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Study Plan 8.3.4.2.4.2
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Study of the Hydrological Properties of the Near-Field Environment

Revision 1

Yucca Mountain Site Characterization Project
Lawrence Livermore National Laboratory

YMP-C21-R3
06/06/94

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
STUDY PLAN APPROVAL FORM

Study Plan Number 8.3.4.2.4.2

Study Plan Title Study of the Hydrological Properties of the Near-Field Environment

Revision Number 1

Prepared by: Lawrence Livermore National Laboratory

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Approved:

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Assistant Manager for Scientific Programs / Date

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Exhibit YAP-2.20.3

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Study Plan 8.3.4.2.4.2
Study of the Hydrological Properties of the Near-Field Environment, Rev. 1: Modeling

Abstract

This study plan describes modeling and experimental activities that fall under Sec. 8.3.4.2.4.2 of the Site Characterization Plan, entitled "Near-Field Environmental Hydrological Properties." The overall objective of this study is to develop a conceptual and quantitative understanding of the thermal-hydrological behavior within the near-field and altered zone of a nuclear waste repository at the potential Yucca Mountain site. This behavior must be understood well enough to allow predictions of expected thermal-hydrological conditions affecting the performance of waste packages and the Engineered Barrier System (EBS). A major factor determining repository performance is how water contacts a waste package, thereby affecting its integrity and (if containment is breached) how radionuclides are dissolved and transported in the EBS and in the unsaturated zone. This thermal-hydrological behavior is controlled by processes that arise within the near-field and altered zone as a result of the interaction of (1) heat-producing waste packages, (2) materials emplaced within (and the configuration of) the EBS, and (3) the ambient hydrological system. Interaction and coupling of thermal-hydrological processes with geochemical and geomechanical processes may also be important. Heat from radioactive decay of waste emplaced in the repository will change the gas- and aqueous-phase fluxes, water content, and other properties of the surrounding rock within a large volume (the Thermally Altered Zone), which may extend vertically from the ground surface to hundreds of meters below the water table, and laterally several kilometers beyond the edge of the repository. The extent of this zone depends on the specific time during the thermal heating and cooling cycle that is being investigated, and on design and operating decisions, such as the areal mass loading (AML, expressed in metric tons of uranium per acre, MTU/acre), the age of waste at emplacement, and how much heat is removed from the repository by the ventilation of emplacement drifts. Analysis of near-field thermal-hydrological behavior requires models extending over these spatial scales. The analysis must also consider a range of potential repository designs under a range of thermal loading conditions.

This study requires the iterative interaction of experimental and modeling activities. The modeling activities include parameter-sensitivity studies that help identify properties and parameters that must be determined in laboratory- and field-scale experiments, and scoping calculations that help in the design of those experiments. As they are determined, these property and parameter values are incorporated in ongoing model calculations (using the V-TOUGH and NUFT codes) of thermal-hydrological behavior in the near-field, the EBS, and altered zone. Laboratory- and field-scale model validation experiments are also needed to confirm that important processes have been adequately incorporated in our conceptual and numerical models of the near-field and altered zone. Model validation is greatly facilitated by hypothesis testing, whereby hypotheses critical to EBS-affecting thermal-hydrological behavior are established and then resolved through a combination of analysis (including bounding analysis) and testing (both laboratory- and field-scale).

Work performed in this study has been divided into three main groups of activities: (1) model development and analysis of thermal-hydrological flow, (2) hydrological property measurements, and (3) laboratory-scale validation experiments. Field-scale validation experiments needed for this study are covered by other study plans.

1. Purpose and Objectives

1.1 Purpose

The purpose of this Study Plan (SP), is to describe studies known as Near-Field Environment Hydrological Properties (NFEHP) in the Site Characterization Plan (SCP) Sec. 8.3.4.2.4.2.

1.2 Objectives

The objectives of this study are to conduct experimental and modeling studies relevant to the entire range of potential thermal loads to:

- Identify hydrological and transport processes at Yucca Mountain that significantly affect WP performance, radionuclide release and transport.
- Develop a detailed conceptual and quantitative understanding of repository-heat-driven flow processes that govern the WP environment, including temperature, relative humidity, and flow conditions throughout the repository and EBS.
- Conduct experiments and develop related models to assess the impact of repository-altered matrix and fracture properties on nonequilibrium fracture flow and to assess the conditions under which nonequilibrium fracture flow will occur.
- Develop and conduct laboratory and *in situ* tests for model validation and hypothesis testing that provide the basis for confidence building and substantiation of compliance with the substantially complete containment and controlled Engineered Barrier System (EBS) release requirements.

The overall objective of this study is to understand the thermal-hydrological processes expected to occur within the near field and altered zone of a nuclear waste repository after WP emplacement. The scope of this SP includes the near-field environment of WPs and the altered zone. The near-field is the region that most directly influences the WP, i.e., it is the region whose properties and processes directly influence the EBS design and performance. The altered zone is the region significantly affected by emplacement of WPs, primarily by the radioactive decay heat. Heat from radioactive decay of waste emplaced in the repository will change the gas- and aqueous-phase fluxes, water content, and other properties of the surrounding rock within a large volume (the Thermally Altered Zone), which may extend vertically from the ground surface to hundreds of meters below the water table, and laterally several kilometers beyond the edge of the repository. The extent of this zone depends on the specific time during the thermal heating and cooling cycle that is being investigated, and on design and operating decisions, such as the areal mass loading (AML, expressed in metric tons of uranium per acre, MTU/acre), the age of waste at emplacement, and how much heat is removed from the repository by the ventilation of emplacement drifts. Analysis of near-field thermal-hydrological behavior requires models extending over these spatial

scales. Depending on the process of concern, the size of the altered zone will be determined by thermal loading conditions.

The thermal-hydrological processes reflect perturbations expected to be induced by the emplacement of nuclear WPs and the subsequent effects due to heat and radiation. They will have significant effects on chemical, mineralogical, hydrological, thermal, and mechanical characteristics of the near-field environment. The characteristics of the near-field environment will affect the performance of the WPs and the release rate of radionuclides from the near field to the far field of a repository.

This study plan describes the modeling and laboratory-scale experimental activities that are required to identify and quantify the thermal-hydrological processes and properties that are important to WP and EBS performance. The study of hydrological properties of the WP environment, as described in Sec. 8.3.4.2.4.2 of the SCP, includes laboratory experiments and model calculations. The results of the laboratory and field-scale experiments will be used to help develop, calibrate, and validate the conceptual and mathematical models required to develop adequate abstractions of EBS performance.

The evolution of the thermal and radiation output of the WPs will result in an environment whose characteristics may change with time. To assure that WP design considerations account for this evolving environment, it is necessary to determine the range of conditions that exist in the pre-emplacement and may develop in the post-emplacement near-field environments.

The primary objective of this study is to develop an understanding of near-field thermal-hydrological behavior that is sufficient for making long-term predictions of the near-field environment (including the WPs and the EBS). More specifically, the primary objective is to develop and build confidence in conceptual and mathematical models of near-field thermal-hydrological behavior that are the basis for subsystem models of the EBS. To meet this objective, the modeling and experimental activities of this study must be conducted in a highly iterative manner (and in a highly iterative manner with activities in other studies). The modeling activities help provide insight into the processes and properties that must be understood and quantified (experimentally), while the experimental activities help confirm the relevance (or importance) of those processes and quantify the key properties and parameters. A combination of laboratory- and field-scale experiments will help confirm that various processes are adequately represented in models at various scales. Model validation is also greatly facilitated by hypothesis testing, whereby hypotheses critical to EBS-affecting thermal-hydrological behavior are established and then resolved through a combination of analysis (including bounding analysis) and testing (both laboratory- and field-scale).

1.3 Relationships to Programmatic Objectives

1.3.1 Site Characterization Plan Issues and Information Needs

The SCP is divided into a series of issues and information needs that address those issues. Issue 1.10 (Post-closure Waste Package Characteristics) deals with the service environment of the waste package. Sec. 8.3.4.2 of the SCP states that, "The waste package environment, upon initial emplacement of the package, will depend on the ambient conditions at the repository level and how those conditions are altered by the repository construction and operation. The environment following emplacement will depend on the initial emplacement conditions and how those conditions are altered by the waste package. Therefore, there is an interactive process between design and environment characterization. The design is initially based on the ambient conditions and a prediction of how those conditions would alter under the stresses applied by repository construction and waste emplacement. Once a design is available, analysis of that design provides a set of environmental stress factors. Testing is then done to determine the effect of those stresses, such as thermal and radiation fields and mechanical stresses, on the package environment. Based on those tests and subsequent analysis, designs may be modified and the test and analysis cycle repeated."

The ability of the waste package to meet the objective of isolating nuclear wastes will depend on the interactions between the waste packages and the environment into which they are emplaced. Performance Issues 1.4 and 1.5, and their associated Information Needs (IN), address these concerns.

Issue 1.4: Will the waste package meet the performance objective for containment as required by 10 Code of Federal Regulations (CFR) 60.113?

IN 1.4.3: Scenarios and models needed to predict the rate of degradation of the containment barrier.

IN 1.4.4: Estimates of the rates and mechanisms of container degradation in the repository environment for anticipated and unanticipated processes and events, and calculation of the failure rate of the container as a function of time.

IN 1.4.5: Determination of whether the requirement for substantially complete containment of the waste packages is met for anticipated processes and events.

Issue 1.5: Will the waste package and repository engineered barrier system meet the performance objective for limiting radionuclide release rates required by 10 CFR 60.113?

IN 1.5.3: Scenarios and models needed to predict the rate of radionuclide release from the waste package and engineered barrier system.

IN 1.5.4: Determination of the release rates of radionuclides from the waste package and engineered barrier system for anticipated and unanticipated events.

IN 1.5.5: Determination of the amount of the radionuclides leaving the near-field environment of the waste package.

The requirements that pertain to specific design attributes of the waste package environment are detailed under IN 1.10.1 and 1.10.4 of Issue 1.10.

Issue 1.10: Have the characteristics and configurations of the waste packages been adequately established to (a) show compliance with the post-closure design criteria of 10 CFR 60.135, and (b) provide information for the resolution of the performance issues?

IN 1.10.1: Design information needed to comply with post-closure criteria from 10 CFR 60.135(a) for consideration of the interactions between the waste package and the near-field environment.

IN 1.10.4: Post-emplacement near-field environment.

1.3.2 Applicable Regulations and Requirements

The activities described in this study plan address the requirements contained in Nuclear Regulatory Commission (NRC) rule 10CFR96 and in Sec. 135(a), rule 10CFR60, which states, in part:

"Packages for high-level waste (HLW) shall be designed so that the in situ chemical, physical, and nuclear properties of the waste package and its interactions with the emplacement environment do not compromise the function of the waste packages or the performance of the underground facility or the geologic setting."

"The design shall include but not be limited to consideration of the following factors: solubility, oxidation/reduction reactions, corrosion, gas generation, thermal effects, mechanical strength, mechanical stress, radiolysis, radiation damage, radionuclide retardation, leaching, fire and explosion hazards, thermal loads, and synergistic interactions."

All quality assurance activities will be conducted in accordance with the U. S. Department of Energy, Office of Civilian Radioactive Waste Management, Quality Assurance Requirements and Description (DOE/RW-0333P). Specific quality assurance Implementing Procedures will provide information required to perform the work described in the Study Plan.

1.3.3 Related Studies

The potential repository horizon at Yucca Mountain is in a devitrified, partially saturated, nonlithophysal, densely welded and fractured tuff. Work to date suggests that the potential repository horizon has a mean matrix porosity of about 11.3% [Nimick and Schwartz, 1987] and a mean water saturation of 65% [Montazer and Wilson, 1984]. Therefore, the rock mass consists of host rock with pore spaces filled with air and water.

Waste package (WP) emplacement will impose thermal and radiation loads on the rock mass. The thermal load will increase the near-field and altered zone environment temperatures and create a region of hot and drier rock around the WP. Rapid evaporation or possible boiling of the vadose water will occur where the temperatures are sufficiently high. A buildup of pore gas pressure is expected to develop in the

unfractured rock mass. Steam and vapor are expected to flow within the fractures and unfractured rock in response to the gas pressure gradients that develop. A region of increased saturation is expected to form adjacent to and outside of the dry rock region as steam condenses within the cooler portions of the rock mass. Part of this condensation will occur along fractures. Some of the condensation may move from the fractures into the matrix due to high suction potential in the matrix. The remaining water in the fracture may remain immobile due to capillary forces, or it may flow along the fracture under gravity, depending on local fracture apertures and orientations. Because the power output of WPs decreases with time, the hot region of the rock mass eventually cools, and the dry region will slowly regain some of the water previously transported to the surrounding areas. The activities described below will provide laboratory tests of concepts in the numerical models that will be used to predict the thermal-hydrological processes in the near-field rock mass after the emplacement of WPs. They will also provide input data to the numerical models and possibly guide revisions of the concepts in the numerical models.

To assure that the WP emplacement configurations do not compromise the lifetime performance of the repository or the WPs, their design must also consider environmental features. Processes affecting the post-emplacement environment will also influence WP performance. The activities described below will provide input to performance assessment models for the near-field environment and the repository.

Four broad categories of activities provide the information necessary to characterize the chemical, mineralogical, hydrological, thermal, and mechanical properties that constitute the post-emplacement near-field environment. A fifth category of activities provides the information necessary to understand the coupled thermal-mechanical-hydrological-geochemical processes in the near-field environment.

Tests, experiments, and numerical geochemical simulations described in Study Plan 8.3.4.2.4.1, entitled "Characterization of Chemical and Mineralogical Changes in the Post-Emplacement Environment," address the category of activities that define the chemistry of water that may contact WPs. The need for this information is specified in the issue resolution strategy for Issues 1.4 and 1.5, where limits are placed on the quality of water that may contact the WPs. The information gained through those activities will characterize the near-field mineralogy and chemistry. The interactions of tuff, water, water vapor, and WP components in the presence of elevated temperature and radiation fields are considered. Those activities will establish the nature of chemical and mineralogical evolution of the near-field environment for anticipated and unanticipated conditions involving various degrees of water saturation.

Study Plan 8.3.4.2.4.5, entitled "Characterization of the Effect of Man-Made Materials, Chemical and Mineralogical Changes in the Post-emplacement Environment," addresses a second category of activities that define the effect of man-made materials in a repository on the chemical and mineralogical changes.

Tests, experiments, and numerical simulations described in Study Plan 8.3.4.2.4.3, entitled "Geomechanical Attributes of the Waste Package Environment," address a third category of activities that establish the near-field thermal and mechanical properties of the tuff in the near-field environment. This category of activities will define the range of

values of parameters that influence borehole or emplacement drift stability and thermal response of the tuff. The study plan describes the rationale and technical attributes of activities that determine these characteristics of the WP environment. The need for this information is specified in the issue resolution strategy for Issue 1.5 where limits are placed on the failure rate of waste containers.

The fourth category of activities, which are described in the present study plan, incorporates numerical model simulations, laboratory measured hydrological properties of tuff, and laboratory model validations to establish the quantity of water that may contact WPs. The model calculations that are developed, calibrated, and validated in this study will be used to compare with the result of field tests, described in Study Plan 8.3.4.2.4.4. These models will also be used to predict the near-field environment that will be used in WP performance assessment. This plan describes the rationale and technical attributes of activities that help determine the quantity of water that may contact the WP. The need for this is specified in the issue resolution strategy of Issue 1.5 where limits are placed on the quantity of water that may contact waste containers. The information gained in these activities will be used to characterize the near-field hydrological properties of the tuff under anticipated and unanticipated conditions as required in Issue 1.10. These activities will define the range of values of parameters for anticipated and certain unanticipated conditions that influence fluid flow processes in the near-field environment.

Tests, experiments, and numerical simulations described in Scientific Investigation Plan (SIP) SIP-NF-02, entitled "Large Block Testing of Coupled Thermal-Mechanical-Hydrological-Chemical Processes," address the fifth category of activities that investigates the coupled processes of heat, geomechanics, hydrology, and geochemistry that may occur in the rock mass in the near-field environment. These activities will investigate the mechanical responses of tuff to the thermal loading of the heat sources; the effect of heat and the mechanical responses of tuff on the movement of moisture around the heat sources; and the chemistry of the aqueous and gas phases that may be affected by heat. The need for this information is specified in the issue resolution strategy for Issues 1.4 and 1.5. This outcrop testing of coupled process will be followed by larger scale field tests in the Exploratory Study Facility (ESF), as described in Study Plan 8.3.4.2.4.4, entitled "Engineered Barrier System Field Tests."

Several YMP studies will measure properties of the ambient hydrological system of the unsaturated zone. The results of these studies will be used in this study. A few ambient property measurements will be made in this study as a quality check. If the ambient results from this study agree with those of the other studies, then there will be increased confidence in the methodology used in this study to obtain higher temperature data. The other studies include the following:

- 8.3.1.2.2.3, Characterization of percolation in the Unsaturated Zone, Surface Based, and
- 8.3.1.2.2.4, Characterization of percolation in the Unsaturated Zone, ESF.

Another YMP study, 8.3.1.20.1.1, Characterization of the Altered Zone, will address the coupling between hydrology, geomechanics, and geochemistry. The results of the present study, thermal-hydrological coupling, will provide input to that study.

1.4 Near-Field Thermal-Hydrological Behavior

This study focuses on thermal-hydrological processes that affect the environment of the Engineered Barrier System (EBS), including backfill, waste package (WP), man-made materials, and waste-form. Functionally, near-field processes are those EBS-affecting processes that are the result of, or are affected by, the EBS itself (including radioactive decay heat from the WPs), and processes that must be understood to predict EBS performance that are not sufficiently covered in other study plans. The spatial extent of near-field processes depends on individual processes and on the EBS design (particularly the thermal design). The interaction and intercoupling of thermal-hydrological processes with geochemistry and geomechanics is also part of this study.

1.4.1 Fundamental Thermal-Hydrological Processes

Thermal-hydrology comprises processes that result from coupling basic thermal and hydrological processes. Thermal processes include the generation and transport of thermal energy. Hydrological processes involve the generation and transport of water in both the liquid and vapor state. The generation and transport of dissolved chemical species, including radionuclides, result from thermal, hydrological, and geochemical process that may be coupled and thus may influence one another.

