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Yucca Mountain Site Characterization Project

# Total-System Performance Assessment for Yucca Mountain – SNL Second Iteration (TSPA-1993)

## **Executive Summary**

Michael L. Wilson, John H. Gauthier, Ralston W. Barnard, George E. Barr, Holly A. Dockery, Ellen Dunn, Roger R. Eaton, David C. Guerin, Ning Lu, Mario J. Martinez, Robert Nilson, Christopher A. Rautman, Thomas H. Robey, Benjamin Ross, Eric E. Ryder, Albert R. Schenker, Sharon A. Shannon, Lee H. Skinner, William G. Halsey, James D. Gansemer, Lynn C. Lewis, Alan D. Lamont, Inés R. Triay, Arend Meijer, David E. Morris

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#### Abstract

Sandia National Laboratories has completed the second iteration of the periodic total-system performance assessments (TSPA-93) for the Yucca Mountain Site Characterization Project (YMP). These analyses estimate the future behavior of a potential repository for high-level nuclear waste at the Yucca Mountain, Nevada, site under consideration by the Department of Energy. TSPA-93 builds upon previous efforts by emphasizing YMP concerns relating to site characterization, design, and regulatory compliance.

Scenarios describing expected conditions (aqueous and gaseous transport of contaminants) and low-probability events (human-intrusion drilling and volcanic intrusion) are modeled. The hydrologic processes modeled include estimates of the perturbations to ambient conditions caused by heating of the repository resulting from radioactive decay of the waste. Hydrologic parameters and parameter probability distributions have been derived from available site data. Possible future climate changes are modeled by considering two separate groundwater infiltration conditions: "wet", with a mean flux of 10 mm/yr, and "dry", with a mean flux of 0.5 mm/yr. Two alternative wastepackage designs and two alternative repository areal thermal power densities are investigated. One waste package is a thin-wall container emplaced in a vertical borehole, and the second is a container designed with corrosion-resistant and corrosion-allowance walls emplaced horizontally in the drift. Thermal power loadings of 57 kW/acre (the loading specified in the original repository conceptual design) and 114 kW/acre (a loading chosen to investigate effects of a "hot repository") are considered.

TSPA-93 incorporates significant new detailed process modeling, including two- and threedimensional modeling of thermal effects, groundwater flow in the saturated-zone aquifers, and gas flow in the unsaturated zone. The saturated-zone model is used to estimate travel times for contaminants through layered, dipping formations. Coupled calculations of gas and heat flow are used to estimate travel times for gaseous CO<sub>2</sub>. Time-dependent temperature distributions in the rock surrounding the potential repository are calculated, using the four repository layouts. A phenomenological model for waste-package degradation is implemented; the model includes temperature-dependent corrosion, fuel alteration, and dissolution.

Probabilistic analyses are performed for aqueous and gaseous flow and transport, human intrusion, and basaltic magmatic activity. Repository performance estimates are sensitive to assumptions made about unsaturated-zone water flow and contact with waste. Two conceptual models of unsaturated-zone water flow are considered — the composite-porosity model, which treats fracture and matrix flow as being strongly coupled; and the weeps model, which allows for flow only through locally saturated zones. The weeps aqueous releases and the human-intrusion direct releases are sensitive to the size of the waste packages that are affected: the larger horizontally-emplaced containers produce greater releases. Releases are generally insensitive to repository thermal effects: a hotter thermal loading protects parts of the repository from contact with liquid water, but other parts experience enhanced water flow due to condensation and diversion. The volcanic scenario, which investigates the effects of magmatic volatiles on the degradation of the waste packages, does not contribute significantly to releases.

Results of the calculations done for TSPA-93 lead to a number of recommendations concerning studies related to site characterization. Primary among these are the recommendations to obtain better information on percolation flux at Yucca Mountain, on the presence or absence of flowing fractures, and on physical and chemical processes influencing gaseous flow. Near-field thermal and chemical processes, and waste-container degradation are also areas where additional investigations may reduce important uncertainties. Recommendations resulting from TSPA-93 for repository and waste-package design studies are: 1) to evaluate the performance implications of large-size containers, and 2) to investigate in more detail the implications of high repository thermal power output on the adjacent host rock and on the spent fuel.

If future repository performance regulations are based on individual dose rather than cumulative release, results suggest that future site-characterization efforts should emphasize investigations of groundwater contact with waste packages in the unsaturated zone and examinations of saturated-zone flow paths. Because dose rates are dependent on the rate of radionuclide releases, it would be useful to investigate container designs that fail "slowly" over long periods of time. Volume 1 contains Chapters 1 through 12

Volume 2 contains Chapters 13 through 25 and the Appendices This report was prepared under the Yucca Mountain Site Characterization Project WBS 1.2.5.4.1. QAGR 1.2.3.4.1 was applied, however, the information and data documented in the report were not developed to meet qualityaffecting standards. Not all the work activities were subject to QA controls. The information in this report is not qualified and is not to be used for licensing.

