Total System Performance Assessment: Modeling Approach and Overview of Results

Presented to:
Nuclear Waste Technical Review Board

Presented by:
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Outline

• Summary of the modeling approach for the Total System Performance Assessment for the License Application (TSPA-LA)

• Scenarios and modeling cases for the TSPA-LA

• Overview of TSPA-LA results
  – Total dose (summed over scenarios)
  – Important scenarios and radionuclides
    ◆ Shape of expected dose history
    ◆ Magnitude of expected dose
    ◆ Uncertainty in expected dose
  – Stability of total dose results

• Water and radionuclide movement in the Engineered Barrier System (EBS): seismic ground motion damage

• Water and radionuclide movement in the EBS: igneous intrusion
Major Steps in Iterative Performance Assessment for Yucca Mountain

- Screen Features, Events, and Processes (FEPs) and develop scenario classes
- Develop models and abstractions, along with their scientific basis, for logical groupings of FEPs within scenario classes
- Evaluate uncertainty in model inputs
- Construct integrated TSPA model using all retained FEPs and perform calculations for the scenario classes and “modeling cases” within scenario classes
- Evaluate total system performance, incorporating uncertainty through Monte Carlo simulation
Postclosure Science Supporting the TSPA
TSPA Architecture

Output Parameters

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Legend

- Response Surface between Process Models
- Preprocessor
- Response Surface from Process Model to GoldSim
- Connection in Outline
TSPA Documentation
MDL-WIS-PA-000005 REV 00 AD 01

Four volumes
4272 pages

11,843 pages of supporting technical documents that provide direct input

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Future Scenarios for Yucca Mountain

Four scenario classes divided into seven modeling cases

- Nominal Scenario Class
  - Nominal Modeling Case

- Early Failure Scenario Class
  - Waste Package Modeling Case
  - Drip Shield Modeling Case

- Igneous Scenario Class
  - Intrusion Modeling Case
  - Eruption Modeling Case

- Seismic Scenario Class
  - Ground Motion Modeling Case
  - Fault Displacement Modeling Case
Scenarios and Modeling Cases

Nominal Scenario Class (1 modeling case)

– No releases until waste package (WP) corrosion creates pathway
– WP failures rare before 100,000 years
– WP failures due to stress corrosion cracking (SCC) of closure welds occur as general corrosion removes annealed layer
  ✷ SCC common by 500,000 years
  ✷ Releases through SCC occur by diffusion only
– Drip shield (DS) failures due to general corrosion occur between 270,000 and 340,000 years
– WP “patch” failures due to general corrosion rarely occur before 500,000 years
  ✷ Mean of 9% of WPs show patch failures at 1 million years
  ✷ Patch failures allow advective releases
Early Failure Scenario Class (2 modeling cases)

Early Failure WP Modeling Case
- Failures occur at time of repository closure
- Median probability of early failure = $4.4 \times 10^{-5}$ per WP
- Probability of 1 or more early failure waste packages = 0.44
- Expected number of early failure waste packages (given early failures occur) = 2.5
- Diffusion until DS failure by corrosion

Early Failure DS Modeling Case
- Failures occur at time of repository closure
- Median probability of early failure = $4.3 \times 10^{-7}$ per DS
- Probability of 1 or more early failure drip shields = 0.017
- Expected number of early failure drip shields (given early failures occur) = 1.1
- Simplifying assumption: WP under early failed DS is also failed in seeping conditions
- Transport by both advection and diffusion
Scenarios and Modeling Cases (Cont)

- Igneous Scenario Class (2 modeling cases)
  - Intrusion Modeling Case
    - Mean frequency $1.7 \times 10^{-8}$/yr (uncertain event frequency)
    - All waste packages and drip shields sufficiently damaged to provide no barrier to flow and transport
    - Seepage equal to percolation flux (no capillary barrier)
  - Eruption Modeling Case
    - Probability of waste intersection by eruption conditional on igneous event is 0.08
    - Mean number of waste packages intersected = 3.8
    - Mean fraction of waste package content ejected = 0.3
    - Ash redistribution by fluvial processes after deposition
Scenarios and Modeling Cases (cont.)

