Fracture-matrix flow and transport
  - Heterogeneity and scaling effects

- Revised waste-package corrosion rate models
  - Corrosion-allowance materials
  - Corrosion-resistant materials and cathodic protection
  - Cladding
Other Issues to be Addressed in TSPA-1995
(Continued)

• Revised radionuclide mobilization and EBS release model
  - Percent of waste package degraded
    » Probabilistic pit generation and growth model
  - Percent of cladding surface degraded
  - Percent of waste-form exposed to water
    » Based on water content fn(time)
  - Percent of continuous water film for diffusion
    » Based on water content fn(time)
  - Revised waste-form dissolution model
  - Revised solubilities
    » Colloidal mobilization and transport
Key Information Needs for TSPA-1995

• Unsaturated Zone Hydrology
  – Infiltration and percolation rate (and variability and uncertainty)
  – Fracture-matrix coupling
    » Matrix imbibition and diffusion
  – Bulk rock characteristic curves in TSw2 (and variability and uncertainty)

• Waste Package/Engineered Barrier System
  – Backfill and invert thermo-hydrologic properties
  – Corrosion initiation criteria (and uncertainty)
  – Corrosion model and parameters (and uncertainty)
    » Corrosion allowance
    » Corrosion resistant
    » Cladding
  – Effective diffusion coefficient at low liquid saturation
  – Spent fuel dissolution model for expected thermo-hydrologic conditions
Conclusions

• Additional sensitivity analyses confirm conclusions made in TSPA-1993 and illustrate importance of assumptions made in waste-package degradation and EBS release

• Preliminary drift-scale thermo-hydrologic analyses indicate importance of
  – Criteria for initiation of corrosion
  – Criteria for initiation of dissolution and release

• Planning for TSPA-1995 is underway, with focus on key components of waste-isolation argument