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## Reference Hydrologic Scenarios Developed from the Nominal Flow Report

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#### Abstract

Earlier work presented a large number of release scenarios arising from the flow of water in liquid or vapor form through and around a hypothetical repository at Yucca Mountain, Nevada. In an effort to expedite final scenario identification, twelve reference cases are now selected from the lengthy list of scenarios previously developed. These reference cases, or "base cases," capture in detail the behavior of the repository as it is currently expected to perform. The base cases are expected to be useful references as further data, exploration, and calculation are produced—some in response to the selection of a particular base case. Two criteria were used in selecting the base cases. First, the complete set of base cases should include all physical phenomena that are reasonably expected to occur, and second, the base cases should include the most likely physical behavior, based on the advice of the PIs. The base cases are both abstracted and expanded from earlier work.

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#### Introduction

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Scenarios Constructed for Nominal Flow in the Presence of a Repository at Yucca Mountain and Vicinity (Barr et al., 1995; referred to here as "the nominal-flow report") presented a large number of release scenarios arising from the flow of water in liquid or vapor form through and around a hypothetical repository at Yucca Mountain, Nevada. Reviewers of the nominal-flow report suggested that it would expedite final scenario identification if a small number of reference cases were selected from the lengthy list of scenarios developed there. These reference cases will be called "base cases." The reviewers requested a limited number of well-posed problems that capture in detail the behavior of the repository as it is currently expected to perform. The base cases are expected to be useful references as further data, exploration, and calculation are produced—some in response to the selection of a particular base case.

Normally, pieces or elements of the scenarios would be examined by many Yucca Mountain Site Characterization Project principal investigators (PIs), who would gradually sort out which can be supported by experiment and calculation and which can not. This process would, over time, provide a vigorous trimming of scenarios. Because current Project scheduling requires the sorting to proceed quickly, we have selected reference scenarios on the basis of literature review and discussions with PIs. We have used two criteria in selecting the base cases. First, the complete set of base cases should include all physical phenomena that are reasonably expected to occur, and second, the base cases should include the most likely physical behavior, based on the advice of the PIs. This memo report is a Project internal document intended to elicit further response from PIs in order to help decide on the most sensible and useful reference scenarios. We ask that such responses include appropriate references, to be used by analysts doing performance assessment.

The base cases are both abstracted and expanded from the nominal-flow report. First, many of the scenarios originally considered seem, in the light of currently available data and calculations, to be unlikely; they are not considered here. Second, scenarios proliferated in the nominal-flow report in part because we attempted to account for how infiltration is distributed over the mountain and how each component of infiltration might be measured. Recent results (Flint and Flint, 1994) have established a distribution function for matrix infiltration for the current climate. That distribution function is presumed here to represent the source for water entering from episodic precipitation events as unsaturated flow plumes and locally saturated flow plumes; hence many of the scenarios in the nominal-flow report collapse into each other. Finally, in some cases the scenarios described in the nominal-flow report needed further expansion of some elements in order to provide well-posed problems.

Selection of base-case scenarios depends on decisions that are made about design, construction, and operation; these decisions constrain the definition of the repository environment. Power density, use of backfill, and container size are examples of factors to be decided; however, decisions about them also depend on the consequences of scenario calculations. The argument is circular, so we have simply started at the current place at which Project PIs have placed the Project and indicate where we believe decisions must be made (or have been made). It is necessary to define the repository environment to sort through the scenarios that have been constructed.

#### General Structure of the Scenarios

The general structure of the scenarios (Figure 1) starts with a query about whether there is infiltration into the mountain and then asks in turn about the thermo-mechanical interaction of any fluids (new or old) in the mountain with the repository heat, container failure, mobilization of contaminants, transport to the water table, and transport in the saturated zone. The answer to the first query of Figure 1—whether there is infiltration—appears to be yes. Recent isotopic studies (e.g., Fabryka-Martin, 1994, chlorine-36) indicated bomb-pulse values in the Calico Hills units beneath the proposed repository horizon. We infer that there is some recharge and flow in a currently active system at Yucca Mountain, although the study was not designed to determine the flux of water through the mountain.

#### **Common Features**

All scenarios share the common features of the tree in Figure 1; resolving how a feature is modeled for a few scenarios will resolve it for many. The large tree from the nominal-flow report (Barr et al., 1995) will be broken up for discussion in this text into expanded segments that share these common features.

The volume of fluid implied by the data and interpretations of Flint and Flint (1994) is still being deduced. Entrance of water into surface fractures is not yet included in any distribution function. As shown below, the permeability of fractures at the surface may be altered as a result of thermo-mechanical coupling, and this distribution function will become important.

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Infiltration. Figure 1 shows three options for the fate of precipitation: infiltration into the mountain, no net infiltration and a draining flow system, and vapor-maintained equilibrium in the mountain. Recent work on chlorine-36 (Fabryka-Martin, 1994) showed apparent rapid flow to depth, suggesting that the most likely choice is infiltration into the mountain. Flint and Flint (1994) provided a distribution function of potential for near-surface moisture over the mountain, other than in fractures. Their distribution function is presumed to be a surrogate for infiltration moving toward the repository. Thermal expansion at the repository is expected in the short term (a few hundred years) to alter fracture permeability at the surface, which could intercept more runoff than current fractures and direct additional water to interact with the repository. As the entire repository block heats up, the thermal expansion is distributed and the fractures initially opened, close. The mountain is probably able to adjust by slippage along existing blocks with some change in fracture permeability. Any infiltration interacts with repository heat at a depth dependent on the volume of water and the time after emplacement. Roughly speaking, percolating water can descend as far as the vaporization isotherm and accumulate there, depressing the isotherm toward the repository. If the volume and rate of an episodic entrance of water is great enough, the flow can break



Figure 1. Decision tree showing general structure of scenarios being discussed.