The following are sources and conditions affecting the thermal energy balance at Yucca Mountain and the potential repository:

- Generation of thermal energy by radioactive decay of nuclear waste.
- Generation of thermal energy by geothermal sources below Yucca Mountain, as evidenced by the geothermal gradient.
- Net energy flux at the ground surface from solar radiation and from eddy diffusion of latent heat from evaporation and latent heat of condensation of water vapor.
- Incoming thermal energy that is advected by infiltrating water.

The following are the basic mechanisms that may be involved in the transport of thermal energy at Yucca Mountain and the potential repository. These will be investigated further to determine the extent to which they are operative at Yucca Mountain:

- Thermal conduction in the bulk rock matrix.
- Aqueous-phase advection, including transport of latent heat of water vapor.
- Gas-phase advection.

- Species diffusion in the aqueous phase.
- Species diffusion in the gas phase.
- Thermal radiation, conduction, and convection from the WP to the drift walls.
- Storage of thermal energy in the rock matrix by heat capacity.
- Change in thermal energy from condensation of water vapor and evaporation of liquid water.

The following are basic hydrological processes involved in the movement of water at Yucca Mountain and the potential repository:

- Aqueous-phase advection of liquid water driven by aqueous-phase pressure gradients.
- Aqueous-phase advection of liquid water driven by matric potential gradients.
- Aqueous-phase advection of liquid water driven by gravitational and buoyancy forces.
- Gas-phase advection of water vapor driven by gas-phase pressure gradients.
- Gas-phase advection of water vapor driven by gravitational and buoyancy forces.
- Gas-phase diffusion of water vapor, possibly including enhanced diffusion [Philip and De Vries, 1957].
- Evaporation of water.
- Condensation of water.
- Partitioning of water between aqueous and gaseous phases.
- Vapor-pressure-lowering phenomena [Edlefsen and Anderson, 1943; Nitao and Bear, 1994].
- Changes in permeability and porosity as a result of dissolution and precipitation of minerals.

The following are chemical and hydrological transport related processes at Yucca Mountain and the potential repository:

- Aqueous-phase advection.
- Gas-phase advection (for gaseous species).
- Aqueous-phase diffusion.
- Gas-phase diffusion.
- Adsorption on solids.
- Colloidal suspensions.
- Dissolution reactions.
- Precipitation reactions.

- Radioactive decay.
- Chemical reactions.

The following are some potential geomechanical processes related to thermal-hydrology at Yucca Mountain and the potential repository:

- Change in fracture permeability as a result of thermal stresses.
- Fracturing of the rock matrix as a result of increased pore pressure during boiling of water in the matrix blocks.
- Microfracturing of rock matrix as a result of increased stresses.
- Increased fracture propagation as a result of the presence of liquid water or steam.
- Change in geomechanical properties of the fracture due to mineral precipitation.
- Change in porosity and geomechanical properties as a result of temperature and saturation changes.

The following are the primary conditions addressed in this study that could bear on WP failure at the potential repository:

- Thermodynamic conditions in the EBS and at the WP surface, including gas-phase pressure P_g, relative humidity RH, and temperature T.
- Aqueous-phase flux distribution in the EBS and at the WP surface.
- Gas-phase flux distribution in the EBS and at the WP surface.

The following are related to the source-term release from breached WPs at the potential repository:

- Amount of water flowing around the waste-form.
- Thermodynamic properties of the water contacting the waste-form, including its chemistry and temperature.
- Diffusion of radionuclides from waste-form to rock.
- Advection of radionuclides from waste-form to rock.

1.4.2 Conceptual Model of Thermal-Hydrological Phenomena

Phenomena of interest in this study result from the interaction of basic physical processes. The following are some current conceptual models of key thermal-hydrological processes that will be studied and analyzed.

1.4.2.1 Fracture-Matrix Aqueous-Phase Flow

Net vertical movement of the aqueous-phase liquid through the rock matrix is very slow, especially in the welded units, because of their very low permeability. Fast movement of water can only occur in fractures. This water may arise from three origins:

- Natural infiltration of rainfall and snowmelt.
- Condensate generated under *boiling conditions*.
- Condensate generated under *sub-boiling conditions*.
- Dehydration of hydrous minerals, such as clays or zeolites.

The first source arises from the ambient system; the second and third are generated by radioactive decay heat, primarily from spent nuclear fuel (SNF). Heat-driven, buoyant vapor flow and the binary diffusion of water vapor and air may play important roles in condensate generation [Buscheck and Nitao, 1994a]. As water flows down a fracture, its movement is slowed by imbibition into the rock matrix. If the flux in the fracture is sufficiently slow, the matric potentials in the fracture and matrix will be nearly equal, and the progress of the front will be very slow. The equivalent continuum approximation (discussed in Sec. 2.3.1.2) is valid is such cases. If the flux into the fracture is large enough, the front will travel rapidly down the fracture [Nitao et al., 1993], and the mathematical model used must account for the disequilibrium between fracture and matrix flow; under these conditions, the equivalent continuum approach is not valid.

Infiltration of liquid water is strongly affected by the connectivity of the fracture network system and by the ability of the matrix to absorb water. Significant attenuation of fracture flow may take place in the vitric nonwelded units (principally PTn and CHnv), which have a higher sorptivity to water [Buscheck et al., 1991]. These units may also be less fractured than the welded units.

1.4.2.2 Fracture-Matrix Gas-Phase Transport of Water Vapor

Gas-phase advective transport of water vapor is driven by (1) gas pressure gradients caused by barometric pumping and generation of water vapor by radioactive decay heat, (2) thermal expansion of the gas phase driven by radioactive decay heat, and (3) density gradients caused by the geothermal gradient, seasonal temperature differences, and temperature gradients created by radioactive decay heat. Gas-phase transport over extended distances will occur primarily by advection in fractures when bulk advective velocities are high. At low velocities, advective gas-phase transport will occur in both matrix and fractures. Diffusion of water vapor into the matrix will retard the overall movement of water vapor for the low-velocity case, where gas-phase transport is not dominated by fracture flow.

Diffusive transport of water vapor is treated by Fick's Law, i.e., the flux is proportional to the local mass fraction gradient of water vapor in the gas phase. If local thermodynamic equilibrium prevails, the mass fraction of water in the gas depends on temperature, total gas pressure, and aqueous-phase saturation. Gradients in any of

these quantities can lead to diffusion of water vapor. For example, all other factors being equal, vapor diffusion will occur from regions of higher to regions of lower temperatures because water vapor mass fraction in the gas phase increases with temperature. Gas-phase diffusion can occur in both the fracture and matrix. Diffusion in the matrix can be affected by the amount of water in the matrix because a higher aqueous saturation will reduce the gas-filled pore space and increase the tortuosity to the gas phase. Diffusion of water vapor can be "enhanced" under a temperature gradient [Philip and De Vries, 1957] relative to the diffusion of a noncondensable gas.

1.4.3 Effect of Radioactive Decay Heat on Moisture Movement

An important feature of the unsaturated zone at Yucca Mountain is its high fracture density. Moreover, the Topopah Spring tuff, which occurs at the potential repository depth, is one of the most densely fractured hydrostratigraphic units. This is significant because, without fractures, the rock throughout most of the unsaturated zone (including the repository horizon) would be extremely impermeable. In general, decay heat moves moisture by (1) vaporization, (2) driving water vapor from high to low gas-phase pressure, (3) condensation, and (4) gravity- or capillary-driven flow of condensate. Without fractures, the rock would be too impermeable to allow significant vaporization and advective movement of water vapor. The flow of condensate would also be very slow. A system of connected fractures facilitates significant repository-heat-driven fluid flow as well as natural infiltration. Enhanced gas-phase diffusion may significantly contribute to water vapor transport in unfractured (relatively impermeable) rock.

Model calculations have indicated that the general thermal-hydrological behavior of the repository can be divided into three sequential periods: drying, quasi-steady, and rewetting [Buscheck and Nitao, 1993a, 1993b]. The concept of these three periods is applicable over dynamically changing *spatial* regimes. Therefore, at a given time, certain locations in a repository (such as the perimeter) may already be in the rewetting regime while other locations (such as the center of the repository) may remain in the drying regime.

During the initial *drying period*, the rate of evaporation is greater than the rate of condensation. Depending on the thermal loading of the repository, the drying period can last from tens of years to up to about two thousand years and can extend several to hundreds of meters vertically [Buscheck and Nitao, 1993a, 1993b]. The important thermal-loading parameters include:

- Areal Mass Loading (AML, expressed in metric tons of uranium per acre, MTU/acre).
- Age of spent nuclear fuel.
- Depth of the repository below the ground surface.

During the drying period, the cumulative volume of water removed from the WP zone increases monotonically. As the repository heating rate decreases and the volume of the boiling region increases, conditions stabilize to a quasi-steady state in which the rate of evaporation is equal, or nearly equal, to the rate of condensation. Temperature, aqueous

saturation, and relative humidity *RH* in the repository change very little during this period. Depending on the AML and SNF age, this *quasi-steady period* may last up to several thousand years, and the drying/rewetting front may be located well away from the repository. As the repository heating rate further decreases, the *rewetting period* begins as temperature, degree of aqueous saturation, and *RH* begin to slowly return to ambient values. During the rewetting period, the net volume of water removed from the WP zone decreases monotonically.

During all three periods, heat is transferred between the WP and the drift walls by a combination of thermal radiation, conduction, and convection. Thermal radiation will play a major role in an open drift, whereas conduction is likely to dominate heat transfer in a backfilled drift. Buoyant gas-phase convective heat transfer may be significant in an open drift or if k_b of the backfill is high enough. The relative contribution of these heat transport processes will be analyzed by drift-scale model calculations. The rise in temperature may change the chemical, mechanical, and thermal-hydrological properties of the backfill material.

Under sufficiently high thermal loading conditions (i.e., high enough global AML or high enough local AML), the heat of decay will raise temperatures in the surrounding rock mass to the boiling point of water within the matrix. Whether the water actually boils, in the sense of forming bubbles within the aqueous phase, or merely evaporates rapidly enough that the partial pressure of water P_v within the matrix is equal to the local saturated vapor pressure of water P_{sat} at the local temperature, the terms "boiling zone," "boiling point," and the like are used in subsequent discussion herein. The term "above-boiling" is used to refer to superheated conditions. Boiling will occur near the fracture surfaces first and proceed into the matrix. The increase in gas pressures in the matrix caused by the generation of steam leads to an advective gas-phase flux that transports steam from within the matrix blocks to the nearest fracture. The increasing gas pressure in the matrix increases the boiling point of the water, so that temperatures in the boiling zone can be above the ambient boiling point, with some water remaining in the pores in the interior of the matrix blocks. Some diffusion of water vapor also drives steam from the matrix to the fractures, but the diffusive flux of water vapor is not significant except for very low matrix permeabilities, in which case advective velocities are low. The progress of the boiling front is relatively slow and is expected to be on the order of a few centimeters per year except during the first few hundred years, during which it could move at decimeters per year to as much as a few meters per year immediately after emplacement.

Once the steam reaches a fracture, it is transported by advection and diffusion. Advective fluxes are driven by gas-pressure and gas-density gradients (buoyancy). If the bulk permeability k_b of the rock mass is high enough, gas pressures in the fracture cannot build up much in the boiling region; under these conditions, density gradients dominate the advective gas-phase flux at the repository, and convection cells may develop. The size of these cells depends on the scale of connectedness of the fracture network. These cells can carry steam from the boiling zone both below and above the repository to a condensation region above the upper boiling zone.

If k_b is not high enough for buoyant gas-phase convection to dominate vapor transport, then the advective gas-phase flux is dominated by the boiling-driven gas-phase pressure gradients, which drive steam from the boiling zone away from the repository, where it condenses. If k_b is low enough, dryout due to boiling may be substantially suppressed (i.e., throttled). This throttling can arise in two ways. Throttling can arise because the gas-phase conductivity in the fractures is low enough to restrict fracture flow and cause a buildup in gas-phase pressure that results in an increase in the saturation temperature T_{sat} (i.e., the boiling point) in the fractures themselves. Throttling that results from restricted fracture flow has been modeled with equivalent continuum models [Buscheck and Nitao, 1993a; Buscheck and Nitao, 1993b], and with discrete fracture-matrix models [Buscheck and Nitao, 1991], and has also been analyzed with an analytical model [Manteufel and Powell, 1994]. Throttling can also result from restricted matrix-to-fracture flow that causes a gas-phase pressure buildup within matrix blocks. Thus, throttling may be more pronounced in sparsely fractured regions (with large matrix blocks) and may be less pronounced in intensely fractured regions (with small matrix blocks). Throttling that occurs because of restricted matrix-to-fracture vapor flow has been modeled with discrete fracture-matrix models [Buscheck and Nitao, 1991]. The discrete fracture-matrix model used by Nitao and Buscheck (1995) can also be extended to address throttling caused by restricted fracture flow and by restricted matrix-to-fracture flow. Where gas-phase advection is throttled, dryout may still be substantial if binary gas-phase diffusion is very enhanced. As boiling continues, water vapor displaces air away from the WPs and may replace it completely for sufficiently high AMLs. Knowing whether (or for how long) air is displaced from the repository is important in assessing the effect of oxidative corrosion on WP integrity.

As liquid water forms in the condensate zone, it will condense within the matrix pores or within the fractures. The potential effects of condensation within the matrix pores are unknown at present, and will be examined by a limited amount of detailed, small-scale modeling. If water condenses within the fractures, it will imbibe into the matrix or flow downward by gravity in a process sometimes called "condensate shedding." The theory of fracture-matrix interaction [Nitao and Buscheck, 1991; Nitao et al., 1993] indicates that if the rate of boiling, and hence the rate of condensate generation, is high enough, then condensate flow is fracture-dominated, and downward flow by gravity can be very fast as long as there is a sufficiently connected fracture network, even if the matrix is not completely saturated. A portion of the condensate drainage above the repository can return directly to WPs, where it reboils if the WP is hot enough. Some of the remaining condensate may drain through the pillars between the emplacement drifts, or through the drifts between the WPs, and leave the vicinity of the repository, resulting in a net removal of water from the near-field environment. Some of this condensate may also drain onto cooler WPs that are not hot enough to reboil this water. The cyclic boiling and condensation of water can set up what has been called a gravity-driven heat pipe. Pruess and others [1984, 1990] were the first to model the heat-pipe effect in the context of thermal-hydrological behavior at Yucca Mountain. Their calculations pertained to a capillary-driven heat pipe. The effect of a gravity-driven heat pipe has been demonstrated in repository- and sub-repository-scale model

calculations [Buscheck and Nitao, 1993a; Buscheck and Nitao, 1993b]. Under most conditions, the heat-pipe mechanism is more efficient than thermal conduction in transporting heat away from the repository.

Initially, the boiling fronts propagate radially away from each of the emplacement drifts. Before these cylindrical boiling zones coalesce, the rate of boiling can be fairly high. Condensate shedding through the repository horizon is most likely to occur during this period. As these zones coalesce, eventually forming a continuous surface or sets of continuous surfaces, and as the coalesced boiling zone propagates farther away from the repository horizon, the specific heat flux (the heat flux per unit area of the boiling front, in W/m^2) at the boiling front decreases. The specific boiling flux (the mass flux of generated steam per unit area of the boiling front, in $kg\ s^{-1}\ m^{-2}$) may become so low that the resulting low condensate flux can be fully imbibed by the matrix until the matrix saturates, at which stage fracture flow occurs. Under these conditions, the continual, long-term refluxing of condensate above the upper boiling region occurs under capillary equilibrium between the fractures and matrix and is, therefore, adequately described by the equivalent continuum approach discussed in Sec. 2.3.1.2 [Buscheck and Nitao, 1993b]. Some condensate may be lost along the sides of the upper boiling region at the outer edges of the repository, or at the edges of repository panels, if there is sufficient fracture connectivity. Natural infiltration fluxes can add to the condensate flux and must be included in "performance analyses" (analyses related to the EBS and to UZ transport).

Vaporization of water can occur even under sub-boiling conditions, because the higher temperatures around the WPs and the surrounding rock increase the mass fraction of water vapor in the gas phase. This higher water vapor concentration in the gas phase can advect and diffuse away from the repository horizon. Advective gaseous transport of water vapor for sub-boiling repositories is dominated by density gradients, because there is little increase in pressure due to vaporization of water. Depending on k_b, density-driven advection can move at least as much water from below to above the repository as the advection driven by an above-boiling repository [Buscheck and Nitao, 1994a].

As mentioned above, buoyant gas-phase convection cells can form at different scales depending on whether k_b at a given scale is large enough. Thus, it is possible to form convection cells at drift, repository, and mountain scales. The location and extent of the cells are controlled by heterogeneities in the natural system. High-k_b rubbelized zones and faults are key candidates for mountain-scale convection cells. These cells may lead to condensate refluxing because of the large vapor flux, and they may dominate the thermal-hydrology, leading to less predictable conditions at the repository.

Repository heat can also induce the formation of convection cells in the saturated zone (SZ), even for a sub-boiling repository [Buscheck and Nitao, 1993b]. These cells may dominate the potential to transport radionuclides in the SZ for tens of thousands of years; they may also significantly affect the heat transfer characteristics of the SZ, which, in turn, can influence heat flow in the UZ and EBS.

Regardless of the AML, repository-heat-driven temperature gradients are expected to extend all the way to the ground surface, resulting in a gradient in water vapor mass

fraction from the repository all the way to the ground surface. Water vapor will therefore diffuse to the ground surface, where it is transferred to the atmosphere by eddy diffusion, whose rate depends on temperature, *RH*, and wind velocity. These conditions can fluctuate diurnally and seasonally. Precipitation and plant transpiration processes may also play a strong role. Ground surface conditions can have a noticeable effect on the overall moisture balance and on local conditions in the EBS. Conversely, repository heat can dominate the moisture transport and aqueous saturation conditions at the ground surface.

During the rewetting period, the mechanisms for restoring the aqueous-phase saturation and *RH* conditions in the repository to ambient (humid) conditions are matric-potential forces and the binary gas-phase diffusion of air and water vapor. The rate of rewetting has important implications for the EBS environment during this period. Rewetting by matric forces may be retarded by fractures or rubbelized zones and by low-permeability regions. Changes in fracture properties, such as filling of apertures by precipitates formed during refluxing, may also retard rewetting. Although temperature decrease in the interior of the repository is largely governed by one-dimensional (vertical) heat flow, heat flow becomes increasingly two-dimensional as the repository edge is approached, thereby increasing the cooling rate [Buscheck and Nitao, 1994b]. This edge-cooling effect reduces both the magnitude and duration of the temperature buildup responsible for driving moisture away from the repository. Rewetting the interior of the repository to ambient conditions is also largely a one-dimensional process, but again the process becomes increasingly two-dimensional as the edge is approached. Edge-cooling/rewetting effects decrease the time required to restore the repository edge to ambient conditions.