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## **Executive Summary**

## **1** Introduction

Yucca Mountain is being investigated by the U.S. Department of Energy (DOE) as the potential site for the permanent disposal of spent fuel from nuclear reactors and highlevel radioactive waste generated by the U.S. Department of Defense. Yucca Mountain is located in a sparsely populated, arid region of the U.S., approximately 120 km northwest of Las Vegas, Nevada, on the border of the DOE's Nevada Test Site. To take advantage of less groundwater, a potential repository at the site would be mined in the unsaturated zone of the mountain, about 300 m below the surface, but over 200 m above the water table (Figure ES-1).



Figure ES-1. Location of Yucca Mountain and a potential high-level radioactive-waste repository.

A repository at Yucca Mountain will have to meet a number of Federal regulations, including regulations concerning long-term waste isolation promulgated by the U.S. Environmental Protection Agency (EPA) and the U.S. Nuclear Regulatory Commission. To determine long-term waste isolation, the Yucca Mountain Site Characterization Project (YMP) of DOE has begun a series of total-system performance assessments (TSPAs). The work described in this report—TSPA-93—is part of the second full iteration in the series (Figure ES-2).



Figure ES-2. Progression of TSPA analyses.

TSPA-93 differs from previous analyses in several important respects. Significant new detailed modeling is undertaken, including three-dimensional geostatistical modeling of the stratigraphy, three-dimensional modeling of the saturated zone, and modeling of repository thermal effects. A phenomenological source term developed by Lawrence Livermore National Laboratory (LLNL) and climate change extrapolated from the paleoclimatic record are included in the probabilistic models. Several different repository designs with different containers and different thermal loadings are evaluated.

Two performance measures are considered in this TSPA iteration: normalized cumulative release, as defined by the EPA in 40 CFR 191.13, and radiation dose to a maximally exposed individual. The Energy Policy Act of 1992 dictates that 40 CFR Part 191 no longer applies to Yucca Mountain, and sets a course of action for specifying a new standard. Individual dose is examined in TSPA-93 to determine the potential impact of such a standard on the performance assessment. To study the impact of longer time periods on repository performance, both cumulative-releases and dose results were calculated for a million-year time period in addition to the typical 10,000-year period.

In one respect, the results of TSPA-93 tend to confirm previous work: cumulative releases from all investigated sources are generally below the EPA standard (40 CFR 191.13), except for gaseous releases of  $^{14}$ C. However, a significant new result is that future peak doses from drinking water in the area could be substantially above background radiation levels. Also, some of the models indicate that larger containers (e.g., the multipurpose container) and hotter repository configurations could lead to worse long-term performance, although a great deal of uncertainty is associated with these results.

## 1.1 TSPA-93 purpose

The ultimate goal of the TSPA process is to determine compliance of a repository with applicable regulations and to support a license application for construction and operation of a repository. However, at this point in the process, the primary goal of TSPA-93 is to provide feedback to YMP particpants on the significance of design and site-characterization information to regulatory compliance. Secondary goals of TSPA-93 involve progress toward performance assessments that are scientifically justified and acceptable for a license application, including refinement of mathematical models of physical processes, features, and events that could influence repository performance; consideration of an individual-dose performance measure; and calculation of conditional estimates of compliance with performance measures for scientific review. A final goal of TSPA-93 is to involve several different organizations within the project in production of a TSPA for Yucca Mountain. Table ES-1 shows the participants who provided input to TSPA-93. In addition, researchers from the Waste Isolation Pilot Project (WIPP) contributed to an independent review of this work.

## 1.2 Scenarios

A TSPA is based on a risk-assessment methodology that contains the following major steps: (1) develop and screen scenarios, (2) develop models of important features, events, and processes, (3) estimate parameter values and uncertainties, (4) make calculations using the models and parameter values, and (5) interpret results. A summary of models, parameters, and results is contained in the following sections. Development and screening of scenarios are independent efforts and are described in separate documents; a brief disscussion follows.

Component	Contributors
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Saturated Zone	USGS (R. Luckey) SNL (G. Barr)
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Table ES-1. Information sources for TSPA-93 analyses.

A scenario consists of an organized list of features, events, and processes (FEPs) that could lead to releases of radionuclides to the accessible environment—either the ground surface or a subsurface boundary 5 km from the repository. Scenario categories consist of groupings of similar scenarios. The general scenario categories considered in TSPA-93 include cases with an undisturbed repository (the "nominal" case), and with a disrupted repository (the "disturbed" cases).

For TSPA-93, the nominal case consists of a heat-generating repository that is subjected to climate-dependent groundwater flow. Two alternative conceptual models of groundwater flow in the unsaturated zone are considered. Waste containers within the repository degrade by a variety of mechanisms, but the most important mechanism is aqueous-induced corrosion. If and when containers fail, radionuclides are available for gaseous or aqueous transport to the accessible environment. For gaseous transport, radionuclides move upward through the unsaturated zone to the ground surface. For aqueous transport, radionuclides move downward through the unsaturated zone, then laterally through the saturated zone past the 5-km subsurface boundary. Radionuclides are tracked in terms of (1) cumulative releases to the accessible environment and (2) the dose an individual might recieve by drinking contaminated water pumped from the saturated zone at the accessible environment.