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through the isotherm and in certain circumstances reach the drifts and waste containers. If a heat pipe regiments established instead of a condensate cap, the flow can suppress and possibly collapse the heat pipe.

Thermo-Mechanical Interaction of Fluids with the Repository. The nominal-flow report discussed three general kinds of thermo-mechanical interactions of fluids with the repository: formation of a condensate cap, venting of vapor to the surface, and formation of a heat pipe. According to Alan Flint, U.S. Geological Survey, there appears to be a saturated zone at the base of the Tiva Canyon unit, well above the proposed level for a repository. Our interpretation is that this makes venting unlikely; venting will be ignored here pending further investigations. Examination of the isotherms associated with the details of loading the repository, with respect to both power density and waste stream, suggest that there are several possibilities for the extent of the condensate zone over drifts and for the interaction of condensate zones with adjacent drifts. These interactions will be considered in more detail, as will the formation of heat-pipes.

Container Failure and Waste Mobilization. The queries in Figure 1 for container failure and waste mobilization focus on the drift and its contents. All scenarios use the same drift size, liner, container type, emplacement mode, spacing (or power density) and absence (or presence) of backfill. Figure 2 is a sketch of a repository drift with waste containers in place. The base cases address how the drift liner and the surrounding rock supply water as a liquid or vapor to the drift and to the waste containers in the drift and what the consequences are to the containers. Oversby (1987) defined container failure as the occurrence of two or more pinholes in the waste container. Container breach is taken here to be a more general collapse of the container. We distinguish between failure and breach because the entry of water vapor or of liquid water through pinholes has different consequences for release and for criticality than a more general collapse of the container.

We also assume that if a flow system is established through the drift, then a signature of the repository is impressed on that flow system, possibly even before there is a release of contaminants from a container. This established flow system with the signature of the repository (which includes temperature, pH, and dissolved construction materials) will be referred to as the "carrier plume." The existence of a carrier plume was not considered in the nominal-flow report.

Exit. Fluids carrying contaminants must leave the drift either through pores in the drift liner or through fractures in the liner in order to enter the flow system. Exit from the drift involves similar chemical reactions for all scenarios. A carrier plume, with a characteristic signature of the repository (possibly different for unsaturated flow and saturated flow), transports the contaminants through the Topopah Spring and Calico Hills units. The Topopah Spring basal vitrophyre will probably be altered below part of the repository. The effects of that alteration will be shared only by scenarios for which leakage from the repository reaches the altered region.

Saturated Zone. All scenarios share the presumed behavior of the saturated zone, which is the principal conveyor of aqueous contaminants to the accessible environment. The



Figure 2. Sketch of a repository drift showing multipurpose containers (MPC) emplaced horizontally on cradles in a lined drift served by a dual-rail system.

description "presumed" is used because various calculations suggest that repository heat can generate convective flow and differential dissolution of rock below the water table (Buscheck and Nitao, 1993; Glassley, unpublished presentation to the Nuclear Waste Technology Review Board). The model of the saturated zone to be used must be tempered with the caution that the properties of the saturated zone are time dependent, and a model must change appropriately with the time of interest to the modeler. If the standard for release changes to a dose-based standard, the model probably must have the outfalls of the flow system identified and the model area expanded for all scenarios.

#### **The Expected Environment**

The repository environment will evolve in time, altering the critical phenomena that must be considered. To establish which scenarios are important, it is necessary to describe the repository environment and how it is expected to change.

When openings are first mined or bored into the rock, the surrounding rock begins to relax into the openings. This relaxation generates radial and concentric fractures near the opening, with the effects extending out to perhaps three drift diameters (Jaeger and Cook, 1979) (Figure 3). The rate of relaxation, or stress relief, by fracture generation depends on rock type and characteristics, which will be measured at Yucca Mountain. Mine ventilation during mining and before waste emplacement will reduce the local moisture content of the rock (Tsang and Pruess, 1989, 1990; Eaton and Reda, 1982). Hot waste containers will probably be emplaced in the drift before much stress relief has occurred. The thermal load of these containers will be radiatively and conductively coupled to the rock in the case of the SCP containers (i.e., the containers described in the Site Characterization Plan, U.S. Department of Energy, 1988) and radiatively, conductively, and convectively coupled to the rock for the MPC (i.e., multipurpose container). Thermal loading (more specifically, the local and average power density), container type (MPC or SCP container), loading scheme, and the use of backfill determine the thermo-mechanical and hydrothermal response of the rock. At present no strategy exists to decide how hot the repository should be, or, since variation of heat output by the waste stream is considerable, what phenomena constrain the local The essential ideas, information, and design that form the basis for such temperature. decisions are now mature enough to proceed with development of such a strategy. As will become clear below, certain decisions are necessary in order to select and model scenarios.