1.4.4 Coupled Thermal-Hydrological and Geochemical Phenomena

The geochemical environment of the near-field and the EBS will affect any liquid water that may contact the WPs, the waste-form, and any radionuclides released into the near-field. The composition of the aqueous phase will depend on the isothermal and nonisothermal flow processes and reaction history experienced by packets of mobile fluid along their respective flow paths. Intermediate flow processes, such as condensate refluxing and evaporation, can concentrate different dissolved components. Condensate may dissolve minerals from fracture walls as it drains down fractures and then precipitate those (or other) minerals as it boils. These changes may significantly increase or decrease fracture apertures along various intervals, thereby altering the bulk permeability distribution. Solubility and dissolution of minerals depend on temperature changes, among other things. The geochemistry of water from surface infiltration contacting WPs will vary depending on whether it drained quickly down fractures or migrated slowly in the matrix, and on whether it was affected by refluxing or buoyant gas-phase convection. It may also depend on the pathways followed by the water and on the temperature gradient along those pathways.

Changes in *RH*, saturation, and temperature can change hydrological properties, such as fracture and matrix permeability, through precipitation, dissolution, or mineral

alteration. Adsorptive properties of various units may be affected by temperature, saturation, and compositional changes.

Changes in temperature and the mixing of groundwater (driven by repository-heat-driven, buoyant, aqueous-phase convection) could alter hydrological and adsorptive properties in the saturated zone and could thereby affect radionuclide transport in the SZ [Buscheck and Nitao, 1993b].

1.4.5 Coupled Thermal-Hydrological and Geomechanical Phenomena

Changes in geomechanical stresses imposed by thermal-hydrological effects could affect hydrological properties. For example, as a result of thermal stresses, fractures may close and open or undergo shear displacement, which would change their permeability. Microfracturing could occur as the result of pressure buildup driven either by boiling of matrix water or by thermally induced stress increases. Mineral alteration arising from changes in temperature and/or the flow of liquid water flow or steam could weaken the rock, thereby facilitating fracture propagation. Swelling of clay minerals could change the strength of the matrix and could contribute to the overall perturbation of the mechanical stress field. The potential for subcritical crack growth depends on the aqueous-phase saturation.

1.5 Waste Package Environment

To safely and permanently store waste, the repository system must limit gas- or liquid-phase transport of radionuclides to the accessible environment. As regards WP performance, the repository system must meet the regulatory requirements for substantially complete containment (SCC) and controlled release from the EBS. A major concern is how water contacts a WP, thereby potentially affecting its integrity and (if containment is breached) affecting radionuclide dissolution and eventual transport to the water table. The degradational mechanisms of greatest concern for WP integrity, such as stress and pitting corrosion or microbial attack, require the presence of liquid water. The rates for many of these mechanisms are increased under warm, humid conditions.

The two primary modes of water contact on the WP are (1) advective aqueous-phase flow and (2) condensation of water vapor on the WP. The critical factors for condensation are *RH* and temperature *T* on the WP. Regardless of whether mobile liquid water is present, ambient *RH* at the repository horizon is humid (approximately 98 to 99%). If the ambient *RH* could be sufficiently reduced, WP corrosion rates would be minimal [Stahl et al., 1994]. Moreover, even for breached WPs, waste-form dissolution and transport are minimal if no mobile liquid water is present. There are two ways to reduce the *RH* on the WP:

1. Drive a large fraction of the initial pore water from the vicinity of the WPs.
2. Maintain a steep enough temperature gradient away from the WP.

The primary means of reducing the pore water are ventilation and repository-heat-generated drying. To reduce *RH* to 70%, the liquid saturation S_l (the fraction of the pore space filled with liquid water) must be reduced to less than 20%. An AML that does not drive repository temperatures well above boiling will reduce average *RH* only slightly.

Even if repository heat does not substantially reduce average *RH* in the repository, it is still possible to substantially reduce *RH* on the WP itself for a considerable period of time. The *RH* on the WP can be quite low even if ambient (humid) *RH* conditions prevail in the host rock immediately adjacent to the emplacement drift. A large difference in *RH* between the emplacement drift wall and the WP can arise as a result of the temperature difference between these locations. It is reasonable to assume that, because of the relatively high gas-phase diffusivity and the possibility of convective gas-phase mixing within the drift, the partial pressure of water P_v will not vary substantially between the drift wall and WP surface. This is equivalent to saying that the absolute humidity (i.e., the mole fraction of water vapor in the gas phase) will not vary substantially with radial distance from the WP surface within the drift. On the other hand, because the WP surface will be hotter than the drift wall, *RH* on the WP surface will be less than that on the drift wall. Under the assumption of a uniform absolute humidity in the drift, the relative humidity RH_{wp} on the WP is given in terms of the ratio of saturation pressures P_{sat}:

$$RH_{wp} = RH_{dw} \frac{P_{sat}(T_{dw})}{P_{sat}(T_{wp})}, \qquad (1)$$

where RH_{dw} is the relative humidity at the drift wall and $P_{sat}(T_{dw})$ and $P_{sat}(T_{wp})$ are the saturation pressures at the drift wall and WP surface temperatures, respectively. For example, if T_{dw} and T_{wp} are 80°C and 100°C, respectively, then the ratio in P_{sat} is 0.468. If the drift wall were at ambient *RH* (98.4%), then *RH* on the WP would be only 46%. Because of its relatively low thermal conductivity, a granular backfill in the drift would result in a substantially and persistently lower temperature at the drift wall than at the surface of the WP. In developing concepts for the EBS, we must consider the possible benefits of an engineered temperature drop between the WP and the drift wall on reducing *RH* on the WP surface.

During the drying and quasi-steady periods, the rock surrounding the drift will become desaturated if the local AML is high enough, resulting in a reduced *RH* on the WP. This reduction in *RH* will persist at least as long as the WP temperature remains high, and may persist long after the WP temperature has dropped below boiling. The reduction in *RH* decreases both the likelihood and amount of WP corrosion, and the reduction in aqueous-phase saturation in the near-field will decrease the rate of aqueous-phase waste-form dissolution and subsequent aqueous-phase diffusion of radionuclides in the backfill and host rock. Under high AMLs, this desirable scenario may last for tens of thousands of years. Under low to intermediate AMLs, the reduced-*RH* period may be substantially shorter, at least for average *RH* conditions in the repository. Nevertheless, the WP may remain substantially hotter and drier than average repository conditions for thousands of years [Buscheck and Nitao, 1994b]. It

may be possible to thermally design a low-AML repository that promotes a persistent temperature drop between the WP and the drift wall, thereby facilitating a substantial reduction in *RH* on the WP that persists well after the host rock has rewetted to ambient *RH* conditions. It is important to note that the local reduction in *RH* on the WP given by Eq. (1) is applicable only if there is thermodynamic and capillary pressure equilibrium between the drift and the host rock. Nonuniform rewetting of the drift (in particular, that caused by nonequilibrium fracture flow) may locally invalidate this assumption in regions of high (or focused) aqueous-phase flux.

Higher AMLs will increase the volume of rock that has reduced aqueous-phase saturation and *RH* conditions. Because of the larger volume that must be rewetted, rewetting the repository to ambient conditions will take longer for a high-AML repository than for a low-AML repository. A large enough increase in the duration of reduced-*RH* conditions will lower the temperatures associated with a given value of *RH*. Consequently, once humid *RH* conditions are eventually restored, repository temperatures will have decreased considerably, which is more favorable for reducing WP corrosion rates. Ideally, WPs should remain relatively dry until they are relatively cool.

Besides *RH* and temperature, the potential for advective aqueous-phase flow reaching the WP is of concern. Condensate flow, whether generated by an above-boiling or sub-boiling repository, is one possible source of advective aqueous-phase flux. On average, the matrix will imbibe condensate fluxes until it becomes saturated. However, heterogeneities in the natural system can cause variations about the average that could focus condensate onto WPs. Counteracting this variability in return condensate flux is the heat flux from the WPs, which will continue to boil any returning condensate. In some cases, a higher AML may result in higher condensate fluxes and more variability, but the correspondingly higher heat flux will mitigate the problem of focused condensate drainage [Buscheck and Nitao, 1993a]. Since the system is nonlinear, optimum thermal loading is difficult to determine without (1) extensive sensitivity analyses, (2) experimental information obtained from *in situ* heater tests, and (3) better information and understanding about how repository heat affects the overall moisture balance in the unsaturated zone (UZ).

Figure 1 shows the various repository-heat-driven processes and ambient site conditions that may significantly affect the moisture balance in the UZ. Repository heat might drive enough water vapor out of the top of the mountain (by advective and diffusive vapor flow) to significantly reduce the UZ moisture content for tens of thousands of years. Conversely, mountain-scale, buoyant, gas-phase convection might drive enough water vapor up from the SZ (into the UZ) to increase the UZ moisture content [Buscheck and Nitao, 1994a; Buscheck et al., 1994] for tens of thousands of years. It is also possible that mountain-scale buoyant gas-phase convection, driven by both repository heat and natural forces, will bring in dry air from the flanks of the mountain and exhaust moist air from the top of the mountain, resulting in net drying of the repository-block UZ. Forced convection from the repository ventilation system can also remove substantial quantities of water. The net effect of these mechanisms will be investigated by appropriate model calculations, constrained where possible by field observations and data. The moisture balance in the UZ (and, in particular, the region

above the repository) may play a very important role in the performance of the EBS, the natural barriers, and the total system.

Microbially induced corrosion, which is also of concern, depends strongly on temperature and *RH*. High temperature and low *RH* are generally detrimental to microbial growth, whereas intermediate temperatures and high *RH* may favor it. The severity of microbially induced corrosion depends on many other factors, such as pH, Eh, and the nutrients present. It is unlikely that compelling arguments can be made for the absence of all factors (other than water and sufficiently low temperatures) that promote growth of some organisms that could induce corrosion.

The primary conditions addressed in this study that could bear on WP failure and on the release and transport of radionuclides in the near field at the potential repository are as follows:

- Thermodynamic conditions in the EBS and at the WP surface, including gas-phase pressure P_g, relative humidity *RH*, and temperature *T*.
- Aqueous-phase advective flux distribution in the EBS and at the WP surface.
- Aqueous-phase diffusive flux distribution in the EBS and at the WP surface.
- Gas-phase advective flux distribution in the EBS and at the WP surface.
- Gas-phase diffusive flux distribution in the EBS and at the WP surface.

Also see Table 1 in Section 2.2.

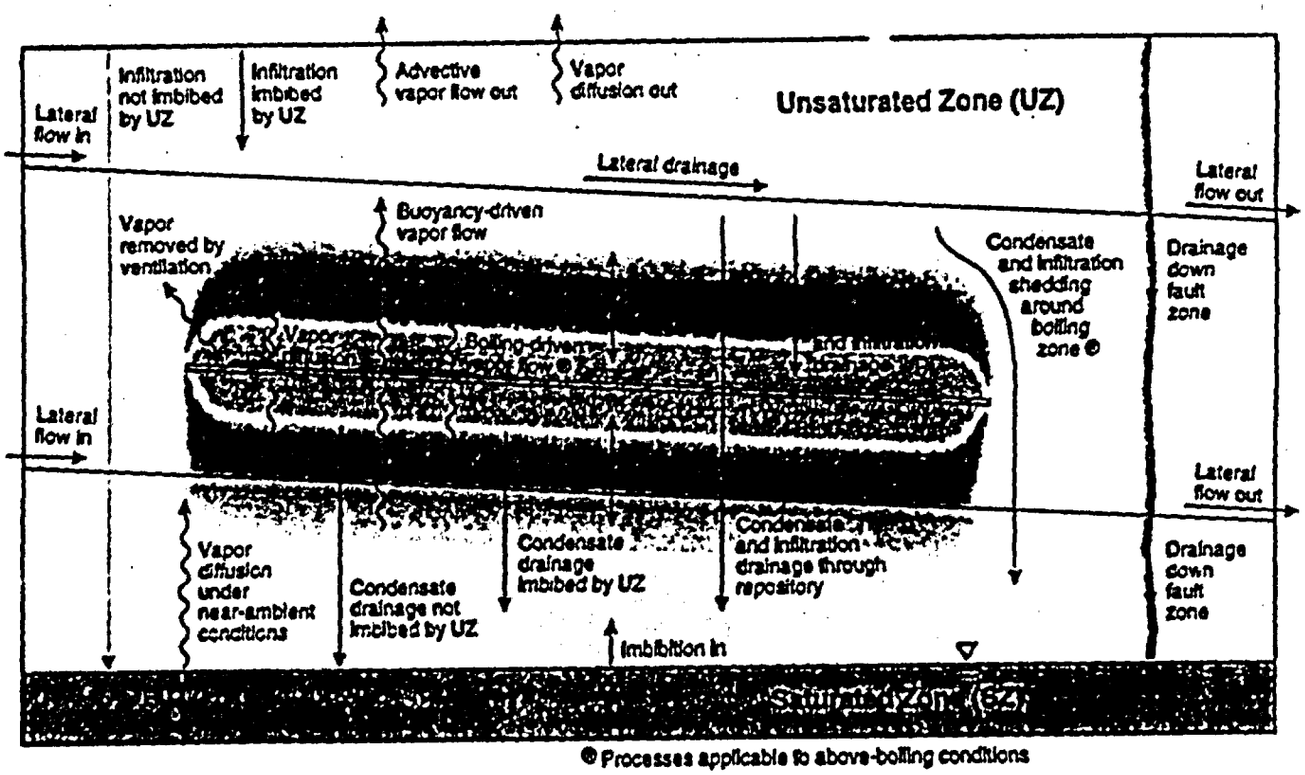
1.5.1 Source-Term Release and Transport

Release of aqueous radionuclides to the natural environment requires that the WP has been breached and that there is enough water that radionuclides can be dissolved and then transported by advection or diffusion from the waste-form to the surrounding rock. The likelihood of this scenario depends strongly on thermal-hydrological processes. The chemistry and temperature, and the advective velocity of the aqueous phase, will play a role in waste-form degradation and in radionuclide dissolution. Possible sources of advective flow are episodic surface infiltration and condensate drainage. If the flux of water leaving the WP is high enough, much of the water will flow down fractures, where it will eventually be imbibed into the matrix or continue to the water table. Radionuclides imbibed in the matrix will be immobilized until the next pulse of fracture flow, whereupon some of the radionuclides will diffuse into the incoming stream if it is at a lower concentration. The remaining radionuclides will continue to imbibe and diffuse deeper into the matrix.

Repository-heat-driven buoyant convection cells can play a dominant role in radionuclide transport in the saturated zone, because the buoyant convective flow velocities can be comparable with or greater than the regional flow velocity [Buscheck and Nitao, 1993b].

Because repository-heat-driven thermal-hydrological effects can dominate advective gas movement, they can have a strong effect on the release and transport of gaseous radionuclides.

Figure 1. Moisture balance in the unsaturated zone (and above the repository itself) is affected by both ambient and repository-heat-driven processes. The two processes labeled with an asterisk (*) are applicable only to above-boiling conditions; all other processes shown can occur under both sub-boiling and above-boiling conditions.



© Processes applicable to above-boiling conditions

2. Scope of Work

2.1 Properties of the Repository Horizon

This study focuses on understanding the thermal-hydrological processes at the potential repository site at Yucca Mountain, Nevada as part of the effort to predict the range of environmental conditions to which the EBS might be subjected. The EBS includes WPs, waste-form, and backfill [NRC, 1991]. This study is part of an integrated group of near-field environmental studies: Of particular concern are conditions that affect (1) corrosion or degradation of WP materials, (2) waste-form dissolution, and (3) radionuclide release from breached WPs. The physical and chemical parameters that characterize EBS conditions are strongly affected by thermal-hydrological processes. These parameters include the flux of liquid water, temperature, relative humidity of the gas phase, chemistry of the aqueous phase, chemistry of the gas phase, and rock mass stresses.

This study will consider near-field thermal-hydrological behavior and related aspects of WP/EBS performance, and the effect on the EBS environment of various WP and repository design options such as WP size, age of SNF, WP spacing, emplacement drift size, emplacement drift spacing, repository size, and repository location. This study will also consider the effect of various options for repository operations, such as WP emplacement scheduling, ventilation, and backfilling.

Thermal-hydrological processes can significantly affect geochemical and geomechanical processes which, in turn, can significantly affect the thermal-hydrological properties of the natural system. The potential interaction and intercoupling of thermal-hydrology with geochemistry and geomechanics must therefore also be studied.

The effect of various natural and man-made processes and events on EBS conditions will vary in time and space. An example of a natural process is the episodic percolation of rainfall, which could result in deep infiltration. An example of a man-made process is the mountain-scale and sub-repository-scale movement of moisture, driven by the radioactive heat of decay from WPs. Conditions at the EBS will be the result of the interaction between natural and man-made processes, such as the interaction of decay heat with naturally occurring infiltration. Because of the dependence of EBS conditions on many processes and events, the uncertainties involved in characterizing the system, the time- and space-varying nature of the problem, and the various engineering options being considered, there is no single EBS environment. The goal of the study will be either to predict a range of possible conditions or to identify parameter regimes that determine a particular type of behavior with regards to EBS performance. Key uncertainties and sensitivities to site properties will be identified to aid the direction of site characterization and *in situ* testing activities.

The activities described in this document have been developed to provide information necessary to satisfy design and performance requirements. These requirements, which are detailed in Issues 1.4, 1.5, and 1.10, emphasize the need to estimate the water quantity that may contact WPs. The water quantity is one of the

attributes of the near-field environment that must be considered in WP design and performance assessment.

The proposed environment in which the suitability of storing high-level radioactive waste is being investigated is a devitrified, densely welded, fractured, nonlithophysal rhyolitic tuff. To satisfy the purpose and objective of the information needs, the effects of WP emplacement on the hydrological properties of the tuff and the hydrological transport processes in the near-field environment must be determined. To establish the nature of these effects, it is necessary to identify and characterize the processes that may influence the near-field hydrology during thermal perturbation of the environment.