- **Seismic Scenario Class (2 Modeling Cases)**
  - **Seismic Ground Motion (GM) Damage Modeling Case**
    - Ground motions result in SCC that allow diffusive releases
      - Frequency of events that damage codisposal (CDSP) packages: ~ $10^{-5}$ / yr
      - Frequency of events that damage transportation, aging, and disposal (TAD) packages for commercial spent nuclear fuel (CSNF): ~ $10^{-8}$ / yr
    - Cracked area accumulates with additional seismic events
    - Repeated damage may cause WP rupture (<$10^{-8}$ / yr)
    - Drip shield thins by general corrosion and fails due to dynamic loading of accumulated rockfall
  - **Nominal corrosion processes included for million-year analyses**
    - Corrosion affects EBS response to ground motion
      - Damage analyses consider thinning of Alloy 22 and titanium
      - SCC allows corrosion of internal steel components
Scenarios and Modeling Cases (cont.)

- Seismic Scenario Class (2 Modeling Cases) (cont.)
  - Seismic Fault Displacement Modeling Case
    - Annual frequency approximately $2 \times 10^{-7}$ / yr
    - Fault displacements rupture waste packages and drip shields, allowing advection and diffusion
      » Size of rupture uncertain, 0 to cross-sectional area of WP
    - mean of ~ 47 waste packages and drip shields damaged
Total System Performance Assessment Results
Total Mean and Median Annual Dose

MDL-WIS-PA-000005 REV 00 AD 01, Figure 8.1-1[a] and Figure 8.1-2[a]
TSPA Results: Modeling Cases Contributing to Total Mean Annual Dose

10,000 years

1,000,000 years

MDL-WIS-PA-000005 REV 00 AD 01, Figure 8.1-3[a].
Terminology

- **“Dose”** – annual dose to the Reasonably Maximally Exposed Individual (RMEI) as a function of time
  - Depends on both aleatory and epistemic uncertainty
  - Summed over all radionuclides

- **“Expected Dose”**
  - Expectation is taken over aleatory quantities
  - Conditional on epistemic uncertainty
  - Calculated for each modeling case

- **“Mean Dose”**
  - Expectation is taken over both epistemic and aleatory
  - Calculated for each modeling case

- **“Total Expected Dose”**
  - Summed over modeling cases by epistemic vector

- **“Total Mean Dose”**
  - Average of Total Expected Dose
Example: Eruptive Dose

Eruptive dose: 40 realizations of aleatory uncertainty conditional on a single eruption of 1 WP at time zero

Eruptive dose averaged over aleatory uncertainty associated with a single eruption of 1 WP, eruptions at multiple times

Expected eruptive dose; 300 realizations, each showing expected dose from a single sampling of epistemic uncertainty with events at all times

Summary curves showing overall mean dose from eruption
Uncertainty in Total Expected Dose (1 million years)
Total Mean Dose
Contribution By Modeling Case

**Figure 8.1-3b[a]**

![Graph showing total mean dose contribution by modeling case](MDL-WIS-000005 REV 00 AD01 Fig 8.1-3b[a])

- Total
- Drip Shield Early Failure
- Waste Package Early Failure
- Seismic Fault Displacement
- Igneous Intrusion
- Seismic Ground Motion
- Volcanic Eruption

Time (years)

0  200000  400000  600000  800000  1000000

Mean Annual Dose (mrem)

10^{-6}  10^{-5}  10^{-4}  10^{-3}  10^{-2}  10^{-1}  10^{0}  10^{1}  10^{2}  10^{3}
Construction of Total Dose

Volcanic Eruption

Seismic GM (+ Nominal)

Igneous Intrusion

+ + +

Total

(MDL-WIS-000005 REV 00 Fig 8.2-8b)

(MDL-WIS-000005 REV 00 Fig 8.2-8b[a])

(MDL-WIS-000005 REV 00 AD01 Fig 8.2-11b[a])

(MDL-WIS-000005 REV 00 AD01 Fig 8.2-7b[a])

(MDL-WIS-000005 REV 00 AD01 Fig 8.1-2[a])
Composition of Dose from Seismic GM

Included

Expected Dose from Nominal processes

Expected Dose from Seismic and Nominal processes

Stylized decomposition

- From seismic damage to CDSP WP (diffusion)
- From SCC failure of CSNF WP (diffusion)
- From general corrosion failure of both WPs (advection)
Radionuclides Important to Mean Dose

E indicates “early” and refers to the time period before ~ 200,000 yr. L indicates “late” and refers to the time period after ~ 200,000 yr.
Stability of Total Dose

Replicated sampling demonstrates that sample size is sufficient

Confidence interval illustrates precision of estimate of total mean dose
Water movement following ground motion