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Thermo-Mechanical Effects. The thermal load causes thermal expansion of the rockexpansion sufficient to overwhelm mechanical stress relief early in the life of the repository. Calculations by Jung and others (1994) indicate that zones of compression will form near the openings and zones of tension will form away from the repository, including at the surface of the mountain. Compression is expected to close many, but not all, of the fractures leading to the underground openings (See NUREG/CR-5390, by Mack et al., 1989). Given the existing stress state of the mountain and the presence of fractures, thermal expansion is likely to produce shear on some fractures. The ability of these fractures to conduct fluids is not currently known, but tension produced by the thermal expansion is expected to alter fracture permeability throughout the mountain, including at the surface.



Figure 3. Possible alterations of the rock due to the presence of the drift.



Figure 4. Formation of condensation cap (or shell) around a drift.

Smeared-source calculations support the formation of such a condensation cap. Individual container calculations: and row (smeared-source) calculations honoring repository layout geometry using conduction models suggest that the vaporization isotherm shows considerable structure (Ryder and Dunn, 1995). The isotherm parallels rows of containers above and below the rows and drops down between rows. The structure becomes lumpy when loading of the repository is connected in detail with inventory from a real waste stream (Ryder and Dunn, 1995). This result reinforces the possibility that a condensation cap over a part of one drift can shed accumulated fluid to another drift or to another part of the same drift (Figure 5). These calculations of the isotherm seem to be more robust than the two-phase smeared-source calculations mentioned above because they are specifically geometry dependent: drift length, separation, perimeter, and loading are included in the calculations.

One thus expects shedding of the condensate cap back to drifts and between drifts. Condensate shed between drifts leaves the repository area and reduces the total water available. One consequence of this two-phase movement of water is local drying around waste containers. The extent of the dryout zone and its persistence is unknown. LLNL has proposed using the pervasiveness and persistence of dryout to extend container lifetime (Ramspott, 1991; Wilder, 1993). This suggestion is being debated because existing calculations are not sufficiently detailed: smeared-source approximations are inadequate to examine the level of dryout (change of saturation in the rock) and simultaneously to allow for return of fluid from a condensation cap showing real structure (Ryder, 1992). Furthermore, "dryout" is not well defined (Pruess and Tsang, 1994). Any decrease in the saturation of the rock constitutes a level of dryout, but what reduction in saturation can usefully extend container life, how can that level of reduction be manipulated, and how much of the repository does it apply to?

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Thermal effects, which appear in rocks all the way to the surface, have additional consequences below the repository. Two-phase calculations (Buscheck and Nitao, 1993) and conduction calculations (Jung et al., 1994) indicate that the water table is not an isothermal boundary. Flow in the water table aquifer (tuff aquifers) is inadequate to carry away enough heat to maintain the original temperature of the aquifer. Conduction calculations produce temperatures in excess of 60 C at the water table, suggesting the possibility of single-phase convective flow being established in the rocks below the water table. Similar calculations for two-phase flow (Buscheck and Nitao, 1993) come to the same conclusion. The thickness of the units (100 to 300 m) and their dip of about 5 degrees also suggest that convective flow would be established in cells as rolls of about the thickness of the units. The faults that appear to bound the repository block (Solitario Canyon fault, Bow Ridge fault, and possibly others) probably constrain this convective flow laterally. The temperature differential of 30 C or more is likely to produce differential solubilities (for silica and calcite, for example) from the water table to the depth at which the convective circulation reaches, perhaps 200 m. There should be mass transport from the water table to this depth with precipitation in pores and fractures in the cooler regions below the edges of the repository and at the bottom of the convective circulation, according to Glassley and Barr. The rates of such precipitation and plugging are unknown, but we recognize four possibilities:



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Figure 5. Formation of a condensation cap over two drifts and its possible structure between drifts.

- 1. the rate is insufficient to affect transmissivity while convective circulation exists,
- 2. transmissivity is reduced,

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- 3. transmissivity is reduced in pores and small fractures but is unaltered in large fractures,
- 4. permeability is increased as solutes are swept way from the vicinity of the repository in the saturated-zone flow system.

Impacts Associated with Construction. The foreign materials introduced during construction and operation are primarily concrete and iron. Under current design, steel mine sets and a concrete liner will be used. A concrete invert will be placed (probably as prepoured segments) to support the rail system (Figure 2). The segment surfaces are in effect vertical fractures, and repeated passes of the transporter down the rail system carrying the containers will probably produce additional fractures in the liner. It appears that fracture flow will be possible through the invert and liner in the floor. Heating will cause some floor and wall buckling because of mineralogical phase changes, differential heating, and differential thermal expansion (say, shear on existing fractures). Whatever fluid is able to enter and leave the drift will carry the signature of the repository, which will include pH, calcium carbonate, iron, and heat. Fluid leaving the drift will form a carrier plume to which are added any contaminants that are released. How far this carrier plume will carry the repository signature into the rock is not known. The distance depends on the dissolved constituents. temperature, and the residence time of the plume (Figure 6) in a rock unit. W. Glassley estimates that the chemical signature of the repository would be buffered out by the rock if the residence time of the plume exceeds a few thousand years.