The hydrological properties of the tuff are a reflection of the degree of welding, extent of secondary mineral growth, magnitude and distribution of fracturing, and degree of water saturation. The rock in the potential repository horizon has a mean matrix porosity of about 11.3% [Nimick and Schwartz, 1987] and a fracture density between 8 and 40 fractures per cubic meter [Scott et al., 1983]. The structural location of this horizon, 213 to 427 meters above the local water table [Ortiz et al., 1985], and the local meteorological conditions, have resulted in a rock that is approximately 65% saturated [Montazer and Wilson, 1984]. Evidence suggests that the net water flux in this unsaturated environment is 1.0 to 2.0 mm/yr upward, although a downward flux of 1.0 $\times 10^{-7}$ to 0.5 mm/yr may occur as a result of matrix flow [Montazer and Wilson, 1984; Montazer et al., 1985]. Extrapolation from Daily and Lin's [1991] data indicates that the matric potential of 65% saturated Topopah Spring tuff at 20°C is about –8 MPa (–80 atm) during dehydration and –3 MPa during imbibition. At 70°C, the matric potentials at 65% water saturation increase to –24.5 MPa and –24.0 MPa respectively. According to Wang and Narasimhan [1985], the stronger suction potential would make fracture flow less possible. However Buscheck et al. [1991] suggested that fracture flow is a strong function of the total flux, not just the suction potential of the matrix. Permeability is another parameter that will affect the occurrence of either fracture flow or matrix flow. The permeability of the matrix of Topopah Spring tuff is on the order of one microdarcy (10^{-18} m^2) [Lin and Daily, 1984; Moore et al. 1986]. The processes that will occur upon emplacement of WPs in the tuff and the effects of these processes on the hydrologic characteristics of the near-field must be established to meet the requirements of Information Need 1.10.4. It should be noted that the scope of this study is the near-field environment and altered zone. Understanding of the near-field environment will be enhanced by studies of the altered zone.

Characterization of the processes affecting the thermal-hydrological properties in the near field requires knowledge of the potential fluid flow pathways under saturated and unsaturated conditions, the influence of thermal stress on fractures, the influence of fractures on fluid flow and degree of relative saturation, the relative importance of convective flow coupled with condensation and evaporation phenomena, the effect of gravity on the movement of vapor and liquid water, and dissolution and precipitation reactions that may influence pore and fracture geometry and openings and, hence, permeabilities to water and gas. The parameters that influence these processes are temperature, temperature gradient, pressure, pressure gradient, effective and total porosity, suction potential and imbibition of vapor and water, and fluid chemistry. These parameters will be evaluated in model simulations, experiments, and tests.

For some scenarios under unanticipated conditions, saturation of the WP host rock may occur. Hydrological processes under saturated conditions may differ in magnitude and nature from those that occur under unsaturated conditions. To satisfy the requirements for resolution of Issues 1.5 and 1.10, the hydrological processes that may occur over a range of saturation conditions must be determined.

Near-field temperatures will be a function of the power output of the WPs as a function of time, the density and distribution of WPs, and of the thermal response of the host rock. The thermal response of the host rock depends on the relative roles of conductive and convective heat transport, which, in turn, reflect interactions between water quantity and fluid flow characteristics of the near-field environment and altered zone. Information obtained in the model simulations and laboratory experiments and tests will contribute to defining the thermal-hydrological behavior of the near-field environment, which addresses IN 1.10.4.

2.2 Rationale for Selected Studies

The activities described in the following sections are designed to provide information necessary to characterize the hydrological properties and processes of the near-field environment and altered zone for anticipated and certain unanticipated conditions. Delay in this work will delay complete definition of the near-field environment needed for WP design, WP performance assessment, and license application. It will also delay definition of the source term to be provided for the Engineered Barrier System release rate and travel time calculations. Completion of the laboratory activities described below relies on the availability of core or blocks of rock from the repository horizon or, for the model validation experiments, alternate materials that have the hydrological properties (such as permeability, porosity, and fracture aperture) that the principal investigator (PI) considers to be appropriate.

The determination of hydrological properties and the model validation experiments to be discussed later will increase our confidence in the thermal-hydrological models by subjecting them to various testing conditions. These experiments and measurements will also improve our understanding of the thermal-hydrological processes by investigating the statistical variations of the measured parameters. The relationship between the measurement/experiment activities and model calculations is summarized in Table 1. They are also included in the description of each activity in Sec. 2.3.

Work performed in support of this study plan has been divided into the following activities for quality assurance (QA) grading. The Study Plan (SP) is for general planning to show the concept of the study and requirements for conducting the tests and modeling. Detailed descriptions of the activities, including test methods, instruments to be used, and test procedures, will be included in Activity Plan(s). It is possible that one single activity plan will be used to cover all of the activities described in this SP. The activity titles and objectives have been revised since publication of the SCP. Current controlled descriptions and titles are maintained in the Site Design and Test Requirements Document.

Table 1. Relationship between Measurement/Experiment and Model Calculations.

Measurement-Experiment	Model Calculation
Hydrological Properties (Secs. 2.3.2.1 through 2.3.2.4)	Input to models using hydrological codes, such as V-TOUGH and NUFT, which will be used for scoping studies of thermal-hydrological-geochemical coupling.
Electrical Conductivity as a Function of Moisture Content (Sec. 2.3.2.5)	Establishment of calibration databases for electrical resistivity tomography, which is used to monitor moisture distribution in rock; the databases are needed for most of the experiments in this study.
Fracture Healing Experiment (Sec. 2.3.3.6)	Determine how fracture permeability may vary. To be used for model development, to validate geochemical codes (e.g., EQ3/6), and to test existing codes that attempt to couple hydrology and geochemistry (e.g., PRECIP and BASIN II).
Drying and Rewetting Experiments on Intact and Fractured Rock (Secs. 2.3.3.1 and 2.3.3.3), 3-D Imbibition Experiment (Sec. 2.3.3.5)	Determine dehydration rate, imbibition rate, pore-pressure gradient; and calculation of relative permeability. To be used to check these parameters calculated by models using the V-TOUGH and NUFT codes.
Infiltration in a Fracture (Sec. 2.3.3.2)	Determination of fracture flow rate and imbibition rate in the matrix. These will be used to test models using the V-TOUGH and NUFT codes.
Vapor Flow and Condensation Along Fractures (Sec. 2.3.3.4)	Measurement of the amount and distribution of condensate along fractures. These parameters will be used to test models using the V-TOUGH and NUFT codes.
Large-Block Test (Lin et al. 1995)	Provide input for hypothesis testing (Table 2) and to provide thermal-hydrological framework to investigate the coupling with geochemical and geomechanical processes.
Drift-Scale *In Situ* Thermal Test (Buscheck et al. 1995)	Provide input for hypothesis testing (Table 2) and to provide thermal-hydrological framework to investigate the coupling with geochemical and geomechanical processes.
Large-Scale, Long-Duration *In Situ* Thermal Test (Buscheck et al. 1993a, 1993b)	Provide input for hypothesis testing (Table 2) and to provide thermal-hydrological framework to investigate the coupling with geochemical and geomechanical processes.

2.2.1 Activity: Model Development and Analysis of Thermal-Hydrological Flow and Transport

To safely and permanently store waste, the repository system must limit gas- or liquid-phase transport of radionuclides to the accessible environment. As regards WP performance, the repository system must meet the regulatory requirements for substantially complete containment and controlled release from the EBS. A major concern is how water contacts a WP, thereby affecting its integrity and (if containment is breached) affecting radionuclide dissolution and transport to the water table. The degradational mechanisms of greatest concern for WP integrity, such as stress and pitting corrosion or microbial attack, require the presence of liquid water. The rates for many of these mechanisms are increased under warm, humid conditions. A major focus of this study is to develop an adequate understanding of how features (such as fault or shear zones), processes (such as heat-driven processes), and events (such as intense infiltration episodes) affect the nature and degree of water contact with WPs and the release and transport of radionuclides. This understanding will be used in the development of WP and EBS subsystem models required for total system performance assessment.

Prediction of the expected range of thermal-hydrological conditions at the EBS is needed for EBS performance analyses, WP performance analyses, and source-term calculations. Analyses of the thermal-hydrological conditions at the EBS are also critically important for the selection of a thermal loading strategy. This strategy will affect WP and repository design decisions about WP size, age of SNF, WP spacing, emplacement drift size, emplacement drift spacing, repository size, and repository location. This strategy will also affect decisions about the operation of the repository, including WP emplacement scheduling, ventilation, and backfilling. Thermal-hydrological analyses of the near-field environment will also affect the analysis of near-field geochemistry, near-field geomechanics, altered-zone processes, far-field transport, and repository-influenced environmental conditions at the ground surface. These analyses will be used in the development of near-field and far-field transport models required for total system performance assessment.

A detailed study of near-field thermal-hydrological processes such as fracture-matrix flow and moisture movement will aid in understanding generic physical processes that occur in the far-field and at the ground surface. The decision on the suitability of the Yucca Mountain site will be based on whether it is possible to design a repository system that will meet regulatory requirements. Therefore, the study also directly affects site suitability and characterization activities. The methods of analysis used in this study, and the insight gained thereby, will also aid in the interpretation of natural analog studies [Bruton et al., 1993].

A major objective of this study (in conjunction with the other near-field environment and altered zone studies) is to support the technical justification for the regulatory requirements of substantially complete containment and controlled release from the EBS. The primary objective of the model development and analysis activities is to conduct modeling studies for the entire range of potential repository thermal loading options and for the entire thermal loading cycle to accomplish the following goals:

- Identify coupled thermal-hydrological-geochemical-geomechanical processes, transport processes, and ambient site conditions (e.g., bulk permeability distribution) that significantly affect the WP and EBS environment (i.e., affecting WP performance and radionuclide dissolution, release, and transport), with emphasis on their effect on temperature, relative humidity, and aqueous-phase flow conditions throughout the repository and EBS.
- Determine the parameter sensitivity of the thermal-hydrological behavior in the near-field and EBS to a range of expected site conditions, WP designs, repository configurations, WP loading scenarios, and repository operational options (e.g., ventilation and backfill). Of particular importance is dryout and rewetting behavior.
- Develop mathematical and numerical models of repository-heat-driven flow and radionuclide transport, with emphasis on the WP and EBS environment. These models should be capable of treating the important coupled thermal-hydrological-geochemical-geomechanical and transport processes occurring in the thermally altered zone, including (1) nonequilibrium fracture-matrix interaction, (2) coupled reactive transport, (3) the effects of coupled fracture-aperture deformation, and (4) the effects of heat-altered thermal and hydrological flow and transport properties.
- Establish hypotheses critical to the prediction of thermal-hydrological behavior and EBS performance. Design laboratory- and field-scale experiments that critically test these hypotheses.
- Develop validated subsystem models of the WP and EBS environment.

In addition to supporting the technical justification for SCC and controlled EBS release, the conceptual and numerical models developed in this study are required to develop an adequate understanding of the thermally altered zone.

2.2.2 Activity: Hydrological Property Measurements

The objectives of this activity are to determine the hydrological properties of repository horizon Topopah Spring Tuff samples and other rock units that may fall within the altered zone. The properties include effective porosity, saturated liquid- and gas-phase permeability, relative liquid- and gas-phase permeability, matric suction potential vs. liquid saturation, effective coefficient for the binary diffusion of air and water vapor, and Klinkenberg coefficient. The properties will be measured under ambient conditions and thermally altered conditions that are relevant to the heating and cooling cycle for a range of potential thermal loads.

As mentioned in the previous section, moisture transport within the tuff of the potential repository horizon occurs by a combination of vapor and liquid water transport through the matrix and fractures [Buscheck et al., 1991]. The relative importance of each flow mechanism is a function of the bulk saturation, the amount of water transported through the rock, the temperature and temperature gradient in the

rock, the fracture characteristics, and the characteristics of the matrix such as suction potential and permeability.

The emplacement of WPs will produce a large thermal perturbation. Buscheck and Nitao [1991] show that even for area power density APD = 57 kW/acre and 30-yr-old SNF, the temperature at t = 557 yr will be above the boiling point of water within a region 90 m above and 60 m below the repository horizon. This thermal load, in turn, will cause water to vaporize and migrate in the near field and will result in an altered thermal-hydrologic regime. Because liquid water is the main corrosive medium for the metal container and the main agent for the dissolution and transport of radionuclides; laboratory, and numerical modeling studies will be used to characterize the flow of water in the Topopah Spring tuff.

Numerical modeling studies of the flow of water in the Topopah Spring tuff, using Vectorized Transport of Unsaturated Groundwater and Heat (V-TOUGH) [Nitao, 1989] and Non-isothermal Unsaturated Flow and Transport (NUFT) [Nitao, 1993] codes, require hydrological properties of the host rock matrix and fractures as input data. The required hydrological properties include saturated water permeability, gas and liquid permeabilities as functions of water saturation and temperature, suction potential as a function of saturation and temperature for drying and wetting, porosity, and Klinkenberg coefficients for Knudsen diffusion. These properties will be determined on tuff samples from the repository horizon.

Due to inevitable limitation of resources and time, the number of measurements of these hydrological properties will be determined by the PI. The number of measurement will depend on the consistency among the measured results in each rock type and the uniformity of the rock mass at the potential repository horizon. The number of experiments also depends on the relative importance of the parameters to be determined. For example, some of the properties, such as effective porosity and water permeability, will be determined on all samples that are studied. Klinkenberg coefficient can be estimated from liquid permeability [Heid et al., 1950]. The Klinkenberg coefficient may be determined in a few samples of Topopah Spring tuff to confirm the relationship between Klinkenberg coefficient and water permeability.

2.2.3 Activity: Laboratory-Scale Model Validation Experiments

The objectives of this activity are to develop and conduct laboratory tests for model validation and hypothesis testing that provide the basis for confidence building and substantiation of compliance with the substantially complete containment and controlled EBS release requirements. The experiments will test the adequacy of the models to represent hydrological and transport processes at Yucca Mountain that significantly affect WP performance, radionuclide release and transport.

Numerical modeling using the V-TOUGH and NUFT codes will be used to understand and predict the hydrological processes in the near-field and altered zone as a function of time and space after the emplacement of the WPs. Development, calibration, and validation of the model are essential so that the numerical prediction of

the hydrological characteristics of the near-field and altered zone can be used for the WP design and the assessment of the performance of the WPs and the repository.

Because the potential repository horizon is partially saturated with water, an interconnected gas phase may be assumed to exist initially at local atmospheric pressure. As the rock mass heats following waste emplacement, pore water will begin to evaporate, and gas pressure will increase. This phase change and the low gas permeability of the matrix relative to the fractures will induce a significant gas-phase pressure gradient between the matrix and fractures. The pressure gradient will drive vapor from the matrix into the fracture system and primarily away from the WP. As heating progresses, a local gas-phase pressure gradient may exist between the matrix and fractures in the boiling zone. This pressure gradient may cause vapor/steam to flow toward the WP, especially if the fracture intersects the WP borehole or drift. This flow will be limited in duration if the emplacement drifts are sealed. Therefore, the dehydration of the near-field region will depend on the distribution and configuration of fractures. Field testing (e.g., Engineered Barrier System Field Test, SCP 8.3.4.2.4.4) would be more appropriate, than the laboratory tests, to study the effects of fracture distribution and configuration on the near-field environment. The tests described in this SP are designed to study the effects of one single fracture on the thermal-hydrological processes that are relevant to the near-field environment.

The flow of vapor in the fractures away from the WPs will result in condensation along the fracture walls in the cooler region. Whether the condensate along the fracture walls will attain liquid-phase saturations sufficient to result in liquid-phase mobility within the fractures, or whether condensate will imbibe into the rock matrix as rapidly as it forms, must be established. The answer to this question depends on the rate of condensation, capillary suction gradient, liquid-phase permeability in the matrix and fractures, fracture orientation, and the effects that secondary minerals along fracture surfaces have on the imbibition of water. Laboratory results indicate that imbibition of water into the tuff during the flow of vapor is much slower than when the vapor is condensed into liquid water [Lin, 1992]. Model predictions of the amount and distribution of condensation in a fracture must be validated. Laboratory determinations of the moisture retention and imbibition in the tuff, and tests on heated blocks with known fracture patterns, are needed to test model predictions.

The size of the dryout region around the WP is inversely dependent on the efficiency of the primary mechanism of heat transfer. When the liquid phase is mobile in the fractures, a highly efficient vapor-liquid counter flow, or "heat pipe," system may be established [Preuss et al., 1984], which may result in a smaller dryout zone around the WP. If heat conduction is the dominant heat transfer mechanism, a far less efficient vapor-liquid counter flow system may develop, potentially resulting in a larger dryout zone [Buscheck et al., 1991]. Within the dehydrated zone around the WP, the only available mechanism of heat transfer is heat conduction, which is far less efficient than convective heat flow in heat pipes. Understanding these effects is necessary for building confidence in thermal-hydrological models of the near field. These effects are best studied in *in situ* tests, such as the Engineered Barrier System Field Tests (SP 8.3.4.2.4.4) to be conducted in the Exploratory Study Facility (ESF). The measurements and tests described in this SP will provide input data to model calculations. Study of some

processes, such as fracture flow vs matrix imbibition, described in this SP, will provide information that will help in analyzing results of field tests.

The thermal output of WPs will diminish with time. Temperature in the rock mass will increase and then decrease, and the water that has been driven away by the heat will rewet the dryout zone through matrix imbibition and liquid flow in fractures. In addition, unanticipated events, such as greater episodic infiltration due to climatic change, could result in scenarios in which rapid flow of water in the vicinity of WPs could episodically rehydrate previously dehydrated host rock. Repeated dehydration/rehydration cycles may thus be a part of some unanticipated scenarios. The effect of such events must be evaluated to satisfy Issue 1.10. Laboratory study of the movement of a water front from a three-dimensional imbibition process will be needed to validate a numerical model that is geared to understanding the rehydration process. Laboratory studies of the infiltration of water into a fracture and how the water is imbibed by the matrix is needed for model validation.