For TSPA-93, two disturbed cases are investigated: (1) inadvertant human intrusion by exploratory drilling, and (2) volcanic activity that introduces corrosion-enhancing heat and volatiles into the repository. For human intrusion, radionuclides exhumed with the drill core and the drilling fluids contribute to releases. For indirect volcanic effects, magmaticinduced corrosion of containers allows earlier releases of radionuclides that are transported in groundwater flowing as described in the nominal case. (Direct volcanic releases were evaluated in TSPA-91.)

## 2 Data development

## 2.1 Repository

The design limit for a repository at Yucca Mountain is 70,000 metric tons of radioactive waste. The approximately 63,000 metric tons of spent fuel emplaced in the repository is considered to be aged 25 years, with burnups of 30,000 MWd/MTU for boiling-water-reactor fuel and 40,000 MWd/MTU for pressurized-water-reactor fuel. The approximately 7,000 metric tons of defense high-level waste is considered to have many of the heavy metal products removed and to be encased in a vitrified waste form. A study performed in conjuction with TSPA-93 examined the significance of each radionuclide contained in the wastes in terms of its potential for contributing to contamination at the accessible environment. Based on this study, the human-intrusion analyses in TSPA-93 consider a broad suite of 43 radionuclides. Nominal case and indirect volcanic effects consider 8 radionuclides, chosen for their transport characteristics (low retardation) or their potential contribution to individual dose.

The waste forms are enclosed in containers; container designs have not been finalized, but those investigated to date consist of cylindrical metal containers with gas-tight closures. Two container types are considered in TSPA-93 (Figure ES-3): (1) a smaller, "vertically emplaced" container proposed in the Site Characterization Plan (SCP) Conceptual Design of 1987, and (2) a larger, "in-drift" container which approximates the multipurpose container (MPC) presently being considered by the Yucca Mountain Project. Vertically emplaced containers are modeled with a surrounding air gap that is sometimes filled with rubble. In-drift containers are modeled with a surrounding backfill, provided to prevent drift collapse. (Consequences of adding a backfill are an increased potential for water pathways to the waste container, and higher container temperatures caused by the backfill acting as a thermal



Figure ES-3. The two container types and emplacement strategies considered in TSPA-93.

insulator.) A 70,000-metric-ton repository requires the use of about 35,000 of the vertically emplaced containers or about 8,500 of the in-drift containers.

The repository layout incorporated in TSPA-93 consists of a series of emplacement drifts that run perpendicular to a main access drift. Length and proximity of the drifts to one another depend on the rock mass and the thermal characteristics of the repository. Decay of the radioactive waste produces heat: approximately 1 kW of heat for every metric ton (at emplacement—heat generation decreases over time). While the heat output depends primarily on the spent-fuel burnup and on the waste-acceptance schedule, the temperatures within the repository depend on the local areal power density (LAPD, expressed in terms of kW/acre), which is primarily a function of the waste-container spacing. It has been proposed that temperatures above boiling could produce a dry environment that would enhance the long-term performance of the repository. The SCP Conceptual Design specified an LAPD of 57 kW/acre (Figure ES-4). More recently, LAPDs up to 114 kW/acre have been considered by the YMP in order to attempt to induce a larger dryout zone.

Four combinations of container/thermal loadings are examined in TSPA-93. A 57kW/acre repository with vertically emplaced containers is the baseline analysis case for TSPA-93, and most like the design described in the SCP and evaluated in TSPA-91. Also



Figure ES-4. Repository layouts for the two thermal loadings considered in TSPA-93.

examined are a 114-kW/acre repository with vertically emplaced containers, a 57-kW/acre repository with in-drift containers, and a 114-kW/acre repository with in-drift containers.

### 2.2 Stratigraphy

A fully three-dimensional stratigraphic model of the potential repository region is developed for TSPA-93. The model uses geostatistics to reduce dependence on qualitative approaches by incorporating as much site-specific information as possible. The model was developed with the long-term goal of determining whether the thicknesses of the strata at the site are important to the modeled performance. For TSPA-93, probabilistic calculations (see below) are conducted using a reference stratigraphy selected from 10 geostatistical simulations performed with this approach.

The model incorporates lithologic data from 22 deep drillholes within or near the potential repository region in an indicator simulation to determine boundaries between welded and nonwelded layers of tuff. More regular structures—the Topopah Spring vitrophyre and the boundary between the vitric and zeolitized Calico Hills layers—are added separately.

Despite the welded/nonwelded indicator having horizontal correlation lengths on the order of kilometers, significant variation is seen in the strata contacts within the repository block for the 10 geostatistical outcomes. The implication is that the lithologic-data drillholes are not spaced closely enough for accurate predictions.

## 2.3 Hydrogeologic parameters

A performance-assessment data base is produced for TSPA-93 for the purpose of standardizing available data and generating probability distributions of parameters used in both the detailed and the probabilistic models. Data are categorized for 15 hydrologic properties (e.g., porosity, hydraulic conductivity, etc.) in 10 strata, both in the unsaturated and saturated formations. Each of the 10 modeled strata is considered homogeneous, and one probability density function (PDF) is developed for each hydrologic property in each layer. Each PDF is either derived directly from available data (where data are abundant), or is derived based on maintaining maximum informational entropy (where data are sparse), in order to minimize the chance of biasing the results. PDFs are also adjusted from lab scale to site scale to make them more representative.