Cooling. The description of the evolution of the environment has so far considered only the immediate changes due to the emplacement of hot objects. The heat sources are not constant; they decay exponentially in heat output from the time of emplacement. For most of the 10,000-year life of the repository, cooling occurs primarily by propagation of heat into the rock. (The characteristic propagation time for the rock is smaller than the characteristic decay time of the source.) Heat leaves the mountain at the top surface, into the atmosphere; at the "bottom," being carried away by the aquifers; and at the sides, by conduction into an ever-larger mass of surrounding rock. The mechanical response to this cooling of the repository is diffusion of thermal expansion throughout the mass of the mountain. Because most of the heat is retained in the mountain during the 10,000-year lifetime of the repository, the net thermal expansion is about the same, but the strain, that is, actual movement on fractures, continues to be redistributed over the entire period of heating.

Rewetting. As the heat output of the source declines, the vaporization isotherm moves back toward the repository. This movement can be followed by corresponding movement of a condensate cap or possibly by re-establishment of a heat pipe regime. Similarly, any influx of water from the surface can interact with repository heat closer to the waste containers and drifts. When the isotherm is close enough, presumably just outside the drift liner, water vapor can enter the drifts. When the outer surface of the drift liner is below the temperature of vaporization, liquid can accumulate against the liner and enter through a structural weakness, most likely a fracture in the liner. Liquid flowing into the drifts either vaporizes or drops on waste containers to evaporate or flow over them. Once the liner temperature permits liquid contact, transport away from the drift is also possible. In addition, if flow



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Figure 6. Contaminants moving in a carrier plume.

from a condensate cap or from water entering from the surface is vigorous enough, liquid water can enter the drift even though the vaporization isotherm is still some distance away from the liner.

Summary. This detailed description of sources of and condition of entry of water and water vapor leads to a particular description of the drift environment. That is, for perhaps several thousand years, beginning with container failure—perhaps 1000 years after emplacement, the drift is hot and moist, with the ambient humidity controlled by the rate of influx and by source temperature. For the longer term the primary controls of humidity will be rock and concrete, which are expected to interact with the water present to control equilibrium humidity as temperature changes. As the temperature declines past the critical temperatures for mineral phase changes, rock volume and structural integrity of the rock will decrease, and not all the changes are reversible. The temperature decline will reduce the compressive stress around the repository and the rock will gradually relax into the openings. Failure of the liner and rock fall will occur locally at various places along the drifts (Figure 7).

#### **Expansion of Trees**

In developing the base cases, we expanded several segments of the nominal-flow event tree (Barr et al., 1995) (Figures 8 through 22). We do not discuss these expansions here; rather we discuss appropriate segments of them as we use them in the reference scenarios. The connections between the expanded segments and the nominal-flow event tree are discussed in the Appendix.

#### **Base Cases**

All of the coupled processes of interest in describing the response of the mountain to heat are rate-dependent, so the time at which one assesses a scenario is important. The relative importance of reference scenarios can change with time. We suggest the following three times for consideration in reference calculations:

- 1. T<sub>1</sub>, after closure, while the basal vitrophyre and saturated zone are not yet affected (probably ~300 years after closure).
- 2.  $T_1 < time < 2T_2$ , where  $T_2$  is the time at which the vaporization isotherm reaches its maximum extent (-1000 years after closure).
- 3.  $2T_2 < \text{time} < 10,000$  years, the "cold" phase of the repository.

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The values of  $T_1$  and  $T_2$  must be determined from experiment and calculation. Each scenario selected for these three periods is individually discussed below. For all of them the particulars of the surface source of water are left to the analyst and are presumed to be based on the moisture distributions of Flint and Flint (1994) (Figure 23) and the volumetric flow rates inferred from isotopic geochemistry.

We define a hot repository to exist when the vaporization isotherm is outside the waste containers, and a cold repository to be one for which the isotherm is inside the container. Scenarios 1 through 8 examine the hot repository; Scenarios 9 through 12 examine the cold



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Figure 7. Local failure of the liner and rock.



Figure 8. Interaction of water with the condensation cap at a hot repository, saturated flow.

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Figure 9. Water enters drift to interact with containers as vapor or as liquid flow.

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Figure 10. Container failure and waste mobilization in a hot repository (cf. Figure 22).









Figure 13. Saturated-zone flow.

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### Figure 15. Transport through liner.



Figure 16. Interaction of water with the condensation cap at a hot repository, unsaturated flow.



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Figure 17. Water enters drift to interact with containers as vapor or as unsaturated flow.

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Figure 19. Development of heat-pipes.



Figure 20. Liquid water enters drift-saturated flow.



Figure 21. Arrival of water at a cold repository.

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Figure 22. Container failure and waste mobilization for a cold repository.

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Figure 23. Estimate of flux, in mm/yr, for the surface grid blocks for the three-dimensional USGS/LBL site model (from Flint and Flint, 1994).

repository. The cold repository scenarios are appropriate for the time period  $2T_2$  to 10,000 years.

Although it is mentioned in some of the trees, criticality is not treated here, for two reasons. First, the kinetics of forming a critical assembly outside the container or in the carcass of the decayed container is the heart of the criticality problem and involves detailed chemical analyses as well as neutronics. Such analyses have not been included in the trees. Second, preliminary calculations by L. Sanchez (SNL, 6341) suggest that the consequences of such a criticality event are irrelevant to safety. Insufficient fission products and heat seem to be generated to affect repository performance, although detailed calculations involving chemical and nuclear dynamics remain to be done.