Laboratory-determined dehydration and imbibition as functions of time and space are necessary to calibrate the numerical model that will be used to characterize the movement of vapor and liquid water in the near-field and altered zone. Lin and Daily [1989 and 1990] and Lin [1991] have reported that flowing liquid water or steam in fractured Topopah Spring tuff samples at temperatures greater than 90°C may cause fractures to heal, resulting in a drastic decrease in permeability. The maximum test temperature of their samples was 160°C. Lee and Ueng [1991] reported an increase in air permeability in the heater borehole after heating the rock mass to about 240°C in a field test in G-Tunnel, Nevada Test Site. The apparent discrepancy may be due to: (1) the difference in testing conditions, such as temperature and confining pressure, (2) the amount of water flowed through the sample, and (3) the scale effect, including size and heterogeneities. Certainly, laboratory experiments cannot complete the study of the scale effect. Laboratory experiments will be conducted to investigate the effects of confining pressure, temperature, and the amount of water flowing through a fractured sample on the fracture healing. In general, the effect of moisture movement on the hydrological properties of the fractured rock mass in the near-field environment and altered zone must be determined to develop a conceptual model that can properly characterize the hydrological processes in the repository block. The reported fracture healing was attributed to dissolution and deposition of minerals along fracture surfaces by hot water or vapor flowing through the sample. Apparently, rock-water interaction will happen in the near field of a nuclear waste repository. The effect of hydrological processes on geochemistry, and vice versa, need to be established. The laboratory tests of rock-water interaction and the coupling between geochemistry and hydrology can be used to evaluate geochemical codes, such as EQ3/6 [Wolery, 1992], and to develop conceptual models that attempt to model the coupled hydrological-geochemical processes, such as PRECIP [Noy, 1990] and BASIN II [Bethke et al., 1993].

In summary, this activity will conduct experiments to test and calibrate thermal-hydrological processes used in model calculations. The experiments include fracture healing, drying and rewetting of intact and fractured rock, electrical conductivity vs moisture content, fracture flow and matrix flow, vapor flow and condensation in a fracture, three-dimensional imbibition, and fracture healing.

2.3 Description of Activities

This study requires the iterative interaction of experimental and modeling activities. The modeling activities include parameter-sensitivity studies that help identify properties and parameters that must be determined in laboratory- and field-scale experiments, and scoping calculations that help in the design of these experiments. As they are determined, these property and parameter values are incorporated in ongoing model calculations (using the V-TOUGH and NUFT codes) of thermal-hydrological behavior in the near-field, the EBS, and altered zone. Laboratory- and field-scale model validation experiments are also needed to confirm that important processes have been adequately incorporated in our conceptual and numerical models of the near-field and altered zone. Model validation is greatly facilitated by hypothesis testing, whereby hypotheses critical to EBS-affecting thermal-hydrological behavior are established and then resolved through a combination of analysis (including bounding analysis) and testing (both laboratory- and field-scale).

Work performed in this study has been divided into three main groups of activities: (1) model development and analysis of thermal-hydrological flow, (2) hydrological property measurements, and (3) laboratory-scale validation experiments. Field-scale validation experiments needed for this study are covered by other study plans.

2.3.1 Model Development and Analysis of Thermal-Hydrological Flow and Transport

2.3.1.1 Overall Methodology and Approach

The following steps articulate the methodology that will be used in the development, refinement, and validation of conceptual and numerical models:

1. Conceptual and Mathematical Model Development.
    - Identify processes and interaction of processes that are important to thermal-hydrological behavior in the near-field and altered zone.
    - Develop a conceptual model of thermal-hydrological behavior in the near-field and altered zone.
    - Develop mathematical models of processes consistent with the conceptual model.
    - Verify the mathematical models.
2. Process Analysis and Parameter-Sensitivity Studies.
    - Develop an understanding of the important thermal-hydrological processes, and their intercoupling with geochemical and geomechanical processes, through the use of mathematical models, including detailed process models.
    - Identify parameter regimes that govern thermal-hydrological flow and transport behavior for natural and man-made processes.

- Quantify the parameter sensitivity of thermal-hydrological behavior to natural and man-made processes.
- Refine conceptual and mathematical models on the basis of results from detailed process models and parameter-sensitivity analyses.

3. Integration with Experiments.
   - Conduct scoping calculations to help design laboratory- and field-scale experiments to quantify important parameters and properties.
   - Refine conceptual and mathematical models on the basis of results from laboratory and field experiments.
4. Hypothesis Testing and Model Validation.
   - Establish hypotheses critical to prediction of thermal-hydrological behavior.
   - Establish hypotheses critical to EBS performance.
   - Conduct scoping calculations to help design laboratory- and field-scale tests that critically test these hypotheses.
   - Test hypotheses on the basis of testing, at the laboratory and field scale, and analysis, including bounding analysis.
   - Validate conceptual and mathematical models on the basis of laboratory and field experiments and hypothesis testing.
5. Subsystem Performance Assessment.
   - Determine the parameter sensitivity of EBS performance to natural and man-made processes.
   - Develop simpler models (abstractions) for EBS and total systems performance assessment.

The steps just described are not necessarily taken in order; the method is a process of iterative refinement as knowledge of the site-repository system increases. The method relies on a combination of mathematical models and laboratory and field data to develop conceptual models and parameter regimes and to test hypotheses.

2.3.1.2 Mathematical Models

The behavior of thermal-hydrological processes, as described in Sec. 1.4, will be predicted using mathematical models. These models are usually partial differential equations describing the balance of energy and the balance of mass of each important chemical species, which can include air and water. A species such as water can occur in both a gas and an aqueous phase. Mathematical models are usually defined at the macroscopic level: that is, they are derived from microscopic balance laws through volume-averaging [see, for example, Bear and Bachmat, 1990] over a representative elementary volume (REV) of the porous medium. Predicted quantities are therefore

averages over the REV, and any variations in these quantities are lost over distances less than the size of the REV.

The following assumptions are typical of macroscopic mathematical models for flow and transport in porous media:

- Darcy's law is assumed to hold for advective fluxes.
- Fick's law is assumed to hold for diffusive and dispersive fluxes.
- Either approximate local or partial thermodynamic equilibrium or assigned disequilibrium is assumed over the REV or macroscopic kinetic rate laws can be used.

Whether or not an REV can be defined that is smaller than the system to be modeled is an open question, as is the question of whether the REV is the same for flow, transport, and heat transfer processes. Developments in the literature will be monitored, and mathematical models used will be tested against experiments as data become available to assess their adequacy for representing important processes and phenomena in fractured porous media. Three principal classes of mathematical treatments have been developed in the past:

1. Equivalent Continuum Model (ECM). Assumes equality of the matric potentials of the fracture and matrix. Single, composite characteristic curves are used to define the unsaturated hydraulic conductivity and matric potential.

Advantages:

- Computationally simple because it uses a single porous medium continuum for both fractures and matrix.

Disadvantages:

- The assumption that the fracture and matrix are in equilibrium is adequate only if fracture fluxes are low enough [Nitao et al., 1993; Buscheck et al., 1991]. This assumption is adequate for modeling condensate drainage during the intermediate and late stages of repository-heat-driven moisture movement, but may be inadequate during early stages when high specific heat flux in the boiling region leads to high condensate drainage fluxes. This assumption is not adequate for modeling intense episodic infiltration events.
- Fractures are not treated as discrete features; rather, their effects are averaged over the whole spatial domain. In effect, fractures are treated as a porous medium.

2. Dual Permeability Model. This model treats the matrix and the fractures as two distinct porous continua with a transfer term to represent the flux between the two continua.

Advantages:

- Less computationally intensive than a discrete representation of fractures (treatment No. 3, below).

- Can handle larger advective fluxes without producing conditions near 100% aqueous-phase saturation in the matrix, because it does not assume capillary equilibrium between fracture and matrix.

Disadvantages:

- More computationally intensive than equivalent continuum method, but of manageable complexity.
- Typical fracture-matrix transfer terms cannot adequately treat fracture-matrix interaction, especially during early and intermediate stages of matrix imbibition.
- Fractures are not treated as discrete features; rather, their effects are averaged over the whole spatial domain. In effect, fractures are treated as a porous medium.

3. Discrete Fracture-Matrix Model. This model spatially discretizes the space occupied by the fractures and the matrix by finite element or finite difference elements. Because the location and morphology of individual fractures is not usually well known, their geometric characteristics are either (1) interpolated from field data, (2) randomly generated, or (3) represented using an idealized geometry.

Advantages:

- Actual fracture geometry is considered, including size of fractures and intersections.

Disadvantages:

- Highly computationally intensive.
- Available data may not justify the approach.

The selection of an approach must weigh the trade-off between computational complexity and physical accuracy. Factors that should be considered include (1) the magnitude of fracture fluxes, (2) the size of the domain being modeled, and (3) the scale over which results are desired. The discrete fracture approach is probably not practical for repository-scale and mountain-scale calculations, but it can be used to determine phenomenological parameters needed for the dual permeability approach. This approach can also be useful in interpreting the results of laboratory-scale experiments. Complementary use of these three approaches is probably the only effective way of incorporating some of the effects of nonequilibrium fracture-matrix behavior at any practical scale of analysis.

Mathematical models have the following limitations:

1. Because they are usually macroscopic (based on volume averaging), the effect of fine-scaled physical processes may be lost.
2. They have somewhat limited ability to incorporate realistic spatial variability of input parameters as a result of geological heterogeneities.

3. They are subject to spatial uncertainty of input parameters as a result of limitations in geological data gathering.

4. All of the detailed physical and chemical processes cannot be implemented because of computational limitations.

An example of the first limitation is "dispersion of the liquid phase," a term used by Nitao and Buscheck [1991] in the context of the deviation in the movement of a liquid front relative to the mean position of the front as a result of viscous fingering and branching at fracture intersections as it percolates down a fracture network. Expressions for phase dispersion will involve deriving higher-order terms in macroscopically averaged models. The effect of the second and third limitations can be reduced by sensitivity analyses, stochastic realizations, and phenomenological models. To reduce the effect of the fourth limitation, conservative and judicious assumptions and simplifications must be used.

2.3.1.3 Numerical Models

The partial differential equations for the macroscopic balance of energy and mass are highly nonlinear for multiphase fluid flow with phase changes (i.e., evaporation and condensation). They must, therefore, be solved numerically. The codes V-TOUGH [Nitao, 1990] and NUFT [Nitao, 1994] will be used for this study. They both use the integrated finite difference method. V-TOUGH considers only the transport of air, water, and energy; NUFT can also consider transport of other species, including radionuclides. NUFT also has mechanical dispersion of components; it has more physical and numerical options, is more flexible, is more computationally efficient, and is more user friendly. It can also handle additional fluid phases, such as a nonaqueous hydrocarbon phase. The following are the important output variables for the two codes:

V-TOUGH: Spatial and temporal distribution of gas- and aqueous-phase pressure, gas- and aqueous-phase saturation, air mass fraction in gas and aqueous phases, water mass fraction in gas and aqueous phases, and temperature.

NUFT: Same as V-TOUGH but, in addition, can solve for mass fraction of other components, including radionuclides.

Planned enhancements to NUFT include the following:

- Dual-permeability models.
- Higher-order models for dispersion and fracture-matrix interaction.
- Radioactive and chemical reactions.
- Geomechanical coupling with thermal-hydrological behavior.
- Extension of the current suite of numerical methods.

Software Quality Assurance (SQA) will be carried out for V-TOUGH and NUFT according to the Individual Software Plan (ISP) developed for each code. The ISP will describe the configuration management and control of the codes, necessary documentation, walk-throughs, and benchmarking problems. Software verification will

include the comparison of results of the codes with analytical solutions and with results of other selected numerical models. Because of uncertainties and heterogeneities, it is difficult to have enough information to explicitly validate a model based on a multiphase, nonisothermal porous media flow and transport code. Partial model validation will be performed using laboratory and field experiments by (1) determining whether calibration of the model is possible and (2) whether the conceptual model predicted by the model is consistent with observations.

2.3.1.4 Parameter Sensitivity and Process Analysis

The general methodology for this part of the study is to perform parameter-sensitivity analyses and to ascertain parameter regimes of characteristic behavior. The following analyses will be performed:

- Theoretical study of fracture-matrix interaction.
- Effect of nonequilibrium fracture flow arising from episodic infiltration events.
- Effect of decay heat on the diffusive flux of water vapor at the ground surface.
- Effect of decay heat on moisture balance in the unsaturated zone.
- Interaction between thermal effects and surface infiltration.
- Nonisothermal processes involved in sub-repository-scale, repository-scale and mountain-scale moisture movement.
- Effect of decay heat on buoyant gas-phase convection in the unsaturated zone and the implications of this convection for heat and moisture flow.
- Effect of decay heat on buoyant aqueous-phase convection in the saturated zone and the implications of this convection for heat and moisture flow.
- Sensitivity study of gas-phase and aqueous-phase rewetting of the repository.
- Impact of heterogeneity on condensate shedding and on the focusing of vapor and condensate flow.
- Effect of heterogeneity on temperature and *RH* in the repository.
- Effect of heterogeneity on advective aqueous-phase flow in the repository.
- Sensitivity study of geomechanical-thermal-hydrological coupling.
- Sensitivity study of geochemical-thermal-hydrological coupling.
- Influence of thermal-hydrological flow processes on the geochemistry of the water contacting the WP.
- Impact of repository depth on thermal-hydrological and thermal-hydrological-geomechanical processes.
- Impact of drift ventilation on thermal-hydrological and thermal-hydrological-geomechanical processes.

- Impact of thermal loading design on temperature and *RH* in the repository and on WPs.
- Optimization of thermal loading design (including repository and WP layout) to improve EBS performance and reduce uncertainty in the EBS environment.
- Determination of processes important to the release and transport of radionuclides from the EBS.
- Bounding analyses related to hypotheses critical to the prediction of thermal-hydrological behavior.
- Bounding analyses related to hypotheses critical to EBS performance.

2.3.1.5 Integration with Laboratory and Field Experiments

The goals of laboratory and field experiments are to (1) measure fundamental material properties for input into the codes, (2) determine consistency of conceptual models with processes observed in experiments, (3) partially validate mathematical models by calibration, and (4) perform hypothesis tests. Conversely, the model will be used to design and interpret data collected during the experiments.

A key issue for the Yucca Mountain Project that will require integration of modeling studies with laboratory and field experiments is evaluating the effect of various thermal loading options on the ability of the Mined Geological Disposal System (MGDS) to contain and isolate radionuclides. With respect to a thermal loading strategy, the DOE Program Approach may adopt the position of starting with a low thermal load (i.e., low AML), while reserving the option of increasing to a higher AML at a later time as *in situ* heater test data and other site characterization data relevant to thermal loading become more readily available. The primary motivation for the initial low AML is to avoid or limit the significance of heat-mobilized fluid flow in the unsaturated zone. The underlying assumption is that by eliminating or limiting the spatial and temporal extent of boiling one minimizes the major significant mechanism of heat-driven fluid flow mobilization. However, there are mechanisms that occur under sub-boiling conditions that must be addressed to justify this assumption.

Hypothesis testing can help determine whether a minimally heated (MH) repository system [Buscheck et al. 1995], can avoid (or limit) heat-mobilized fluid flow in the UZ. The primary hypotheses concern:

MH-1 Whether buoyant, gas-phase convection significantly affects UZ moisture movement.

MH-2 Whether binary gas-phase diffusion significantly affects UZ moisture movement.

MH-3 Whether heterogeneity in the heat load distribution and/or gas- and liquid-phase pathways focus enough percolation and condensate flux to

cause this heat-mobilized water to contact WPs and drive radionuclide transport.

Heterogeneity in UZ flow pathways, both small-scale (fractures and fracture networks) and large-scale (faults) is being investigated in Study 8.3.1.2.2.4 by several activities shown in Table 2.1-2, page 2.1-12, YMP-USGS-SP 8.3.1.2.2.4, R1. For example, the questions of the validity of the equivalent continuum model (also called the effective continuum model and the equivalent porous medium model) and the REV are addressed in Activities 8.3.1.2.2.4.1 and 8.3.1.2.2.4.3 of the referenced study plan. Although this and other related studies consider only natural conditions without the disturbance imposed by decay heat, they will produce useful results for helping to understand the hydrological properties of the near-field environment. These will be incorporated as appropriate and as they become available. Overall integration of this Study with others will be performed by the YMP M&O.

For repository systems with thermal loads that significantly mobilize fluid flow, as is certainly the case with a high-AML repository, these hypotheses address how that mobilization occurs.

Field tests, including the Large-Block Test (LBT), to be performed at Fran Ridge [Lin et al 1994], and *in situ* heater tests to be conducted in the ESF (e.g., the Engineered Barrier System Field Test) will aid in evaluating issues associated with thermal loading, including resolution of the major hypotheses. These tests are described in separate Study Plans. Portions of these heater tests should be conducted under sub-boiling conditions to support the resolution of these major hypotheses for a low-AML repository system and for the post-boiling period of a high-AML repository system. Portions of the heater tests will be conducted under above-boiling conditions to address the effect of boiling for either a low- or high-AML repository system, and it is also important for establishing the technical justification for an increase in the repository AML.

Hypothesis testing can help determine the extent to which a constructively heated (CH) repository [Buscheck et al. 1995] system can generate conditions in the repository that promote WP integrity and reduce the potential for radionuclide dissolution and transport. The primary hypotheses concern the following unknowns:

CH-1 Whether heat conduction dominates heat flow.

CH-2 Whether boiling-driven rock dryout and/or the temperature difference between the WP and drift wall result in a significant reduction in *RH* and limited mobile liquid water near WPs.

CH-3 How long rewetting the WP environment to humid conditions lags behind the end of the boiling period (or how long the temperature difference between the WP and drift wall results in a significant reduction in *RH* on the WP).

CH-4 Whether enough condensate buildup occurs to significantly affect drying and rewetting.

The relationship between experimental activities and the resolution of these thermal-hydrological hypotheses is given in Table 2.

Table 2: Experimental Activities Providing Input to Thermal-Hydrological Hypothesis Testing.

Hypothesis	Lab-Scale Tests	Large-Block Test[1]	Pneumatic Tests	Drift-Scale *In Situ* Thermal Test[2]	Large-Scale, Long-Duration *In Situ* Thermal Test[3]	Performance Confirmation
MH-1	L	P	P	S	C	C
MH-2	P	P	N	S	C	C
MH-3	L	P	P	S	C	C
CH-1	L	P	P	S	C	C
CH-2	L	P	P	S	C	C
CH-3	L	P	L	S	C	C
CH-4	L	P	L	S	C	C

N = no information; L = limited information; P = preliminary indication;

S = substantial understanding; C = confirmation

[1] Described in Lin et al. (1995).

[2] E.g., the single-drift, winged thermal test described in Buscheck and Nitao (1995).

[3] E.g., the 3- and 5-drift heater tests described in Buscheck et al. (1993a, 1993b).

The above-boiling portions of the heater tests are needed to support the resolution of this second set of major hypotheses and to further support the resolution of the first set of hypotheses. It is easier to evaluate the significance of buoyant, gas-phase convection when thermal testing is conducted under above-boiling conditions [Buscheck et al. 1993b].