A new accomplishment with this effort is the development of a method for determining fracture characteristics that are consistent with site data. Distributions of bulkpermeability, fracture-frequency, and fracture-dip data from drillholes are used as input to a parallel-plate model, allowing calculation of fracture apertures, hydraulic conductivities, porosities, etc.

### 2.4 Climate change

Groundwater flow could be the most important process affecting the performance of a repository at Yucca Mountain (analysis of TSPA-91 and TSPA-93 results show a significant sensitivity to the groundwater-flux parameter). Although the present groundwater flow through Yucca Mountain is thought to be relatively insignificant, few quantitative data are available. The strategy for TSPA-93 is to examine the paleoclimatic record and data from analog sites, then extrapolate future infiltration and percolation at Yucca Mountain. The paleoclimatic record shows that an ice-age cycle of 100,000 years has existed during the recent Pleistocene, and researchers have noted that Yucca Mountain experienced probably 40% but perhaps up to 200% more annual precipitation during the last ice age. Recent data from the U. S. Geological Survey (USGS) has also indicated that the water table under Yucca Mountain was higher by 85 m or more during the last ice age.

For TSPA-93, a series of "wet" (ice-age) and "dry" (interglacial) climates are specified, with a cycle of 100,000 years, but with the dividing time between wet and dry selected at random. Flow is modeled as a sequence of steady states. Infiltration rates average 10 mm/yr for wet climates, and 0.5 mm/yr for dry climates. The water table is allowed to rise up to 120 m during wet climates. These values are greater than what often is believed for the region. Percolation from meteoric sources is assumed to equal infiltration in the TSPA model that describes groundwater flow in fractures (the weeps model) but, for the model that describes flow in both matrix and fractures (the composite-porosity model), percolation is reduced to account for lateral diversion of flow above the repository. For TSPA-93, groundwater mobilized by a repository thermal pulse (see below) is added onto the direct meteoric influx and both are diverted around the dried region where temperatures are above boiling.

## 2.5 Solubility and sorption parameters

Distributions of solubility and sorption parameters for TSPA-93 were obtained through elicitation of experts from Los Alamos National Laboratory (LANL) and Sandia National Laboratories (SNL). Their decisions are based primarily on laboratory data, while keeping in mind that solubility and sorption characteristics of radionuclides are especially dependent on site-specific groundwater chemistry and somewhat dependent on temperature. The experts reaffirmed that most of the actinides are relatively insoluble and highly sorbing in conditions typical of Yucca Mountain. However, neptunium does not adsorb well to tuffs and under oxidizing conditions is relatively soluble. The solubility and sorption values offered by the experts resulted in neptunium often being a major contributor to aqueous releases and doses for the nominal-case scenarios.

## **3** Detailed calculations

## 3.1 Thermal effects

It has become increasingly apparent over the last few years that heat generated by radioactive decay within a repository will influence the environment around it. For TSPA-93, thermal effects related to the thermal dryout, perturbation of the flow field, container corrosion, and spent-fuel alteration are considered.

For TSPA-93, three-dimensional heat-flow calculations were performed to determine parameters thought to be the most critical in defining the impact of the repository thermal pulse. Only heat conduction was considered in the calculations; hydrologic and mechanical effects were not explicitly modeled. All four repository configurations were explicitly modeled, however, accounting for each container location, container thermal output, and container emplacement time. In addition, LLNL supplied TSPA-93 with results of twodimensional hydrothermal calculations with a smeared heat source for comparison (see below).

Critical parameters that are produced relate to the extent that the thermal pulse protects the repository from groundwater by forming a region above boiling temperature (called the protected, or "dryout fraction," of the repository), as well as the extent that it perturbs the environment by displacing vaporized water (water is displaced from the "dryout volume") and diverting meteoric water. In addition, container-wall temperatures and internal waste tempertures are produced. The parameters are used in the probabilistic calculations to redistribute groundwater flow and to adjust the source term. For example, the source term used in the probabilistic calculations allows aqueous corrosion of a container only when liquid water is contacting the container and the container-wall temperature is below 100°C.

Some major results of the thermal modeling are as follows. The boiling isotherm, and therefore the perturbation in the environment, reaches substantial proportions around both the 57-kW/acre repositories and the 114-kW/acre repositories, although more so for the higher thermal loading (Figure ES-5). (For a period, at 114-kW/acre, the entire repository is dried out.) Comparison of the SNL and LLNL thermal modeling shows that repository geometry and the discrete nature of the heat sources are important: the center of 114-kW/acre repositories drops below boiling at around 5000 years with a discretely modeled repository, but at around 9000 years when the repository is modeled as a smeared heat source. Also, the in-drift containers are large discrete heat sources that produce a nonuniform dryout zone at early times. Thermal loading, backfill, and container size have a significant effect on container temperatures: the in-drift containers could see temperatures well above 500°C under certain conditions in a 114 kW/acre repository; the vertically emplaced containers reach temperatures slightly above 200°C in a 57 kW/acre repository.