- Nominal seepage model accounts for capillary and thermal effects around drift
  - Nominal model shows seepage in a mean of 40% of WP locations, mean seepage rates are 2-11% of percolation flux
- Seepage model adjusted for rockfall accumulation
  - Additional seepage model developed for rubble-filled drifts; seepage for seismic GM case in a mean of 70% of WP locations, mean seepage rates are up to 48% of percolation flux
  - Lithophysal rock (~85% of emplacement area): nominal model used when rubble < 5 m³/m; rubble-filled model used when rubble > 60 m³/m
    - Linear interpolation between nominal and rubble-filled seepage based on calculated amount of rubble
  - Non-lithophysal rock (~15% of emplacement area): collapse events rare, percolation flux used when rubble > 0.5 m³/m
Mean TSPA Seepage Rates

Units are m$^3$/5.1m of drift, also shown as kg/yr per waste package; mean of all realizations

MDL-WIS-PA-000005 REV 00 AD 01 Figure 8.3-3b[a]
Water and Radionuclide Movement in the EBS Seismic Ground Motion Motion Case (cont.)

- Water movement following ground motion (cont.)
  - Flow through EBS components
    - **Drip Shields**
      - Flow through SCC in drip shield is negligible, screened out from TSPA (see discussion in FEP 2.1.03.10.0B)
      - After general corrosion thinning and failure due to accumulated rockfall (approx. 300,000 yr), DS no longer provides flow barrier
    - **Waste Packages**
      - Diffusion of water through SCC in WPs assumed to be sufficient to degrade stainless steel internal components
      - Flow occurs through general corrosion WP patch failures and rare WP ruptures or punctures
      - Flow fraction entering WP is proportional to ratio of patch failure length to WP length: conceptually, GC failures along crown of WP allow all available flow to enter WP when a small fraction (mean of 4%) of patches have failed
      - Flow allowed to leave WP at same rate it enters
  - Flow in invert same as in nominal case
Water and Radionuclide Movement in the EBS Seismic Ground Motion Modeling Case (cont.)

- Radionuclide transport following ground motion
  - Diffusion is the only release mechanism prior to patch failures by general corrosion or rupture/puncture
    - Diffusion of water into WPs allows waste form degradation
    - Diffusion of radionuclides occurs through continuous water films from waste form to invert when relative humidity > 95%
      » High solubility, non-sorbing nuclides dominate dose: $^{99}$Tc and $^{129}$I
      » Rate of diffusion controlled by cross-sectional area of cracks, path length, concentration gradient
  - After patch failures, advective releases dominate
    - Long-lived actinides dominate dose: $^{242}$Pu, $^{237}$Np, $^{239}$Pu
    - Water flux, solubility limits, sorption processes in WP affect rate of release
Water and Radionuclide Movement in the EBS Igneous Intrusion Modeling Case

- Water movement following igneous intrusion
  - Seepage model replaced with percolation flux to bound uncertainty associated with capillary properties of magma-filled drifts
    - Seepage equal to percolation flux occurs at all waste package locations
    - Water re-enters drifts when temperatures drop below boiling
      » Temperatures fall below boiling within a few years at post-thermal times, ambient temperatures are reached after ~ 100 yr
  - All water entering drifts reaches waste
    - Magmatic material filling drifts assumed to have properties equivalent to fractured tuff
    - Drip shield and waste packages provide no barrier to flow
  - Water flow in invert is unchanged from nominal case
Water and Radionuclide Movement in the EBS Igneous Intrusion Modeling Case (cont.)

- Radionuclide transport following intrusion
  - CSNF and HLW waste forms assumed to be fully degraded by high temperature of intrusion
  - Waste package geometry and materials assumed to be intact for purposes of water chemistry and radionuclide transport
    - In-package chemistry model used to determine solubility limits
    - Transport pathways are the same as for nominal case with patch failures
  - Contents of all waste packages are available for advective transport
Summary of TSPA Results

- Total mean dose determined by occurrence of igneous events, seismic damage and general corrosion

- Major contributors to dose are $^{99}\text{Tc}$, $^{129}\text{I}$, $^{239}\text{Pu}$, $^{242}\text{Pu}$, $^{226}\text{Ra}$, and $^{237}\text{Np}$

- 10,000-yr total estimated maximum mean annual dose: 0.24 mrem/yr
  - Largest contributor is $^{99}\text{Tc}$ from co-disposed waste, dominant pathway is diffusion through stress corrosion cracks following ground motion damage