Assumptions. Because no final design decisions have been made, we have made certain assumptions about design, namely that there will be horizontal, in-drift emplacement of an MPC without backfill, in a lined drift, with an invert of concrete segments to support a rail transporter.

Features of the flow system as altered by repository heat must include the following:

- a. a condensate zone whose geometry will be selected on the basis of existing conduction calculations.
- b. heat-pipes, including chemical alterations to the flow paths,
- c. episodic recharge events, which feed rewetting and may collapse any condensate zone or shut off a heat pipe,
- d. flow to a cold repository in which the permeability has been chemically altered.
- e. chemical alteration of the Topopah Spring basal vitrophyre.
- f. chemical alteration of the saturated-zone aquifer (water-table aquifer).

Hot repository, Scenario 1:  $T_1$  to  $2T_2$  Years After Closure. The scenario for a hot repository during the period  $T_1$  to  $2T_2$  years after closure appears in schematic form in Figure 24. The discussion of the scenario follows the tree, with discontinuous branches for paths not taken, so the reader can see the alternatives.

 $T_1$  is a time when heat and circulating moisture have not yet altered the basal vitrophyre and the tuff aquifer.  $T_2$  is the time when the vaporization isotherm reaches its maximum extent, probably around 1000 years, and the Topopah Spring basal vitrophyre and the saturated-zone are modified. Heating of the rock has caused the initial expansion of the rock mass and has begun to modify fracture openings in the mountain. (See NUREG/CR-5390, by Mack et al., 1989, for estimates of the closure of fractures [roughly a factor of 2] and consideration of the effect of the thermal stress on fractures subject to shear.) Modeling of flow in fractures, particularly hot fractures, requires considerable experimental support to define and characterize controlling mechanisms.

It is presumed that water in the rock adjacent to the drifts is moved by heating as twophase flow to a cooler region, where condensation occurs ("2-phase Flow with Condensation Cap"). Numerous numerical models suggest the formation of such a condensate zone (Buscheck and Nitao, 1992, 1993; Nitao, 1988; Pruess and Tsang, 1993, 1994; Tsang and



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Figure 24. Hot Repository, Scenario 1.

Pruess, 1989, 1990). Such a zone could extend around the drifts, below and to the side as well as above. The tree shows several alternative choices for the size and shape of the condensate zone (see Figure 5). The alternative with localized condensation over adjacent panels was selected on the basis of conduction calculations of the vaporization isotherm for a model of the repository that includes the details of individual waste containers (Ryder, 1992). The formation of the condensate required substantial movement of water in the rock, which has presumably altered the permeability of both pores and fractures. Any modeling of two-phase flow will require evaluation of these changes (see, e.g., Steefel and Lasaga, 1992, for a discussion of this problem). Because of the temperature of the rock and of the waste container, the scenario requires a saturated return of water from the condensate zone, down the connected fractures extending from the condensate, to the drift liner. This scenario is moot if the volume of water available from the condensate zone is inadequate to chill the fractures sufficiently to allow vapor to reach the drift. The water in the condensate can be augmented by an episodic flow from the surface, however, which may allow such chilling and add to the flow to the drift as an auto-catalytic effect (Grant, 1981).

The scenario assumes that return flow will be condensate that forms over one hot panel and is shed to an adjacent, cooler panel. Certain repository loading schemes, as for example, area mass loading (AML), will allow substantial temperature differences between panels. Modeling of this scenario thus requires a defined loading scheme in order to consider the temperature differences that control shedding. The tree shows that panel edge effects should be considered; this is to maximize the structure of the condensate zone. When water vapor enters the drift, if in fact the drift has been water-vapor free (another condition to be derived from the modeling), its introduction is likely to result in rapid failure of any metallic container.

We distinguish container failure (development of two or more pinholes in the container) from container breach or collapse in order to recognize that a container can have an effective lifetime for retention of water and contaminants after it has been compromised (Oversby, 1987). The distinction becomes important for criticality and for the chemical reactions of container and waste that control speciation. Container breach or collapse is necessary for substantial mobilization of contaminants.

The first hot-repository scenario continues with the idea that sufficient water must enter the drift and reach the container and debris to interact with the contaminants. Fracture flow to the back of the drift would allow water to drip onto the breached container. Either the waste must be cool enough to allow liquid water to persist, or the inflow must be sufficient to cool the debris to allow interactions between the liquid and the waste.

At this point this scenario assumes that the primary interaction with the waste will produce dissolution of various contaminant species. Pigford and others (1992) reviewed some of the problems of modeling dissolution and precipitation in both porous and fractured rock. Flow of water occurs through fractures into the drift and out again, forming a flow system that exists before contaminants dissolve. That flow acquires the signature of the repository with respect to temperature, pH, dissolved carbonate, dissolved iron from containers and mine sets, etc (Figure 25). This signature is an important factor in determining speciation



Figure 25. Typical movement of the carrier plume in fractures.