57 kW/acre repository

114 kW/acre repository



Max dryout volume  $1.5 \times 10^8 (2 \times 10^8) \text{ m}^3$  at 300 (1000) yr. Total collapse by 1300 (2500) yr.

Max dryout volume 6 x  $10^8$  m<sup>3</sup> at 800 yr. Total collapse by 5000 (9000 ) yr.

Figure ES-5. Extent and duration of the volume encompassed by the boiling isotherm (the dryout volume). Where different, the values calculated with a smeared heat source are shown in parentheses.

## 3.2 Saturated zone

A three-dimensional model of steady-state groundwater flow in the saturated zone is constructed for TSPA-93. Geometry for the model consists of an approximately 8-km square section extending from the water table down 200 m. Five strata are included, which because of the tilt of the units intersect the water table at an angle. Two different flow models are superimposed on this geometry: nondiversionary flow, where all fluid entering the "highgradient region" (to the northeast of the repository block) in the tuff aquifers continues to move through the tuff aquifers; and diversionary flow, where part of the fluid entering the high-gradient region is diverted from the saturated tuff downward to continue its flow path in the carbonate aquifers. Flow boundary conditions are taken from a regional saturatedzone flow model. Both the nondiversionary and the diversionary models calibrate to within a meter of water-table elevation at almost all drillholes.

Tracer transport times through the complicated three-dimensional structure are estimated for both models by transport calculations. The calculations involve a nonsorbing tracer released at various points under the repository block. Transport-time distributions are changed to velocity distributions for use in the probabilistic models.

Model calculations indicate that tracer transport times over the 5 km to the accessible environment tend to be less than 1000 years, and they tend to be shorter for the diversionary flow model than for the nondiversionary model. The short transport times, as well as the structure exhibited by the tracer concentrations during transport, indicate that threedimensional modeling is important in the saturated zone. Accurate calibration of the flow systems required that reduced hydraulic conductivities be assigned to the Solitario Canyon fault and the Drill Hole Wash fault; these faults should be investigated for these properties.

## 3.3 Gas flow

A two-dimensional, nonisothermal, transient model of gas flow and  $^{14}CO_2$  transport provide gaseous-transport-time distributions for use in the TSPA-93 probabilitic models. Geometry for the model is taken from three parallel east-west cross sections that incorporate the latest information about site topography and stratigraphy. Only a 57-kW/acre repository is considered. For each calculation, transport times are determined for gas particles traveling from points distributed throughout the repository area to the ground surface. Transport-time distributions for  $^{14}CO_2$  particles are output at 1000-year intervals.

Major results of the gas-flow calculations indicate that  ${}^{14}CO_2$  transport times are short enough to have only marginal effect on cumulative releases. Gas flow depends primarily on temperature and the bulk-permeability distribution within the mountain. Retardation by exchange of  ${}^{14}CO_2$  with bicarbonate in the groundwater is included in the model, and significantly slows transport—typically by an order of magnitude or more. Adsorption onto minerals in the rock is not included, but is potentially important.

## 4 Probabilistic modeling

The models for probabilistic analyses are abstractions of process models. The input parameters for these models come primarily from the data development and detailed modeling activities discussed above. To address uncertainty in parameters, the probabilistic models are used to perform thousands of calculations with parameters picked from probability distributions (the Monte Carlo method). To address uncertainty in models, two alternative conceptual models of groundwater flow in the unsaturated zone are analyzed. To simplify the process, aqueous, gaseous, human-intrusion, and basaltic-volcanism releases are modeled separately.

### 4.1 Nominal-case models

Two alternative conceptual models of flow in the unsaturated zone form the foundation of the nominal-case calculations. These two models were used in TSPA-91, but are refined for TSPA-93 to include an abstracted thermal-effects model (based on the results of the detailed thermal-effects calculations discussed above) and climate change. To calculate aqueous releases and doses, each of these models incorporates: (1) a phemonenological source-term model to calculate radionuclide releases from containers, (2) a transport model to calculate spread of radionuclides through the groundwater, (3) a simplified saturated-zone model (using parameters from the detailed saturated-zone calculations discussed above), (4) a simple drinking-water-dose model, and (5) a simplified gas-flow model (based on the detailed gas-flow modeling discussed above).

#### 4.1.1 The composite-porosity model

The composite-porosity model (also known as the equivalent-continuum model) describes flow through an equivalent porous medium of matrix and fractures using Darcy's law. The major assumption in the model is that a local pressure equilibrium tightly couples flow in the matrix and flow in the fractures; thus, groundwater flow is dominated by capillary forces and only occurs in the fractures when the matrix is saturated. The result is a relatively uniform flow (Figure ES-6). Radionuclide transport also is modeled assuming tight coupling between matrix and fracture transport; thus, when fracture flow does occur in the calculations, diffusion of radionuclides into the matrix slows the transport considerably. At the onset of a climate change, the water table is modeled to rise abruptly, and all radionuclides in the inundated part of the unsaturated zone are transfered immediately to the saturated zone, shortly thereafter forming a spike in the releases at the accessible environment.