An important part of this study is to conduct thermal-hydrological scoping calculations to design LBT and ESF heater tests that provide useful and timely information for resolution of the major hypotheses and to observe potentially critical coupling between thermal-hydrological processes and geomechanical and geochemical processes. How the heat load is applied to the rock during the heater tests must be done so that it is relevant to repository conditions, and the experimental design must allow the resolution of hypothesis tests. A primary concern is that the heated area of rock must be large enough to accomplish the following:

- Incorporate a network of fractures that is sufficiently connected to examine important heat-driven processes such as buoyant gas-phase convection.

- Allow the development of condensate perching above the boiling zone.
- Examine whether heterogeneities in the gas- and liquid-phase pathways focus enough condensate drainage to cause water to drip onto WPs.
- Prevent edge-cooling effects from dominating thermal-hydrological flow processes.
- Determine the significance of buoyant gas-phase convection on moisture movement and heat flow.

Model calculations are being carried out [e.g., Buscheck et al. 1993a; Buscheck et al. 1993b] to address the question of *in situ* heater test size.

Resolution of these hypotheses is critical to addressing the geohydrology qualifying condition for Technical Site Suitability (TSS) that states "Geohydrologic setting is compatible with waste containment and isolation." [DOE, 1994] Resolution of these hypotheses is also important in addressing the disqualifying condition that states "Groundwater travel time is less than 1000 years along paths of likely and significant radionuclide travel." [DOE, 1994]

Because of limited time before the License Application Deadline (LAD), some of the *in situ* heater tests will have to be accelerated relative to actual thermal loading conditions. A major objective of this study is to examine the trade-offs between test duration (and heating rate) and generating thermal-hydrological conditions applicable to repository performance during the entire thermal loading cycle, including heating and cooldown. For both the heating and cooldown phases, the heater test will accelerate changes in time and space, including:

1. The transition from sub-boiling to boiling conditions.
2. The transition from boiling to above-boiling conditions.
3. The transition from above-boiling to sub-boiling conditions.

It is important that the accelerated thermal cycle not preclude the occurrence of coupled thermal-hydrological-geomechanical and thermal-hydrological-geomechanical phenomena that may be important to boiling, dryout, and re-wetting under actual repository conditions. It is equally important that the accelerated thermal cycle not introduce complex phenomena that are not relevant to actual repository conditions.

To determine the size and duration of the *in situ* heater tests, the following criteria should also be considered:

1. Volume of the dryout zone.
2. Rate of change of temperature.
3. Peak rock temperatures.
4. Size and duration of condensate perching.
5. Velocity of the dryout front.

The first criterion relates to the scale of the dryout zone relative to the scale of the heterogeneity of the fracture properties, particularly the fracture spacing and

connectivity. Because buoyant, gas-phase convection is very dependent on the fracture system, it is necessary to dry out a sufficient volume of rock to include an interconnected fracture system. If the dryout zone is small relative to the scale of heterogeneity or connectivity, dryout, buoyant, gas-phase convection and condensate drainage may be completely dominated by the local heterogeneity. Moreover, models that incorporate bulk averages of matrix and fracture properties require tests in which bulk averages are statistically meaningful. For thermal-hydrological processes to perch condensate, it is necessary to coalesce the boiling zones, thereby precluding condensate from being easily shed off the sides of the individual boiling zones around each heater.

The second and third criteria relate to the potential for geomechanical and geochemical effects to significantly alter the thermal-hydrological properties in a way that is not representative of repository thermal loading conditions. The fourth and fifth criteria relate primarily to thermal-hydrological-geochemical coupling at the refluxing front, which may result in geochemical alteration of fracture and matrix properties. If the dryout front is driven too quickly, there will be inadequate time for geochemical effects to occur. Note that an increase in boiling (and dryout rate) will also be accompanied by an increase in the return flux of condensate. One might therefore expect that the increased rate of condensate flow would compensate for the reduced overall time that a given region of fractured rock is exposed to refluxing conditions. If condensate sheds off the sides of the boiling zone, there will be a net loss of fluid from the refluxing system, increasing the overall rate of dryout. If condensate shedding is particularly effective, substantial overdriving of the dryout rate (relative to applicable repository conditions) will have the effect of reducing the potential for reflux-driven redistribution of minerals in fractures.

2.3.1.6 Modeling and Analysis Study Activities

This study involves six major modeling and analysis activities that are conducted in a highly iterative fashion. It is difficult to prescribe the precise order in which successive activities would be conducted because such a sequence is highly dependent on the particular application or physical processes being modeled. Activities that concern establishing the proper use of a particular model (such as determining that adequate grid resolution, sufficient spatial model domain, and appropriate mathematical models were being used) would precede the application of that model to process analysis and parameter-sensitivity studies. Various process models will be used to design and plan laboratory-scale and field-scale tests. As appropriate, results from those tests will be used to update parameter values and assumptions used in various process models.

A major purpose of the modeling and analysis activities is to help resolve hypotheses of thermal-hydrological behavior and EBS performance (Table 2). Resolution of those hypotheses will provide an important part of the scientific basis for building confidence in process models that will be the basis for simplified (abstracted) subsystem models of the EBS (i.e., the WP environment) and radionuclide transport in the near field. These subsystem models are required for total systems performance assessment.

The major activities of the study will include the following applications of mathematical models (equivalent continuum models, dual permeability models, and discrete fracture-matrix models) appropriate to the phenomena being studied and to the spatial and temporal scales:

1. Conceptual and Mathematical Model Development. Development, refinement, and validation of a complementary suite of complex numerical and analytical models (at various scales) of thermal-hydrological behavior, thermal-hydrological-geochemical behavior, and thermal-hydrological-geomechanical behavior in the near-field and altered zone. This will include the following:

- Development of the models.
- Proper usage of the models, including the determination of parameter domain of applicability.
- Proper usage of models, including the determination of sufficient grid resolution and spatial model domain for a given model application.
- Proper usage of models, including the determination of sufficient mathematical models (e.g., dual permeability model) for a given model application.
- Verification of mathematical models.
- Calibration of mathematical models.
- Qualification of codes according to the respective Individual Software Plan (ISP) and applicable Software Quality Assurance (SQA) procedures.
- A family of qualified codes will be maintained under the configuration management system and will be available on request.
- Provide documentation of the validation of conceptual and mathematical models on the basis of results from laboratory and field experiments and hypothesis testing.
- Provide input to the Near-Field Environment Report (NFER) and Altered Zone Report (AZR).

2. Process Analysis and Parameter-Sensitivity Studies. Development of an understanding of the processes and parameters critical to near-field and EBS performance. This will include the following:

- Identification of potentially important processes.
- Parameter-dependence studies to help establish the key processes and dependences.
- Parameter-sensitivity studies to help quantify the key dependences.
- Identification of parameter and thermal-hydrological flow regimes.
- Development and refinement of conceptual models on the basis of laboratory and field testing, including results of related studies by M&O Teammates and the USGS, as they become available.

- Provide input to the NFER and AZR.

3. **Sensitivity Studies of Site Conditions and Design Options.** Provide the results of predictive studies of the sensitivity of near-field and EBS behavior to natural and man-made effects, including consideration of the following:

- A range of expected (present and future) ambient site conditions, including steady, quasi-steady, and transient events. Future conditions include future climate, thermally altered conditions, and conditions that are altered by the construction and operation of the repository. Results of sensitivity analysis of ambient site conditions will be regularly shared with site characterization efforts.
- A range of options for the design and operation of the repository system, including repository design, WP design and layout, WP emplacement schedules, man-made materials, ventilation, and backfill. Particular emphasis will be placed on evaluating a range of thermal loading strategies. Results of sensitivity analysis of design and operational considerations will be regularly shared with WP and repository design efforts.
- Provide input to the NFER and AZR.

4. **Test Integration.** Provide calculational support for LLNL site characterization, laboratory-scale experiments, and field tests. Integration of these hydrological and thermal-hydrological studies with related work by other M&O Teammates and the USGS will be implemented by M&O Scientific Program Operations.

- Provide results of the analysis of the sensitivity of thermal-hydrological behavior to ambient site conditions to provide a context for understanding the relative importance of various hydrogeological properties, features, and boundary conditions that will be determined during site characterization.
- Provide results of the analysis of repository-altered thermal-hydrological behavior to provide input for near-field geochemistry studies, altered zone studies, geomechanical studies, and far-field transport studies.
- Provide results of scoping calculations for laboratory-scale hydrological experiments.
- Provide results of scoping calculations for field-scale tests, including *in situ* heater tests.
- Provide documentation of the interpretation of laboratory and field tests.
- Provide input to the NFER and AZR.

5. **Hypothesis Testing.** Development and resolution of hypotheses critical to thermal-hydrological behavior and EBS performance.

- Establish hypotheses critical to prediction of thermal-hydrological behavior.
- Establish hypotheses critical to prediction of EBS performance.

- Provide scoping calculations to help design laboratory- and field-scale tests that critically test these hypotheses.
- Provide resolution of hypothesis testing on the basis of the synthesis of results from laboratory and field testing and theoretical analysis, including bounding analysis.
- Provide input to the NFER and AZR.

6. Performance Assessment. Support the development of simplified performance assessment subsystem models of the near-field and EBS, abstracted from calculations of near-field and EBS thermal-hydrological behavior using complex numerical and analytical process models.

- Provide results of analyses of parameter sensitivity of EBS performance to natural and man-made conditions (including thermal loading conditions).
- Develop simpler models (abstractions) for EBS and total systems performance assessment.
- Provide input to the NFER and AZR.

2.3.2 Hydrological Property Measurements

Hydrological properties of rock samples from the repository horizon will be determined. If other rock types or materials are used in the experiment for model calibration and testing (as described in Sec. 2.3.3), as deemed appropriate by the PI, then the hydrological properties of the alternate materials will also be determined. The tuff to be used in the experiments described in this section is the repository horizon Topopah Spring tuff that is divitrified, densely welded, and nonlithophysal. These properties will be used as input data to numerical model analysis and to characterize the samples used in model calibration and validation experiments. The hydrological properties to be determined include saturated aqueous phase permeability, suction potential as a function of water saturation for drying and wetting (moisture retention curves), matrix porosity, and Klinkenberg coefficient for Knudsen diffusion. The moisture retention curves and the imbibition history of water in tuff will be used to solve the inverse problem of Richard's equation for relative permeability, which is an essential parameter in understanding the flow of both gas and liquid in an unsaturated medium.

Methods to determine these hydrologic properties are described below. The PI will have the flexibility of using other methods to determine these properties. As mentioned in Sec. 2.2.1, the PI will also have the flexibility to determine the number of measurements to be performed on certain properties, based on the variability of the measured results. Samples will be collected so that they represent the spatial variability of the rock types in the near-field as much as possible. The detailed information of sampling and number of measurements will be included in Activity Plan(s). Modification of the experimental method and/or adding new methods of determining these hydrological properties will be documented in scientific notebooks.

J-13 water will be used as the pore fluid in most of the tests described in this section. Because of the functional requirement of the constant humidity chamber, deionized water will be used for the moisture retention curve experiments. If J-13 water is not available, the PI may decide to use water with similar chemistry as the J-13 water.

2.3.2.1 Effective Matrix Porosity

A sample without visible fractures will be used for the determination of effective matrix porosity. The sample material will be machined into an appropriately sized cylinder. The accuracy of the dimensions of the sample should be better than 0.5%. The sample volume is calculated from its dimensions. The sample will be dried in a vacuum oven at temperatures low enough to prevent any alteration in mineralogy or thermal cracking. Normally, temperatures below 35°C will be used. The sample will be weighed periodically to monitor the decrease of sample weight due to drying. The sample is considered dried when its weight remains unchanged for at least one day. The dry density of the sample is calculated by dividing the dry weight of the sample by its volume.

Samples will also be dried in a humidity chamber at low humidity levels, such as 20% relative humidity. The dry density of a sample determined using a vacuum oven at low temperature will be compared with that determined in a low humidity environment. This comparison will indicate residual saturation in a sample that has been dried under low humidity conditions.

The dry sample will then be saturated with water. To do this, the sample will be placed under vacuum, and then water will be allowed to flood and cover the sample. The sample will be left in water and continuously placed under vacuum for a few hours to remove the air in the water. The weight of the sample is measured periodically. The sample is considered saturated when its weight remains unchanged for at least one day (initial steady state). The sample will usually remain in water for several days after the initial steady state. Scoping studies indicate that the weight change after the initial steady state does not contribute to the uncertainty of effective porosity greater than the desired accuracy. The saturated density of the sample is calculated by dividing the saturated weight of the sample by its volume. The effective matrix porosity of the sample is the difference between its saturated density and dry density, divided by the density of water. The effective matrix porosity determined by this method is considered to be relevant for studying the transport of water.

Measurement Uncertainty

The accuracy of the determined effective porosity should be within about 1%. The largest source of uncertainty is in determining the volume of the sample in which a 1% accuracy must be obtainable.

Range of Expected Results

The tuff samples are the densely welded nonlithophysal Topopah Spring tuff. There is very little pumice in the rock. The RIB [1992] reports the expected value of the effective matrix porosity of the welded Topopah Spring tuff (TSw2) is between 8.5 and

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15.7%. A welded tuff sample from the Topopah member (outcrop at Fran Ridge, NTS) was found, using mercury porosimetry, to have a porosity of 6.51% [Knauss et al., 1985].

2.3.2.2 Saturated Aqueous-Phase Permeability

A steady state flow-through method will be used to measure the saturated aqueous phase permeability. Further details of the procedures are contained in Lin and Daily [1984] and Daily and Lin [1985].

Fractured and intact cylindrical samples will be saturated with water. The saturation procedures are the same as described in Sec. 2.3.2.1. The saturated sample will be jacketed and placed in a pressure vessel. The sample will be brought to the desired confining pressure, pore pressure, and temperature. A small pore-pressure gradient will be created across the longitudinal axis of the sample so that the pore fluid will flow at a measurable rate. The pore-pressure gradient will be kept as small as possible so that the effective pressure in the sample is virtually uniform and the flow rate is small enough that the flow is not turbulent. The measured steady state flow rate of the pore fluid, the pore-pressure gradient, the cross sectional area of the sample, and the viscosity of the pore fluid (which may be obtained from a handbook of physical properties of water) will be used to calculate permeability, using Darcy's law:

$$k = q\mu l / Ap ,$$

where

k is permeability in darcies

q is volumetric flow rate in cm^3 per second

μ is viscosity of water in centipoise

l is the sample length in cm

A is the cross sectional area of the sample in cm^2

p is the pore-pressure difference across the sample in atm.

The water that flows through the sample will be collected and analyzed for the primary constituents of the rock and water to evaluate the rock-water interaction process. Analysis for the elements Si, Al, Ca, Na, K, Mg, Fe, and B is done by inductively coupled plasma atomic emission spectroscopy (ICP). This technique is used because it provides reproducible, high-precision (±10% for all elements except K, which is ±20%) results on small volume (5 mL) samples. High accuracy in the sub-parts per million range is obtainable with the ICP method for most of the elements of interest. Atomic absorption spectroscopy (AA) is used as a supplementary means for obtaining K analyses in the ±10% range. Ion chromatography (IC) is used to obtain analyses for the anions F^-, Cl^-, NO_3^-, and $SO_4^=$. Alkalinity, primarily in the form of bicarbonate (HCO_3^-), is determined using an automated total alkalinity titration technique. AA, IC,

and alkalinity titration provide analyses of high precision and accuracy (±10%) in the parts per million range, which covers the concentration range for species of interest in these solutions and which provides the accuracy necessary for determining reaction processes.

Measurement Uncertainty

The main uncertainty in the measured permeability is in the determination of the pore-pressure gradient and the volumetric flow rate. For low permeability (on the order of one microdarcy), the uncertainty is about 20 to 50% of the determined permeability. For greater permeability, the uncertainty is about 10 to 20%. The required tolerance of the permeability measurement should be determined by the sensitivity analysis of model studies.

Range of Expected Results

The expected range of saturated water permeability of intact welded Topopah Spring tuff is between 0.1 and 10 μd. Previous scoping studies suggest that the saturated water permeability of an intact welded tuff sample does not change with increasing temperature [Lin and Daily, 1984]. The saturated water permeability of a fractured sample depends on the fracture apertures and the number of fractures in the test sample. With an axially oriented single hairline fracture (of less than 0.1 mm apparent separation on the surface), the expected permeability is on the order of one millidarcy. Previous studies suggest that permeability of fractured samples decreases with increasing temperature [Lin and Daily, 1984; Daily et al., 1987].

2.3.2.3 Moisture Retention Curves

The matric potential will be determined by measuring relative humidity in equilibrium with a sample at fixed temperatures. For the imbibition of water in tuff, the suction potential is almost equal to the matric potential, because the water and the rock are relatively free of solutes. The degree of saturation will be determined by comparing the sample weight with its dry weight and saturated weight. Various degrees of saturation will be achieved by equilibrating samples with known relative humidities or adding a known amount of water to the sample. Repeating these measurements over a range of saturations allows determination of the curve that defines the variation of suction potential with degree of saturation (moisture retention curve) at each fixed temperature. The measurements will be repeated for other temperatures. Matric potential is defined by Kelvin's law as

$$P_s = \beta RT \log_e(e/e_0)/M ,$$

where

P_s = matric potential, in MPa

β = density of water (g/cm^3) at the temperature of interest

R = universal gas constant (8.31 J/K-mole)

T = temperature (K)

M = molecular weight of water (18 g/mole)

e/e_0 = relative humidity.

A constant humidity chamber will be used to determine the moisture retention curve of rock samples in vapor. For the wetting phase, a dry sample will be placed in a constant humidity chamber. The chamber is brought to the desired temperature and relative humidity. The sample will then be weighed periodically to determine when it has reached an equilibrium weight. The relative humidity is used to calculate the matric potential, and the total weight change allows computation of the degree of saturation. The measurement will be repeated at higher humidities, at the same temperature, until the maximum relative humidity in the chamber is reached, which is about 98%. The measurement process will then be reversed to measure the matric potential in a drying phase. The cycle of measurement will then be repeated at another temperature. The highest level of saturation that can be attained in a sample using this method is about 30% of its pore volume [Lin, 1992]. This may be because the saturation process was started from a dry sample. Other procedures will also be tried, such as starting with a water saturated sample to complete the measurements in a drying phase until the saturation level is irreducible in a constant humidity chamber, then starting the measurements in the wetting phase. The two methods of drying a sample, in a vacuum oven at near-ambient temperature and at a low humidity level in a humidity chamber, will be compared to evaluate their effect on drying the Topopah Spring tuff samples.