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and rates of dissolution of contaminants (Savage et al., 1992; Nitsche et al., 1992) and must be a component of the near-container transport model. Changes in the chemical character of this carrier plume by buffering by the rock are expected to alter the mobility of the various contaminants; that is, sorption is in part controlled by the persistence and extent of the carrier plume.

The alternative that was ignored, colloidal formation, will be brought up explicitly in other scenarios. In reality, contaminants are distributed between colloids and solutes, depending on waste form, temperature, and so on, and the real description of mobilization requires that the distribution be known. For spent fuel, Forsyth and Werme (1992) suggested that contaminants dissolve without producing colloids; however, their analysis is appropriate for 25 C, without a container. The actual range of temperature is 95 to 30 C, with a massive iron container.

The next element in the tree is transport of the contaminants through the invert (the filling forming the bottom of the drift), which supports the rail system. Some designs indicate that the invert will be constructed of precast concrete segments. Whether the invert is concrete or tuff ballast, it may affect the residence time of contaminants in the drift and influence the signature of the carrier plume. It is part of any modeling. A concrete liner is part of some designs (Figure 2). Fracture flow is assumed to occur through the liner in order to accommodate rapid exit of the flow volume required earlier for dissolution.

For the time period considered for this scenario, it is expected that at least part of the Topopah Spring basal vitrophyre will be altered (according to Wm. Glassley, LLNL, on the basis of unpublished experiments). The alteration changes the vitrophyre to clays and zeolites and produces an increase of volume of about 10%. Figures 26 and 27 map the top and thickness of the Topopah Spring basal vitrophyre. Figures 28 through 30 show the location of differential conduction isotherms below the repository for several times. These figures are intended to give the reader some idea of how much of the basal vitrophyre might be altered and at what time. Figure 31 shows possible alterations at the repository.

The scenario continues with transport through the Calico Hills units. These units will be thermally altered by the repository, and locally they may experience thermal stress similar to the Topopah Spring units but of reduced extent. There is an excellent compilation of current Calico Hills hydrologic data (Loeven, 1993), but no corrections are yet published for alterations that the repository will induce.

The scenario next considers the condition of the tuff water-table aquifer that the contaminants and the carrier plume will see. Repository heat is expected to induce convective flow in the aquifer below the water table. Buscheck and Nitao (1993) has calculated such convection for an idealized porous medium representation. Discussions of this problem and these calculations in Hydrology Integration Task Force (HITF) meetings have suggested that convective circulation to a depth of a few hundred meters might be possible (Figure 32). The temperature differential between the aquifer at the water table and the aquifer at depth is expected to cause differential solubility of silica and calcite, which could be precipitated in the cooler regions below and parallel to the edge of the repository projection into the tuff



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Figure 26. Structure contour map of the top of the lower vitrophyre of the Topopah Spring Tuff (from the Lynx data base; courtesy of William Zelinski, Sandia National Laboratories). Units are feet.



Figure 27. Isopach map showing thickness in feet of the lower vitrophyre of the Topopah Spring Tuff (from the Lynx data base; courtesy of William Zelinski, Sandia National Laboratories).



Figure 28. Differential isotherms (in degrees C) 50 m below the repository 120 years after closure (courtesy of Eric Ryder, Sandia National Laboratories.) (Add 30 C to obtain the temperature.)



Figure 29. Differential isotherms (in degrees C) 70 m below the repository 300 years after closure (courtesy of Eric Ryder, Sandia National Laboratories.) (Add 30 C to obtain the temperature.)



Figure 30. Differential isotherms (in degrees C) 110 m below the repository 800 years after closure (courtesy of Eric Ryder, Sandia National Laboratories.) (Add 30 C to obtain the temperature.)



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Figure 32. Schematic diagram showing the three-dimensional relationships among the potential repository, the stratigraphic units, and the major faults. Also shown is the postulated convective circulation induced in the saturated zone by a hot repository. aquifer (as suggested by Wm. Glassley, LLNL, and G. Barr, SNL). The rate (mass/unit time) of such dissolution and precipitation is unknown. For vigorous-enough circulation rewould be possible for primary and possibly secondary porosity to be altered. This scenario presumes that the rate of such alteration is too slow to have affected permeability in the tuff aquifer in the 2000-or-so years in which repository heat could drive convection.

Hot Repository, Scenario 2: time  $< T_I$ . The second scenario for a hot repository (Figure 33) differs from the previous scenario in that it occurs earlier in the failure history of a container. In particular, this scenario is presumed to occur at time T1, which is too early for there to be significant changes in the basal vitrophyre and the tuff aquifer (probably T1 < 300 years).

The scenario is identical to the previous one up to "Steam Corrosion of the Container to Failure." At this point the alternative path, allowing liquid to enter the failed container, is selected. Liquid water enters the container and contacts the waste. Boiling (i.e., possibly two-phase) reactions occur between waste and water with contaminant dissolution. Given the circumstances of the reactions it is possible that speciation differs from that in Scenario 1. The reactions continue, breach (or massive failure) of the container ensues, and contaminants are mobilized in the carrier plume. Given a residence time for the contents of the container to cook, it is likely that the carrier plume would have a somewhat different signature than the plume associated with the first scenario. Rapid exit is necessary to preclude drying and precipitation and allow the contaminants to escape, so the tree shows fracture flow through the invert and drift liner. The basal vitrophyre and saturated-zones are chemically unaltered—by assumption; however, there can be thermal stress effects on fractures in the basal vitrophyre and Calico Hills units. Transport is then through the otherwise unaltered saturated zone.