- 1,000,000 total estimated maximum median annual dose: 0.96 mrem/yr (mean annual dose at 1,000,000 yr: 2.0 mrem/yr)
  - Largest contributors are $^{242}\text{Pu}$, $^{237}\text{Np}$, $^{226}\text{Ra}$, $^{239}\text{Pu}$, and $^{129}\text{I}$
    - Actinide releases occur due to advective transport following igneous intrusion and general corrosion patch failure
    - Iodine releases are dominated by diffusive pathways through stress corrosion cracks
  - Nominal general corrosion processes dominate at 1 million years
Backup
Water Mass Balance in the EBS

- Liquid water balance is maintained within the unsaturated zone flow, thermal hydrology, seepage and EBS flow models
  - Water entering drifts is equal to water leaving drifts
  - Exception:
    - Removal of vapor-phase water by evaporation is not included; addition of water from condensation is included during the first 2000 years (evaporation/condensation processes are not explicitly balanced)

- Consumption of water by chemical reactions (e.g., in degradation of engineered materials) is assumed to be insignificant

- Movement of water vapor through SCCs is assumed to be sufficient to sustain degradation reactions and maintain continuous water films that allow diffusive transport
Radionuclide Mass Balance in the EBS

- Radionuclide mass balance maintained in EBS submodel in GoldSim
  - $^{99}$Tc example shown for ground motion case, single sampling of aleatory uncertainty (event at 1000 years), 300 realizations of epistemic uncertainty
  - Mean mass balance discrepancy is approximately 0.001%

LS016_v5.005_SMK_000: $^{99}$Tc Mass Balance
300 Epistemic Realizations (150 plotted), Seismic-GM Modeling Case
Event Time = 1,000-ys, Damage Fraction = $10^{-6}$

Mean mass balance discrepancy is approximately 0.001%
Localized Corrosion in the TSPA

- **Drip Shields**
  - Localized corrosion is screened out
    - FEP 2.1.09.28.0B; Localized corrosion on drip shield surfaces due to deliquescence
    - FEP 2.1.03.03.0B; Localized corrosion of drip shields

- **Waste Packages**
  - Localized corrosion of Alloy-22 due to dust deliquescence is screened out
    - FEP 2.1.09.28.0A; Localized corrosion on waste package outer surface due to deliquescence
  - Localized corrosion in seepage water is included in TSPA
    - FEP 2.1.03.03.0A; Localized corrosion of waste packages
Localized Corrosion of Alloy-22

Note: This overhead contains an error. See correction letter of April 30, 2009, for the corrected version of this overhead. The letter may be reached via the "meetings" page.

- Environmental conditions for LC initiation are analyzed using TSPA model independent of the drip shield (MDL-WIS-PA-000005 REV 003 AD 01, Appendix 0)
  - Temperature, pH, and nitrate/chloride ratios modeled as a function of time for 3,264 nodes in repository
  - The potential for LC peaks in the first few hundred years when temperatures are highest
    - LC conditions could exist at approximately 10% of modeled WP locations at early time
    - By 5000 years, less than 0.1% of WP locations have LC conditions
    - LC conditions do not occur at any locations after 12,000 years
- LC is included by bounding assumptions for modeling cases in which the DS is compromised before 12,000 years
  - For DS Early Failure case, failure of WP due to LC is assumed for all seeping locations, regardless of actual environment
  - For Seismic Fault Displacement, WP is assumed to be sheared by the fault displacement event
  - For Igneous modeling cases, WPs are assumed to be fully compromised by the event
Localized Corrosion in TSPA (cont.)

Note: This overhead contains an error. See correction letter of April 30, 2009, for the corrected version of this overhead. The letter may be reached via the "meetings" page.
Localized Corrosion in TSPA (cont.)

Localized corrosion has the potential to initiate when $E_{corr} \geq E_{crit}$, where $E_{crit}$ is the crevice repassivation potential $E_{rcrev}$

$$E_{critical} = E_{rcrev} = a_o + a_1 T + a_2 \ln[Cl^-] + a_3 \frac{[NO_3^-]}{[Cl^-]} + a_4 T[Cl^-] + \varepsilon_{rcrev}$$

$$E_{corr} = c_o + c_1 T + c_2 pH + c_3 \frac{[NO_3^-]}{[Cl^-]} + c_4 T \frac{[NO_3^-]}{[Cl^-]} + c_5 pH \frac{[NO_3^-]}{[Cl^-]} + c_6 pH \ln[Cl^-] + \varepsilon_{corr}$$

MDL-WIS-000005 REV 00 AD01 Appendix O, Equations O-1 and O-2