To determine the moisture retention curve of rock samples at higher levels of water saturation, the relative humidity will be measured in a sealed rock sample, and the saturation level will be changed by adding water to the sample or drying the sample. The saturation level of the sample is determined by weighing it, as described in the preceding paragraph. The device for measuring relative humidity in a sample can be a chilled-mirror psychrometer [Flint et al., 1992] or a resonant cavity. A Chilled-mirror psychrometer is limited to near-ambient temperature application and a range of suction potentials from -10 to -30×10^4 m of water head (-1 to -3×10^3 atm). A resonant cavity does not have these limitations.

Both methods of measuring moisture retention curves allow the determination of hysteresis between drying and wetting conditions. The effect of drying and wetting on the hydrological properties of the sample, especially at elevated temperatures, must be assessed. To determine the effect of sample history, some of the samples with similar moisture retention curves at room temperature will be divided into three groups. The samples in one of the three groups will be subjected to a complete drying and wetting cycle at high temperature; samples in the other two groups will be subjected to either the drying or wetting phase only. The results from these three groups will be compared to determine the effect of prior drying and wetting at high temperature on the moisture retention curve.

Range of Expected Results

Based on the data obtained at room temperature reported by Klavetter and Peters [1987] and the room-temperature and high-temperature results reported by Daily and Lin [1991], the expected range in suction potential is from 0 to 10^4 atm, when the sample is between saturated and dry conditions respectively.

Measurement Uncertainty

Two measurements are involved in the determination of moisture retention curves: weight and relative humidity. The accuracy of determining the weight of a sample is better than 0.01%. The high-temperature constant humidity chamber can maintain a humidity level within ± 2% relative humidity of a set value. The accuracy of the humidity measurement is about 2 to 5%. The corresponding uncertainty in matric potential is about 100% at 95% relative humidity (a matric potential of 7 MPa) and about 5 to 7% at 40% relative humidity (a matric potential of 123 MPa).

2.3.2.4 Klinkenberg Coefficient

The Klinkenberg coefficient will be used to calculate the Knudsen diffusion coefficient of gas. The Klinkenberg coefficient as a function of temperature beyond the boiling point of water will be determined. In the matrix part of a rock mass, Knudsen diffusion may exist at temperatures greater than the boiling point of water, dependent upon the pore pressure. As mentioned in Sec. 2.2.1, the Klinkenberg coefficient at room temperature will be determined in a few Topopah Spring tuff samples to confirm the relationship between Klinkenberg coefficient and liquid permeability suggested by Heid et al. [1950]. The effect of temperature on gas permeability in the tuff will be measured to determine whether the relationship between Klinkenberg coefficient and liquid permeability can be extended to greater temperatures. The method of determining the Klinkenberg coefficient is described by Reda [1987]. Basically, gas permeability in a dry intact tuff sample will be measured at various levels of pore fluid pressure, while the effective pressure on the sample (effective pressure = confining pressure – pore fluid pressure) is maintained constant. The slope of a plot of the gas permeability vs the inverse of the pore-fluid pressure is the product of the Klinkenberg coefficient and the saturated water permeability of the sample. Therefore, the saturated water permeability of the sample should be determined first. The water permeability can be determined following the procedures described in Sec. 2.3.2.2. The effective porosity of the sample will also be determined, following the procedures described in Sec. 2.3.2.1. Because a dry sample is used, it is not expected that the water saturated permeability and the effective porosity of samples will change due to the measurement of gas permeability. However, these properties will be remeasured after the measurement of the Klinkenberg coefficient.

The procedures for measuring gas permeability are basically the same as measuring water permeability (Sec. 2.3.2.2). The sample for the gas permeability measurement must be dried before jacketing. The sample will be dried in a vacuum oven at a temperature no higher than 35°C until its weight remains unchanged for at least one day. The dry sample is then jacketed and put in a pressure vessel to be saturated with

dry gas (usually N_2) at a certain level of pore pressure. Then, the permeability is measured using the steady-state flow rate method. As mentioned in Sec. 2.3.2.2, the flow rate of the gas will be kept at a minimum measurable level so that the inertial and turbulent effects are minimized. In addition, permeability will be measured as a function of flow rate in some of the samples to test the inertial and turbulent effects.

The gas permeability will also be measured in a sample with residual water saturation, instead of dried in a vacuum oven. A sample will be dried in a humidity chamber, the saturation level will be determined as a function of decreasing relative humidity. The sample will be considered to contain residual water when its saturation can not be significantly reduced. The Klinkenberg coefficient will be determined in such a sample. The sample must not be allowed to dry out during the measurement. A semipermeable membrane that only allows gas to pass may be used to help keep the sample from drying out. The sample will be weighed before and after testing to check its saturation condition.

Range of Expected Results

The measured gas permeability depends on the pore-fluid pressure. According to Reda [1987], the gas permeability may be as high as ten times the water permeability. Therefore the gas permeability of intact, densely welded Topopah Spring tuff is in the range of several microdarcies to hundreds of microdarcies. There are not enough data to establish an expected range of value of the Klinkenberg coefficient. One measurement by Reda [1987] shows that the Klinkenberg coefficient of densely welded tuff is about 0.76 MPa.

Measurement Uncertainty

The accuracy of the gas permeability measurement is about the same as that of the water permeability measurement, in the range of 10 to 15%. The accuracy of the pore-pressure measurement is about 1%. The accuracy of the calculated Klinkenberg coefficient is difficult to assess, because it involves curve fitting and calculation of slope. With good data, i.e., good linear relation between permeability and inverse pore pressure, the uncertainty is expected to be about 20%. The acceptable uncertainty of the calculated Klinkenberg coefficient should be determined by a sensitivity analysis (model) study.

2.3.2.5 Electrical Conductivity vs Moisture Content

In most of the experiments to validate the thermal-hydrological model, the spatial and temporal distributions of moisture in a test sample will be determined. Measurements of electrical conductivity, such as two-electrode measurement and impedance imaging, are among the methods that will be used to determine the spatial and temporal distribution of moisture in a sample. In order to obtain quantitative measurements of the moisture distribution, a relationship between the measured electrical conductivity and water content will be established. The purpose of this activity is to determine the almost-DC electrical conductivity of test material at various

degrees of water content for both draining and imbibition conditions at various temperatures.

In addition to moisture content, conduction of electrical current in rock may also be affected by cation exchange between minerals. Although cation exchange is not expected to have significant effect on electrical conductivity of this Topopah Spring tuff, the cation exchange capacity of the samples used in this activity will be determined using the methodology of Sec. 2.3.3.6. The equation by Waxman and Smits [1968] will be used to evaluate the effect of cation exchange on the measured electrical conductivity.

Samples will be machined to disks approximately 5 cm in diameter with four thicknesses: approximately 1, 2, 3, and 4 mm. Ten samples of each thickness will be measured. The effective porosity of these disk samples will be determined following the procedures described in Sec. 2.3.2.1. The rock core adjacent to these disk samples will be used to determine saturated water permeability, (as described in Sec. 2.3.2.2), cation exchange capacity, mineralogy, and pore size distribution. Platinum or gold electrodes will be vapor deposited on the flat surfaces of each sample. The two-terminal electrical resistance of each sample will be measured at various degrees of water content. The electrical conductivity of the water will be determined by a commercial grade conductance probe. Enough time between each change of water content will be allowed for the water to be uniformly distributed in the sample. The measured electrical conductivity as a function of time will be used to determine whether the sample has reached equilibrium. The measurements will be repeated so that a complete cycle of drying and imbibition is covered.

The measured electrical resistance value of each thickness will be linearly extrapolated to zero thickness to determine the electrode contact resistance which will then be subtracted from each measurement. Each corrected resistance value will be converted to resistivity by multiplying it by the ratio of the surface area of the electrode to the sample thickness. Conductivity is the inverse of resistivity.

The measurements will be repeated at elevated temperatures. Electrical conductivity at four or five different temperatures will be determined so that the effect of temperature on the relation between conductivity and water content can be established. The temperature of the sample will be kept below the boiling point of water.

Material adjacent to the test samples and the test samples themselves will be used in microprobe analysis to determine mineralogical changes before and after the experiment. These results can provide information on the cation exchange capacity of the minerals. The cation exchange capacity will be used to evaluate the effect of water saturation on the bulk electrical conductivity of tuff [Waxman and Smits, 1968].

2.3.3 Laboratory-Scale Model Validation Experiments

Model calculations are used to predict the movement of moisture in a repository for tens of thousands of years based on the results of laboratory and field measurements on a finite number of samples and locations in a relatively short period of time (several years at most). The model takes into consideration the effect of evaporation and boiling

of water caused by decay heat from the WPs. In the model calculations, the effects of fractures on the transport of water, steam, vapor, and heat also need to be considered. The thermal-hydrological processes used in the model calculations should be tested by laboratory experiments under controlled conditions and by field tests. Some of the laboratory experiments, such as the fracture healing experiment, will be used to develop conceptual models of the thermal-hydrological processes. The laboratory calibration and validation experiments are described below. The field tests for model validation are described in a separate study plan (SP 8.3.4.2.4.4).

The experiments described below are for general planning purposes only. More detailed experimental procedures will be included in Activity Plan(s). Scoping calculations will determine the experimental requirements, error analysis, etc. Experimental design and procedures may be changed to reflect the evolving understanding of the thermal-hydrological processes in a nuclear waste repository. New experiments will be added if deemed necessary by the PI. Modifications of the initially planned experiments and initiation of new experiments will be documented in scientific notebooks and, if appropriate, in a revised version of this study plan.

2.3.3.1 Drying and Rewetting of Intact Rock

The rates of one-dimensional dehydration and imbibition can be used along with the moisture retention curve during draining and imbibition to calculate the relative permeability as a function of saturation. The calculation of relative permeability will be discussed in activity plans. An intact sample machined into a cylinder or block will be used for this experiment. At least three samples of each rock type will be tested. J-13 or other appropriate water will be used as pore fluid. The hydrological properties of the material (as specified in Sec. 2.3.2), except the Klinkenberg coefficient, will be determined. The test samples will be oriented such that the imbibition and dehydration processes are either with gravity, against gravity, or perpendicular to gravity.

A cylindrical or block sample of at least 2.5 cm diameter (or square) and 10 cm in length will be used in the test. The sample will be instrumented with electrodes and pressure transducers. It will also be jacketed so that no moisture can be transported in or out of the sample except through one end. The test will begin with a saturated sample which will be heated uniformly and gradually from all sides to encourage dehydration. The temperature in the sample will be maintained below the boiling point of the pore fluid. The dehydration rate will be measured as a function of time by weighing the sample periodically. The drying front will be located using the electrical resistivity measurement and/or x-ray CT scan. Pore pressure in the sample will be measured using a pressure transducer.

When the sample is dry, water will be placed in contact with the open end and allowed to be imbibed into the sample. The imbibition rate will be determined as a function of time. The distribution of moisture in the sample will be determined, again using electrical resistivity measurement. Pore pressure will also be measured.

Another set of one dimensional imbibition experiments will allow air to escape the sample during the imbibition process. Cylindrical samples as described above will be

jacketed on the side, leaving both ends exposed. The samples will be equipped with the same monitoring sensors as described above. One end of the samples will be brought in contact with water. The imbibition rate, the moisture distribution, and pore pressure will be measured as a function of time. The result of this imbibition experiment will be compared with the one described above, in which air is not allowed to leave the sample. This is to understand how the air pressure within an intact sample would affect the imbibition process.

2.3.3.2 Infiltration in a Fracture

The speed of infiltration of water in a fracture and the imbibition of water into the matrix from the fracture at elevated temperatures will be studied. The results will be used for numerical model validation. This study will be done at room pressure. A long sample will be used. The sample may be a circular cylinder or a rectangular column. The hydrological properties (as specified in Sec. 2.3.2) of the same material will be determined before the test.

A sample about 1 m long with a fracture or saw cut along its axis will be used. The aperture of the saw cut will be controlled within a range from about 20 to 100 μm. Pieces of inert metal, such as platinum, shimmed with various thicknesses will be used to control the aperture. The surfaces of the saw cut will be polished flat and smooth to within a typical grain size and cleaned to be free of debris. The sample will be equipped with vapor deposited electrodes on the fracture surfaces, transverse to the main flow direction, to monitor the flow of water in the fracture. The distribution of moisture content in the matrix will be monitored by electrical resistivity tomography and/or CT scanning, using electrodes on the sample surface. A moisture barrier will be mounted on the sides of the sample. The sample will be externally heated either uniformly or from one end such that the water flows along the thermal gradient. The maximum temperature in the sample will be kept below the boiling point of water. Temperature in the sample will be measured.

The experiment will start with a sample of known moisture content. A line source of water will be applied along the fracture at one end of the sample (the upstream end). The water head will be controlled. The water speed in the fracture and the distribution of moisture content in the matrix as a function of time will be measured.

The procedures may be repeated for samples with various degrees of water saturation. In that case, a predetermined amount of water will be added to a dry sample. The added water will be allowed to uniformly redistribute in the sample before the experiment begins.

2.3.3.3 Drying and Rewetting of Fractured Rock

The rate of dehydration as a function of time and space in a cylindrical sample with a fracture or saw cut along its axis will be determined. When the sample is dry, it will be rehydrated, and the imbibition rate and the moisture distribution in the sample will be

determined. The results will be used for model validation. This experiment is similar to that described in Sec. 2.3.3.1, except that the sample will contain a fracture or saw-cut instead of being intact. The hydrological properties (as specified in Sec. 2.3.2) of the same material as the sample will be determined before the experiment is started. The information for the matrix part will be measured using a piece of material from the same block as the sample used in this experiment. The fracture permeability will be determined on the sample actually being tested in the experiment.

A cylindrical sample of at least 2.5 cm diameter and 10 cm length will be used. The sample will have a fracture or saw-cut along its axis. The saw-cut surfaces will be prepared as described in Sec. 2.3.3.2. The aperture of the saw-cut will be controlled. The sample will be saturated with J-13 water or other appropriate liquid. Electrodes will be mounted on the sample surface. Pore fluid pressure in the matrix near the sealed end of the sample will be measured. The sample will be jacketed so that vapor will not escape except through one end. Drying will occur by heating the sample gradually either from all sides or from one end. The heating rate and maximum temperature will be determined by scoping calculations. Total water content, pore pressure, and vapor flowing out of the sample will be determined as a function of time. Electrical resistance tomography will be used to monitor the distribution of water in the sample as a function of time.

After drying is essentially complete, water will be brought in contact with the open end of the sample. Total water content, pore pressure, and the distribution of water in the sample will be determined as function of time. The imbibition will be against gravity, with gravity, and perpendicular to gravity (in separate tests). The fracture surfaces and the matrix of the sample will be examined for mineralogical alteration and/or salt deposition, as described in Sec. 2.3.3.6. A set of imbibition experiments will also be conducted in which air is allowed to escape the sample during imbibition, as described in Sec. 2.3.3.1.

2.3.3.4 Vapor Flow and Condensation in a Fracture

The amount and distribution of vapor condensing in a fracture at room conditions will be determined. This study is to understand the basic phenomenon of vapor condensation and the distribution of the condensate along the fracture. Therefore, the sample must be kept below the dew point of the vapor. Results will be used for model validation. A cylindrical sample of Topopah Spring tuff or equivalent material with a fracture or saw-cut will be used. The sample may be either a circular cylinder or a square column. The hydrological properties (as specified in Sec. 2.3.2) of the material adjacent to the sample will be determined before the experiment is conducted. These properties of the matrix part of the sample will be measured on a piece of the material from the same block as the sample used in this experiment. The fracture permeability will be measured on the sample actually being tested in the experiment.

A sample of at least 2.54 cm in diameter (or square) and 20 cm in length will be used in the experiment. The sample will contain a longitudinal fracture or saw-cut parallel to its axis. The saw-cut surfaces will be prepared as specified in Sec. 2.3.3.2. The saw-cut

aperture will be controlled. Electrodes will be vapor deposited on the sample and on the saw-cut. Steam or moist air will be injected into the saw cut. The entire sample will be kept under the dew point. Total water content will be measured as a function of time. Electrical resistivity measurements will be used to monitor the position of condensed water on the saw-cut surfaces. Electrical resistance tomography will be used to monitor the water distribution in the sample as a function of time. The same procedures will be repeated on samples with various degrees of initial water saturation.

2.3.3.5 Three-Dimensional Imbibition

The movement of a water front from a three-dimensional imbibition process in a tuff sample or equivalent material will be determined. Results will be used to compare with model prediction and for model validation. The hydrological properties (as specified in Sec. 2.3.2) of the material adjacent to the sample will be determined before the experiment. These properties will be measured using several pieces of material from the same block as the sample used in this experiment, so that the block scale variability of matrix properties can be determined. An intact sample of at least 7.5 cm in diameter and 10 cm in length will be used. Electrodes will be vapor deposited on the sample surface to facilitate the use of electrical resistance tomography to monitor the distribution of moisture in the sample.

A dry sample will be used. The sample will be submerged in either water or water vapor at room temperature and pressure. The total imbibition rate will be determined by either measuring the total weight change of the sample when it is in water, or measuring the volume change of the imbibing water. Electrical resistivity tomography will be used to locate the imbibition front of water as a function of time. The procedures will be repeated for samples with various degrees of initial moisture content.

2.3.3.6 Fracture Healing Experiment

It has been observed in the laboratory that flowing water at temperatures greater than 90°C through a fractured Topopah Spring tuff sample causes a drastic decrease in permeability [Lin and Daily, 1984; Daily et al., 1987; Lin and Daily, 1989; Lin and Daily, 1990]. Lin [1991] reported that flowing (probably) wet steam through a naturally fractured tuff sample at a temperature of 127°C decreases N_2 permeability. The fracture healing was observed in samples with a natural fracture, an induced tensile fracture, and a saw cut [Lin and Daily, 1989]. They also showed that N_2 permeability in a dry tuff sample at the same confining pressure was not affected by temperature. However, Lee and Ueng [1991] reported an increase in gas permeability in the heater hole of the field test in G-Tunnel, Nevada Test Site. In the laboratory experiments, the sample was under a constant confining pressure of 5 MPa. The confining pressure is probably one of the major factors influencing the laboratory results. Another factor that may affect fracture healing is the amount of water or steam flowed through a sample before the fracture begins to heal. In this experiment, the fracture healing will be studied at various confining pressures, and the amount of pore fluid that flows through the sample will be

measured. Water flowed through the sample will be analyzed for chemical changes; the fracture surfaces will be examined before and after the experiment for mineralogical changes. Results of this experiment will be used in development of the thermal-hydrological model, using the V-TOUGH and NUFT codes, that will include considerations of variable hydrological properties, such as permeability and fracture aperture. The results will also be used to validate the geochemical model using EQ3/6 and to develop thermal-hydrological-geochemical coupling codes (e.g., PRECIP and BASIN II).