Figure ES-6. The composite-porosity model (large-scale regular percolation).

For TSPA-93, flow and transport through the unsaturated zone is modeled in 8 (for the 57-kW/acre repositories) or 5 (for the 114-kW/acre repositories) vertical flow tubes. Each unsaturated-zone flow tube is matched with a horizontal flow tube in the saturated zone.

Calculations using the composite-porosity model indicate that a relatively uniform flow pattern causes a large number of containers to be in a moist or a wet environment. Subsequent aqueous corrosion of these containers leads to widespread failure. (With the sourceterm being used, most aqueous corrosion occurs during the collapse of the repository thermal pulse, when water contacts containers that are near 100°C—see below.) Slow, constant percolation causes slow, constant leaching of waste from the failed waste containers. Long travel times afforded by the slowly percolating water in the unsaturated zone limit cumulative releases over 10,000 years, but are not sufficient to significantly limit peak doses that could occur in a 1,000,000-year period.

The parameters most important to performance depend on the performance measure applied, i.e., cumulative releases or individual dose. For the EPA measure from 40 CFR 191.13, percolation flux is the dominant parameter; when cumulative releases are measured at 10,000 years, the leading edge of a long-term pulse of releases is being measured, and the percolation flux determines how much of that leading edge crosses the boundary to the accessible environment within 10,000 years. For the individual-dose measure, without any time limit, dilution in the environment is most important, but parameters relating to releases from containers are also important. For example, backfill allows more water contact with in-drift containers, causing a substantial number of failures and subsequent radioactive releases.

### 4.1.2 The weeps model

The weeps model describes groundwater flow restricted to locally saturated fractures, which only contact the repository at discrete points (Figure ES-7). Weep location in time and space depends on thermal effects and climate change, and is treated as an inherently probabilistic process. Degradation of containers and releases of radionuclides are limited to the intersections of weeps and containers. Transport of radionuclides through the unsaturated zone is assumed to be instantaneous. The saturated zone is modeled with a single flow tube.

Weeps-model calculations indicate that flowing fractures contacting containers are relatively rare occurrences, and that many containers within a repository remain relatively dry



Figure ES-7. The weeps model (episodic pulses of flow in locally saturated zones, e.g. fractures).

and intact. In-drift containers present a larger cross section to vertical weeps than vertically emplaced containers, and are more readily contacted. Most contacts occur because of the flow perturbation from repository thermal effects or during a wet climate. Although it is typically of shorter duration, the flow perturbation caused by thermal effects is more significant in terms of releases than the increased flow caused by a wet climate. The reason is because the waste containers are susceptible to corrosion primarily when their temperature is above ambient (about 25°C), and especially when near 100°C, which occurs during the collapse of the thermal pulse. At later times when climate change is most often modeled to occur, container temperatures have fallen to levels where the corrosion rates are insignificant. Releases during wet climates typically only occur from a few previously failed containers. Consequently, peak doses occur most often within the first 20,000 years of repository life, and cumulative releases do not increase much after this time.

## 4.1.3 Radionuclide source-term model

For TSPA-93, the YMIM source-term model, developed at LLNL, is directly incorporated into the nominal-case probabilistic models. YMIM is a phenomenological model that calculates container corrosion (including oxidation, general aqueous corrosion, and localized corrosion—pitting), oxidation alteration of spent fuel, and dissolution of radionuclides within spent fuel. Temperature dependence of these processes is included in the model, although the temperature dependence of solubility is not considered in TSPA-93. Inputs include near-field hydrology, container and fuel-rod temperature, and water chemistry. Defective or mechanically failed containers (known as juvenile failures) are consider probabilistically. Several important processes (e.g., steam corrosion and cathodic protection of containers) are not yet included in YMIM.

Use of YMIM within the composite-porosity and weeps models provides two important results: (1) dry oxidation destroys the corrosion-allowance steel outer wall of the in-drift containers during the high-temperature period following backfill, and (2) aqueous corrosion is only significant while container temperatures are above ambient (about 25°C), and it can be especially rapid while temperatures are near 100°C.

### 4.2 Disturbed-case models

#### 4.2.1 Human intrusion

The human-intrusion analysis is based on a FEP sequence involving exploratory drilling, waste container breakage, and radionuclide release via extracted drill core and entrainment in the drilling fluid. Extraction of contaminated rock from a near miss of a failed container is also considered. Present-day drilling technology is assumed. Drilling frequency is based on guidance given in 40 CFR Part 191. A more comprehensive source term that distinguishes between spent-fuel and defense-high-level-waste containers is used in TSPA-93 than was used in TSPA-91. The only performance measure calculated is normalized cumulative release—individual doses are not considered.

Because of the more detailed source term, more variation is seen in the results when compared with the results for TSPA-91. As with TSPA-91, drilling frequency is the most important parameter (and one of the most difficult to predict). The in-drift containers, being larger, are more often hit by drilling and lead to greater releases; however, if it is assumed that only part of the container is exhumed commensurate with the size of the drill, then releases from in-drift containers are similar to releases from vertically emplaced containers.