Hot Repository, Scenario 3:  $T_1 < time < 2T_2$ . The third scenario for a hot repository (Figure 34) differs from Scenario 1 only by thermo-chemical alteration of the saturated zone. The difference, that primary porosity will be plugged and that any transport will occur in small and large fractures, is not a durable feature that is suddenly introduced. Rather, the chemical and hydrological interactions are continuous and modifications to the flow system need to be derived as a function of the elapsed time since waste emplacement. Modeling therefore must be supported by a description of fracture flow and of the undisturbed flow system, determined experimentally, so that the evolution of the tuff aquifer can be reasonably described.

Hot Repository, Scenario 4:  $T_1 < time < 2T_2$ . The fourth scenario for a hot repository (Figure 35) is an extension of Scenario 2 for longer times; both the basal vitrophyre and the saturated zone are being altered as transport occurs from the drift. The fact that water enters the waste container and more vigorous reactions can occur should provide an alternative speciation in the carrier plume for interaction in the basal vitrophyre and the saturated zone.

The next four scenarios involve establishment of a heat-pipe around the waste container and in the rock surrounding the drifts. (See Winter and Barsch, 1971, for an exhaustive discussion of engineered heat-pipes.)



Figure 33. Hot repository, Scenario 2.



Figure 34. Hot Repository, Scenario 3.



Figure 35. Hot Repository, Scenario 4.

Hot Repository, Scenario 5. The fifth scenario for a hot repository (Figure 36) addresses the consequences of occurrence of the refluxing condition known as a heat pipe (Figure 37). Such a refluxing condition is presumed to occur at individual containers. This may be the case for containers with older waste in a heterogeneous waste stream. The tree shows two choices— an evolving heat pipe and a continuing heat pipe. The distinction is that an evolving heat pipe is defined to be one in which alteration of the rock adjacent to the drift produces local dryout and shuts off circulation, while a continuing heat pipe is defined to be one for which circulation continues until the heat source is too weak to provide thermal gradients required to drive the circulation. The evolving branch is chosen for this scenario. It is presumed that the heat pipe will function long enough that water vapor (steam) will circulate past the container at a rate sufficient to cause container failure before plugging of pores and fractures blocks escape from and return to the drift.

Once refluxing is shut off, some local drying can continue. Dryout does not preclude the presence of water in the rock, it merely means that the water is in local equilibrium with the rock. Moisture available in the drift to contribute to container corrosion is controlled by equilibrium of moisture in the air with water in the rock and drift liner and by the rate of corrosion. It is assumed that moisture from the heat pipe has readjusted throughout the mountain by increasing the saturation of rock units. Conceivably the evolving heat pipe is simply an initial stage of the condensate cap, but that possibility is ignored here. Any influx of water is presumed to be an episodic fracture flow from the surface. At this early time, with the expected temperatures, rapid or voluminous flow is required to reach the drifts.

The tree continues with water arriving at the drift first entering as vapor, which completes the destruction of the container. When sufficient water has arrived to cool the debris there is localized flooding (essentially puddles on the floor) and boiling interactions between waste and liquid water. It is assumed that these vigorous reactions result in dissolution of contaminants rather than formation of colloids. The scenario continues with fracture flow for the carrier plume and the contaminants. A rapid exit is necessary to prevent the water from evaporating in the hot rock below the repository. We suspect that the evolving heat pipe will shut off before the Topopah Spring basal vitrophyre and the saturated zone are altered. The alterations may be just beginning, and modeling of transport through the basal vitrophyre will have to consider the rate and the affects of such alteration.

Hot Repository, Scenario 6. The sixth scenario for a hot repository is similar to Scenario 5, except that a heat pipe extends around and is driven by several containers in a drift (Figure 38). It requires specification of the thermal outputs of adjacent waste containers and thus reflects how the details of the thermal loading strategy and the waste stream affect the interaction between containers in a drift. One could, for example, anticipate that there would be considerable variation of the extent of plugging along a drift, mirroring the variation in thermal output of the containers. That variation would then be expected to influence where water first reaches a drift and how it is distributed along the drift.

Hot Repository, Scenario 7. Scenario 7 for the hot repository describes a continuing heat pipe at a single container (Figure 39). Such a heat pipe is presumed to be active, that is, to drive fluid movement, until the thermal gradient it supplies is inadequate to support the



Figure 36. Hot Repository, Scenario 5.



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Figure 37. Heat-pipe circulation in the rock adjacent to a drift with hot waste containers.



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Figure 38. Hot Repository, Scenario 6.



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Figure 39. Hot Repository, Scenario 7.

refluxing flow. The tree calls this circumstance "Extinction of Heat Pipe." The precipitation in pores and fractures must be inadequate to shut cff flow, either because the rate of plugging is too slow or because the plugging is incomplete. The tree continues with two entries, "Liquid Enters Existing Failures" and "Container Breach/Collapse," that are probably redundant. The continuing heat pipe will have exposed containers to a steam bath until the heat pipe became extinct. Those containers have probably already collapsed. The events are always uncertain in the absence of data, however, and need some corroboration, particularly because the time of extinction of the heat pipe is unknown. The time at which this scenario could occur has not been determined.