Naturally fractured cylindrical samples of the tuff or equivalent material of at least 2.5 cm diameter and 10 cm length will be used. The samples will be saturated with J-13 water or other appropriate fluid, and then jacketed in a soft jacket that has an operational temperature rating of at least 150°C. The pore fluid pressure should be greater than the steam pressure at the testing temperature so that the pore water will remain in liquid form, which is about 0.5 MPa at 150°C. Saturated water permeability will be measured at a confining pressure of just a few tenths of MPa greater than the pore fluid pressure, and the testing temperatures will be varied from room temperature to at least 150°C and returned to room temperature. A minimal amount of water flow through the sample in each permeability measurement will be permitted. If no decrease in permeability is observed, the experiment will be repeated with the same sample at a slightly greater confining pressure, but with the same pore pressure. Thus, the influence of effective pressure on fracture healing will be determined. If fracture healing is observed for the lowest confining pressure case, then an experiment at room pressure and elevated temperatures will be conducted. In this case, the sample will be sealed with adhesive material, and water will be flowed through the sample by gravity force only. Temperature will be kept below the boiling point of water.

Another experiment will be conducted to test the effect of amount of water flow through the sample on fracture healing. The experimental procedures described in previous paragraph will be applied to a new fractured sample at a confining pressure less than that in which fracture healing occurs, as determined in previous experiment, and at a high temperature between 95 and 150°C. Water permeability will be determined as a function of the amount of water flowed through the sample.

Also planned is an experiment in which the water is recycled through the same sample in both situations (i.e., fracture healing occurs and does not occur). This experiment will test the effect of refluxing water on fracture healing. It will also provide information on the geochemical processes related to refluxing.

The water that flows through the sample during the fracture healing experiment will be collected and analyzed so that the quantity can be determined and its chemical composition can be compared with that of the virgin water. These analyses will be conducted under the control of another study plan, SP 8.3.4.2.4.1. Scanning electron microscopy (SEM), microprobe analysis of elements, and fracture surface image analysis will be done on the fracture surfaces of the test sample (post-experiment) and on a piece of the surface adjacent to that being tested for fracture healing (pre-experiment) to examine mineralogical changes associated with fracture healing. These tests will provide information on geochemical processes including rock-water interaction,

mineralogical changes, and cation exchange capacity of the minerals that may be associated with fracture healing. This information will be used to evaluate the geochemical code EQ3/6.

3. Application of Results

The laboratory determined hydrological properties of Topopah Spring tuff, as described in Sec. 2.3.2, will provide input data for numerical model calculations that will predict the hydrological processes in the near-field environment of a nuclear waste repository. The model validation experiments, as described in Sec. 2.3.3, will provide part of the validation and calibration of the conceptual and mathematical models. Thermal-hydrological behavior in the near-field environment will be sufficiently understood so that the radionuclide release and transport models can be developed and the Waste Package Performance Assessment can be accomplished. The results of these studies will be used in WP design in the area of waste package interactions with the emplacement environment. A more detailed discussion of the products of modeling and analysis activities is given in Sec. 2.3.1.6.

The information derived from these activities will be used in addressing the following specific Information Needs (IN) and corresponding descriptions in the Site Characterization Plan (SCP):

SCP 8.3.5.9.3 (IN 1.4.3): Scenarios and models needed to predict the rate of degradation of the container material.

SCP 8.3.5.9.4 (IN 1.4.4): Estimates of the rates and mechanisms of container degradation in the repository environment for anticipated and unanticipated processes and events, and calculation of the failure rate of the container as a function of time.

SCP 8.3.5.10.3 (IN 1.5.3): Scenarios and models needed to predict the rate of radionuclide release from the waste package and engineered barrier system.

SCP 8.3.5.10.4 (IN 1.5.4): Determination of the release rates of radionuclides from the waste package and engineered barrier system for anticipated and unanticipated events.

SCP 7.2.1.3.1 (IN 1.10.1): Design information needed to comply with post-closure criteria from 10 CFR 60.135(a) for consideration of the interactions between the waste package and its environment.

SCP 7.4.5.4.5: Waste package environment model to evaluate the flow of water, steam, and air that can affect the waste package barriers and the waste form.

4. Schedule

The schedule of this study is shown in Fig. 2. This schedule is for planning purposes only and illustrates a generic sequence of experiments, analyses, and information feeds to successive updates of the Near-Field Environment Report (called the Near-Field Report in Fig. 2). Note that all of the experimental activities shown in Fig. 2 include supporting model calculations required to interpret the experiments. Also note that the EBSFT design activities also include supporting model calculations [see e.g., Buscheck and Nitao, 1995] required to optimize the heater layout, heatup and cooldown schedules, and instrument layout. The EBSFT analysis activities include supporting model calculations required to (1) interpret test results, (2) help resolve hypotheses associated with thermal-hydrological behavior and EBS performance, and (3) build confidence in process models of thermal-hydrological behavior in the EBS and near field.

Detailed schedules will be included in Activity Plan(s). The schedule may be changed due to the constraints of time and resources. The changed schedule will be included in the Activity Plan(s). The data obtained from the activity of determining the hydrological properties will be fed to the activity of model validation experiments continuously. The interface between the two categories of activities at the end of every fiscal year, as shown in Fig. 2, is just for illustration purpose only. The determination of hydrological properties will utilize samples from the existing cores, the Large Block Test (LBT) samples, the surface based cores, and the ESF samples. The interface between this study and the Engineered Barrier System Field Tests (EBSFT) is also continuous. In Years 1 and 2 the results of this study will be used as input to the analysis of LBT results and the design of EBSFT. In the later years the results of this study will be used to help analyze the results of the EBSFT. The results from this study will be used to update the Near-Field Environment Report when needed.

The activities of determining the hydrological properties, as listed in Sec. 2.3.2, are grouped together under one single activity, Hydrological Properties, in Fig. 2. This is because most of these measurements will be conducted almost simultaneously.

Before the approval of this Study Plan and associated Activity Plan(s), the activities of determining the hydrological properties and conducting model validation experiments are scoping in nature and are controlled by a Scientific Investigation Plan (SIP), SIP-7, entitled Nevada Nuclear Storage Investigations: Waste Package Environment. The scoping activities have been graded as not quality affecting. The results of these scoping activities were used to prepare this Study Plan, and will be used in preparation of the Activity Plan(s) and to help design the subsequent experiments.

Figure 2. Tentative schedule of the laboratory study of hydrological properties in the near-field environment.

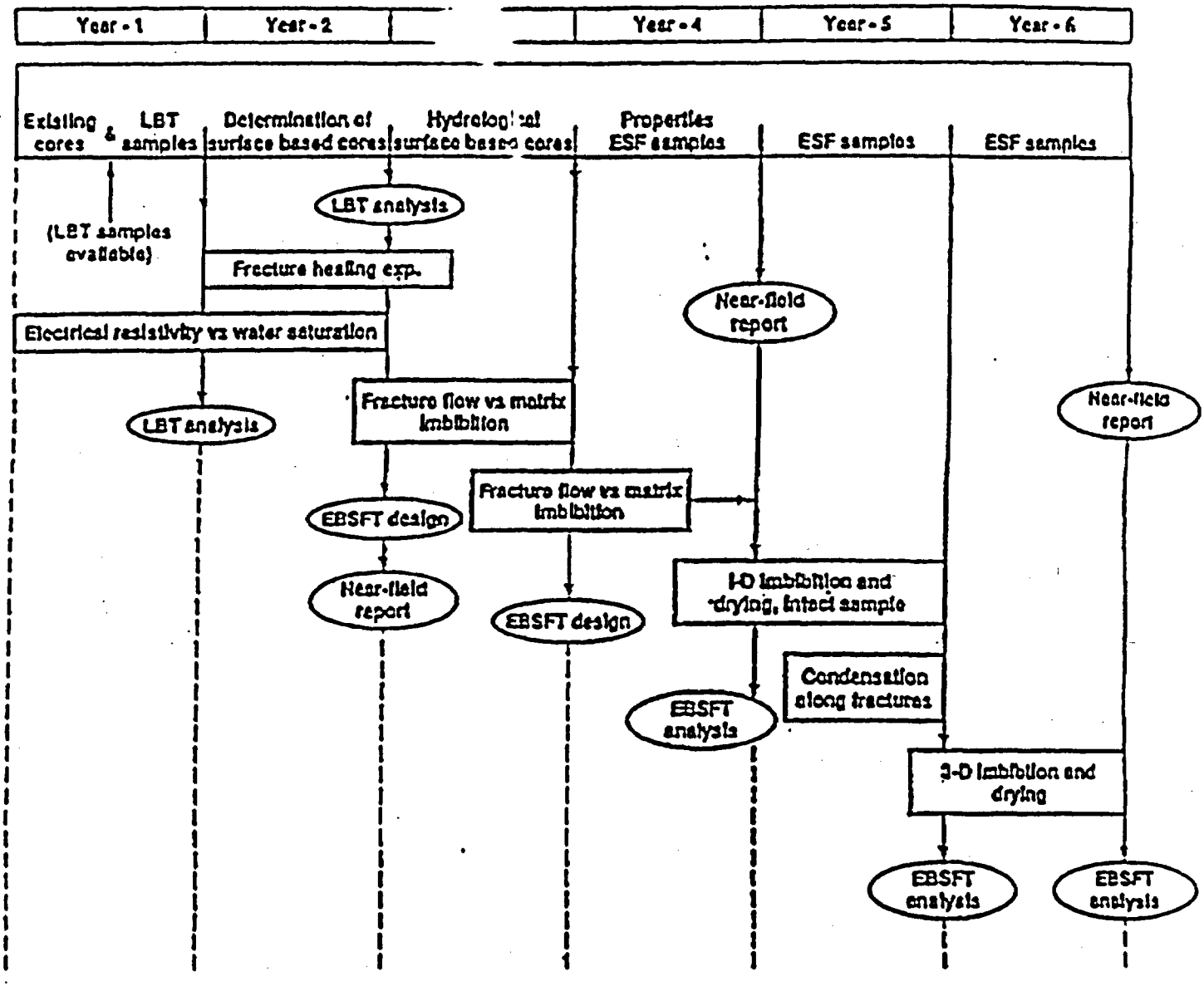

Figure 2. Tentative schedule.

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6. Abbreviations and Acronyms

AA	Atomic absorption spectroscopy
AML	Areal Mass Loading
AZR	Altered Zone Report
CFR	Code of Federal Regulations
EBS	Engineered Barrier System
EBSFT	Engineered Barrier System Field Tests
ECM	Equivalent Continuum Model
ESF	Exploratory Study Facility
HLW	high-level waste
IC	Ion chromatography
ICP	inductively coupled plasma spectroscopy
IN	Information Needs
ISP	Individual Software Plan
LA	License Application
LAD	License Application Deadline
LBT	Large-Block Test
MGDS	Mined Geological Disposal System
MTU	metric tons of uranium
NFEHP	Near-Field Environment Hydrological Properties
NFER	Near-Field Environment Report
NRC	Nuclear Regulatory Commission
NTS	Nevada Test Site
PI	principal investigator
QA	Quality Assurance
REV	representative elementary volume
RIB	Reference Information Base
SCC	substantially complete containment
SCP	Site Characterization Plan
SEM	Scanning electron microscopy
SIP	Scientific Investigation Plan
SNF	spent nuclear fuel

SP	Study Plan
SQA	Software Quality Assurance
SZ	saturated zone
TSS	Technical Site Suitability
UZ	unsaturated zone
WP	waste package

7. Glossary

areal mass loading (AML): a measure of the mass of spent nuclear fuel per unit horizontal area of repository; usually expressed in either metric tons of uranium per acre (MTU/acre) or in kilograms of uranium per square meter (kg/m^2); this term is often used to quantify the average thermal loading conditions over the repository; a high-AML repository is associated with a high specific heat flux that results in thousands of years of above-boiling temperatures in the repository; a low-AML repository is associated with a low specific heat flux that results in a relatively short boiling period or no boiling at all; this term can also be used to characterize local heat generation characteristics.

advection: movement of a substance or material (i.e., an extensive quantity such as internal energy or the mass of a species) arising from the motion of a fluid phase.

advective velocity: the weighted average of the velocity of each species within the averaging volume associated with the microscopic point of the phase; usually the weighting is by the relative mass or relative number of moles of the species.

altered zone processes: the physical and chemical processes that are the result of the repository itself and that could affect EBS and total system performance; these processes include the effects of radioactive-decay heat on moisture and gas movement, geochemical reactions, and geomechanical stresses.

buoyant convection: motion of a fluid arising from changes in fluid density caused by temperature gradients; an example is when heat creates a lighter column of fluid that rises, thus reducing the pressure around the bottom of the column and drawing in cooler surrounding fluid, which also rises as it is heated.

capillary forces: forces arising from surface tension.

capillary imbibition: see imbibition.

condensate: liquid water resulting from condensation of water vapor, usually derived from water evaporated by decay heat from WPs; can also refer to condensation of water vapor driven by geothermal gradients.

convection: the transport of heat by fluid advection.

diffusion: movement of an extensive quantity relative to the advective velocity (usually mass-weighted or molar-weighted velocity) of a phase; molecular diffusion of a species, such as water vapor in the gas phase, leads to a diffusive flux of that species according to Fick's law of diffusion, which states that the diffusive flux is proportional to the gradient in concentration of that species; the relevant concentration is mass fraction or mole fraction, depending on whether the diffusive flux is relative to the mass-weighted or mole-weighted advective velocity, respectively.

dispersion: macroscopic movement of an extensive quantity relative to the macroscopic advective velocity of the underlying phase; an example is the dispersion of a chemical species that results in a deviation of the microscopic concentration of the species from the macroscopic concentration.

engineered barrier system (EBS): defined in 10 CFR 60 [NRC 1991] to mean "the waste packages and the underground facility," where the underground facility is "the underground structure, including openings and backfill materials, but excluding shafts, boreholes, and their seals."

extensive quantity: a physical quantity that is additive over volumes, such as mass, energy, and momentum.

gas phase: in the context of this document, the gas phase is a mixture of air, water vapor, and any gaseous radionuclides or other gaseous chemical species relevant to EBS performance.

heat-pipe effect: an advective heat-transfer mechanism whereby latent heat is transported by a vapor from a hotter region, where liquid is evaporated, to a cooler region, where the vapor recondenses to a liquid; the liquid returns to the hotter region either through matrix suction (including capillarity) or by gravity; in a fractured medium with a porous matrix, the return flow can be driven by gravity in the fractures and by matrix suction.

hydrologic processes: usually means flow and transport processes occurring in an aqueous phase, but in this document we also include transport in the gas phase.

imbibition: process whereby a fluid phase is drawn into a porous medium by a matric potential acting on that fluid phase.

macroscopic: refers to quantities obtained from volume-averaging microscopic quantities over representative elementary volumes; quantities predicted by numerical models of porous media are usually macroscopic quantities.

macroscopic point: it is often assumed that each point in space has a representative elementary volume associated with it over which macroscopic quantities can be defined by averaging.

mass fraction: ratio of the mass of a component to the total mass in a fluid phase of a particular system, often taken to be a very small volume at a point in space.

matric potential: the Gibbs free energy necessary to remove a unit amount (mass or volume) of the aqueous phase from the porous medium to a reference reservoir outside the medium; includes both capillary and adsorptive forces from the solid surfaces; does not include osmotic effects, i.e., change in free energy because of chemical concentrations; measurement at a given temperature gives the matric potential as a function of saturation

microscopic: refers to quantities defined at each (microscopic) point in space.

microscopic point: from statistical thermodynamics, each point in space has associated with it a small volume of space over which fundamental thermodynamic quantities are defined such as temperature, pressure, and concentrations.

near-field-affecting processes: the physical and chemical processes that directly determine the waste package environment and affect the release of nuclides; for an unsaturated repository, these processes may occur over large distances.

phase (fluid): a mixture of species whose composition and thermodynamic properties, such as viscosity, are uniquely defined functions of thermodynamic conditions specific to that phase.

refluxing: the continual cyclic boiling and evaporation of condensate in a heat pipe.

relative humidity: the mole percentage of water vapor in the gas phase relative to the mole percentage of water vapor at equilibrium saturation at a given temperature and pressure; also, approximately equal to the partial pressure of water P_v divided by the saturated vapor pressure $P_{sat}(T)$ at a given temperature T.

representative elementary volume: a volume of space around each point in space over which microscopic quantities are averaged in order to obtain macroscopic quantities; this volume must have the property that small changes in the volume do not significantly affect the value of the macroscopic quantities.

saturation pressure: the saturated vapor pressure of water in an open system (i.e., a system without surface or capillary forces); it is purely a function of temperature and is given in the steam tables for pure water.

source term: the flux of each radionuclide leaving the waste package.

thermal loading conditions: this term generally encompasses the spatial and temporal characteristics of the radioactive-decay heat generated by the spent nuclear fuel (SNF); the most general parameter quantifying thermal loading is the areal mass loading (AML) averaged over the entire repository; the AML quantifies the time-integrated amount of thermal energy that will be released from the SNF per unit horizontal area of the repository; together with the AML, the age of SNF determines initial specific heat flux; thermal loading conditions can also include a detailed accounting of heating on WP-by-WP waste package basis.

thermal-hydrology: refers to thermal and hydrological processes, including intercoupling between these two sets of processes.

thermal processes: those processes having to do with the storage and transport of heat energy.

vapor-pressure lowering: the lowering of the saturated vapor pressure of water in a porous medium because of increasing matric tension (the negative of matric potential) at lower aqueous phase saturations.

waste package (WP): the "waste-form and any containers, shielding, packing, and other absorbent materials immediately surrounding an individual waste container" [10 CFR 60].

waste package environment: the chemical, geomechanical, thermal-hydrological, microbial, and radiological conditions at the waste package.

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