### 4.2.2 Indirect volcanic effects

For TSPA-91, direct releases of radionuclides caused by intrusion of a basaltic dike into the repository were investigated; for TSPA-93, indirect releases are investigated. The FEP sequence modeled addresses magma intruding rock units near the repository and accelerating waste-container degradation because of the effects of heat and aggressive volatiles. These effects result in changes to the aqueous-transport source term. Dike length, location, and thickness are calculated probabilistically. The temperature of rock adjacent to a magmatic intrusion is calculated as a function of basaltic dike temperature and thickness, distance into the rock, and time. Waste-container corrosion rates are adjusted 10<sup>4</sup> higher to account for aggressive magmatic volatiles. This value is consistent with sulfidization rates.

Analysis results show penetration of heat from a dike only on the order of a few meters. Magmatic volatiles are assumed to intrude only the same distance. Also, the probability of magmatic intrusion, based on geologically realistic values for the volcanic recurrence rate in the Yucca Mountain region and scaled for the two possible areas of the repository, is extremely low over 10,000 years ( $\sim 10^{-4}$  probability of occurrence), and even when extrapolated to 1,000,000 years ( $\sim 10^{-2}$  probability of occurrence). Thus, little contribution from indirect volcanic effects to the nominal-case aqueous releases is observed.

## **5** Results

Results of the TSPA-93 probabilistic modeling are in the form of conditional complementary cumulative distribution functions (CCDFs). The CCDFs show the probability of exceeding a given value of either the EPA sum (i.e., the cumulative release normalized as specified in 40 CFR 191.13) or peak individual dose for a given realization of a probabilistic model. The distributions are conditional because they do not as yet include all possible scenarios. Figure ES-8 shows calculated CCDFs of 10,000-year normalized cumulative release using the composite-porosity model, for all modeled release mechanisms. Only results for a 57-kW/acre repository with vertically emplaced containers are shown; however, with the composite-porosity model, all repository configurations produce similar results (see below). Gaseous releases are predicted to be the most significant, exceeding the EPA standard. Several factors contribute to the large gaseous releases: relatively uniform flow causes a large number of containers to be contacted by water when they are warm (near 100°C) and susceptible to corrosion; upon container failure,  $^{14}CO_2$  is readily released (there is a sizable prompt fraction of  $^{14}C$ , but also, when temperatures are elevated, oxidation alteration of spent fuel proceeds rapidly and allows  $^{14}C$  to escape); and  $^{14}CO_2$  has a short transport time to the ground surface. Releases caused by human intrusion and nominal-case aqueous releases are important, but do not violate the standard. Indirect releases caused by volcanism are both few and low; direct releases caused by volcanism (a TSPA-91 result) are low primarily because the probability of a basaltic dike intruding in the repository in 10,000 years is very low.

As mentioned, the composite-porosity model predicts little influence of the four repository designs on performance. Container size is immaterial because slow, uniform percolation



Figure ES-8. Base-case normalized cumulative release predicted by the composite-porosity model.

of groundwater leads to widescale contact irrespective of size. A slight effect is seen in the normalized cumulative releases over 10,000 years, where the dryout zone created by the hotter repositories results in a several thousand year increase in container lifetime. But for dose calculations over 1,000,000 years, container lifetime and thermal perturbations are too short to make much difference.

The CCDFs of 10,000-year normalized cumulative release calculated using the weeps model are shown in Figure ES-9. Normalized cumulative releases are predicted to be lower for the weeps model than for the composite-porosity model (compare total releases in Figure ES-8 with those shown in Figure ES-9). Releases caused by human intrusion are often predicted to be greater than the nominal-case releases predicted by the weeps model. The reason is that weeps rarely contact waste containers. And within 10,000 years, most weep contacts are caused by groundwater shed around the dryout volume onto unprotected parts of the repository (although many of the resulting contacts are for short periods of time). Gaseous releases are greater than aqueous releases at the highest probabilities because of juvenile failures that release  ${}^{14}CO_2$  without weep contact. Indirect releases caused by volcanism are not calculated for the weeps model and do not appear in the figure. (This figure only represents the base-case design; repository design does influence releases predicted by the weeps model, as discussed below.)



Figure ES-9. Base-case normalized cumulative release predicted by the weeps model.

A comparison of peak individual doses for the two unsaturated-zone flow models is shown in Figure ES-10. The doses shown are for drinking water only and are the peak doses realized within a 1,000,000-yr period. The figure shows that both models predict doses from the repository at levels above background dose (approximately 300 mrem/yr): over 90% of the composite-porosity realizations and about 1% of the weeps model realizations exceed background. These doses are primarily caused by neptunium. Peak doses predicted by the composite-porosity model typically occur because of high percolation rates and watertable rise of a wet climate; those predicted by the weeps model typically occur because of water shed on easily corroded containers (the number of containers contacted by water is a probabilistic result) as the repository thermal perturbation dissipates.

Because transport time is not an issue (except that some actinides decay away before they reach the accessible environment), peak doses are primarily a function of radionuclide release rate from the repository and dilution in the environment. Arid environments typically have little dilution. The release rate is greater, and thus the doses are greater, for the composite-porosity model than for the weeps model because of the larger number of containers that are contacted by water and fail.

Figure ES-11 presents weeps-model peak doses calculated for the four repository designs. The weeps model predicts that larger containers, because of the larger cross section



Figure ES-10. Peak drinking-water dose within 1,000,000 years.

they offer for vertical weeps, have worse performance. A secondary effect is that hotter repositories cause worse performance, because hotter repositories cause a greater perturbation in groundwater flow and an increased probability of containers being contacted by weeps. (These findings are predicated on a number of factors, including that the repository drifts do not divert or concentrate weep flow, that flow returns to the dryout volume coincident with its collapse, etc.) The weeps model predicts similar behavior with the EPA performance measure, although none of the repository designs violate this standard.



Figure ES-11. Peak doses for four repository configurations as predicted by the weeps model.

## 6 Conclusions and recommendations

The large difference in the results of the alternative conceptual models leads to questions about what model best approximates the behavior of the groundwater flow system. Calculations of peak individual drinking-water dose over 1,000,000 years indicate that radionuclides released from a Yucca Mountain repository could experience little dilution, and extremely low release rates from the repository—either from a highly engineered waste container or a system for reducing water contact with containers—might be needed to achieve low individual dose rates. Two possible impacts of repository design on long-term performance are also identified: (1) larger containers could be more readily contacted by weeps and drilling; (2) hotter repositories could cause a greater perturbation in the flow field, resulting in more containers being contacted by weeps. Results from the composite-porosity model indicate that normalized cumulative releases and doses are relatively insensitive to thermal loading and container size and emplacement. The YMIM corrosion models used by both the composite-porosity model and the weeps model predict that most container failures significant to performance occur during decay of the repository thermal pulse---within the first few thousand years. A 10-cm corrosion-allowance overpack for in-drift containers is predicted to be oxidized away within a few hundred years, with no contribution to performance. (The overpack could be more important than indicated because of processes not included in the models currently being used.) Indirect releases from volcanic activity are not found to be significant contributors to overall releases.

Recommendations regarding site-data needs derive primarily from nominal-condition results because human-intrusion results are largely site-independent and volcanism results are comparatively insignificant. The following recommendations are made acknowledging limitations and assumptions in the present models, as well as uncertainities in our knowledge of physical conditions within Yucca Mountain and future events. It should also be mentioned that data are being collected in a number of these areas and an effort is being made to ascertain that the data are useful to determining long-term performance.

- Because of the substantial difference between the results of the two groundwater flow models, the first priority should be the determination of the dominant flow mechanisms (in both time and space) operating in the unsaturated zone at Yucca Mountain.
- Concerning gaseous releases, more data are needed on the spatial distribution of bulk permeability throughout Yucca Mountain and on adsorption of CO<sub>2</sub> to tuff.
- Concerning aqueous releases, characterization at the repository horizon of percolationflux magnitude and distribution (in both time and space) is a high priority.
- Concerning individual doses, a high priority is characterization of the amount of horizontal and vertical dispersion (factors in dilution) in the saturated zone.
- Additional hydrogeologic data from new drillholes are also needed, as is research on scaling of properties and hydraulic characterization of unsaturated fractures in the rock matrix.
- Additional information is needed on heterogeneity and spatial correlations for geostatistical modeling and on cross-correlations among parameters.
- Thermal and hydraulic properties of proposed backfill materials should be determined, and fault-zone hydrogeologic properties should be characterized.
- To develop reliable models of near-field interactions, integrated testing is needed in the areas of waste-container/groundwater contact, radionuclide transport from degraded

containers, coupled thermal-mechanical-hydrologic-chemical processes, and the interactions between natural and man-made system components.

• Further work is also recommended on waste-form alteration and container corrosion under realistic conditions.

Repository design must meet a number of requirements, with long-term performance being but one. Recommendations concerning long-term performance typically come from models that contain a number of limitations. Acknowledging this situation, the following design-related recommendations are made based on the TSPA-93 results.

- Calculated waste-container temperatures are very high for the in-drift cases, well above the thermal goals defined in the SCP. To approach the thermal goals, any backfill used with in-drift emplacement needs to be designed to allow for heat transfer.
- The biggest difference in the performance measures for the four repository configurations that are considered is a result of the difference in container "target size." Reduction in target size or engineered measures to reduce contact between containers and weeps or drilling paths is recommended.
- Container emplacement should be designed to reduce moisture contact with containers (both weeps and uniformly percolating water). Borehole emplacement attempts to achieve this reduction by specifying an air gap surrounding the container. For in-drift emplacement, backfill or a system within the backfill could possibly be engineered to control water contact.

Regulatory change could affect performance assessment for radioactive-waste disposal. If the radioactive-release standard changes to a measure based on individual dose rates over a time period much longer than 10,000 years, significant changes in site-characterization program priorities might be needed, with more emphasis on determining radionuclide release rates. If the standard is changed to an individual-dose standard but the regulated time period remains at 10,000 years, impact on the site-characterization needs would be lessened. Dose calculations require more information than cumulative-release calculations and would require additional characterization of the biosphere in the vicinity of Yucca Mountain. Information extrapolated into the distant future will introduce additional uncertainty into the calculations.

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