The scenario continues with liquid water reactions with the waste and introduces the possibility of formation of contaminant colloids. Apparently the possibility of colloid formation becomes more likely as the temperature of the waste decreases. For high-level-waste glass, experiments at 25 C have shown that essentially 100% of plutonium and americium appear on colloids (Bates et al., 1992). For spent fuel, experiments that looked for colloids and found none (Forsyth and Werme, 1992) were performed outside the temperature range of interest to Yucca Mountain-at 25 C rather than 95 to 30 C-and without the container. The massive iron container is expected to form iron hydroxide colloids to which contaminants could attach. Colloids are generally in the size range of 0.001 to 1 micron (van der Lee, 1992; Ramsay, 1988), compared with expected pore sizes that are in two populations (Peters et al., 1984) of 5 and 200 microns. Typical fracture apertures are 10<sup>-4</sup> m and larger (Wilson et al., 1994). The scenario assumes that there will be rapid transport of colloids down fractures through and around the invert and through the liner. The tree then shows transport in the saturated carrier plume to the basal vitrophyre. It is not clear whether colloids will be filtered by the pores and be solely able to move down fractures, because the continuing heat pipe functioned to extinction, implying that enough permeability persisted to allow the heat pipe to work. The limits of that functioning, that is, how much plugging still allows the heat pipe to work, needs to be derived from modeling the early parts of this scenario. Transport through the altered basal vitrophyre is in fractures. Therefore, how the basal vitrophyre changes, mechanically and chemically, becomes an important part of any sorption calculations in the transport. Transport in the saturated zone is taken to be through a tuff aquifer whose primary porosity is being plugged while the transport is occurring.

Hot Repository, Scenario 8. Scenario 8 for the hot repository (Figure 40) is similar to Scenario 7, except that the multiple containers contribute to the continuing heat pipe, and the bottom of the tree shows alternative changes to the basal vitrophyre. The large-scale coupling of the thermal interactions of a drift-load of containers suggests the possibility of more profound alteration to the basal vitrophyre. If the basal vitrophyre is massively changed so its top is a continuous layer of clay and zeolites, it could be a barrier to continued vertical flow and would allow perching of the carrier plume and its load of colloidal contaminants. The topographical structure of the top of the basal vitrophyre (Figure 25) could redirect the transport of contaminants to enter the Calico Hills units and arrive at the water table elsewhere than expected, perhaps outside the projected footprint of the repository on the water table. This possibility is mentioned because the tree continues with transport in a tuff aquifer that is partially altered; therefore the extent and the current dynamics of the alteration become necessary components of the modeling analysis.



Figure 40. Hot Repository, Scenario 8.

Cold Repository, Scenario 9: time >  $2T_2$ . The first scenario for a cold repository, icenario 9 (Figure 41), starts with the arrival of an unsaturated flow plume from the surface to interact with the repository. The unsaturated flow reaches the drifts through the altered region around them. As the temperature of the rock declines, thermal compression diminishes, and the stressed region around the drifts relaxes into the openings. This relaxation, along with any structural weaknesses produced by mineralogical phase changes during heating, will result in localized collapse of the liner and surrounding rock into the drifts.

The tree shows two alternatives for the water reaching the containers, "Unsaturated Flow to Containers" and "Philip's Drip on Containers." Figure 7, which shows collapse of the liner and rock in contact with a container, illustrates the difficulty of unsaturated flow of any importance reaching the container. For that reason, "Philip's Drip" was selected as a more significant path. "Philip's Drip" (Philip et al., 1989; Shimojima et al., 1993) provides a mechanism for focusing unsaturated flow to an underground opening and producing local saturation, e.g., drip onto a waste container. Philip and others (1989) observed that an opening in unsaturated rock alters the hydraulic potential, affecting local saturation around the opening and redirecting the flow. Some of that flow is directed to the opening, as illustrated in dimensionless form in Figure 42. The tree continues with the drip on the container eventually producing container breach or collapse. Liquid water reactions are assumed to occur with the waste, dissolving contaminants for transport. Because water enters the drift at a low rate, the scenario continues with unsaturated flow and transport through and around the invert and through the liner. Contaminants are carried to the basal vitrophyre in an unsaturated carrier plume. By this time the basal vitrophyre has been altered extensively, so the unsaturated carrier plume is assumed to move through this altered basal vitrophyre. Since unsaturated flow is presumed, experimentally derived characteristic curves as well as sorption data are required for the basal vitrophyre in order to model flow and transport. The scenario concludes with unsaturated transport through the Calico Hills units and arrival of the contaminants at the water table. When time  $> 2T_2$ , we expect that the thermal gradients in the saturated zone are becoming too weak to drive the convective flow that plugged the aquifer.

Cold Repository, Scenario 10: time >  $2T_2$ . The second scenario for a cold repository, Scenario 10 (Figure 43), is a variation of Scenario 9. The difference is that unsaturated flow is presumed to occur through and around the invert and that there are no significant changes to either the saturated zone or the basal vitrophyre. This scenario forms a reference for comparison of changes to the residence time of contaminants because of thermo-chemical alterations to the basal vitrophyre and the saturated zone.

Cold Repository, Scenario 11: time >  $2T_2$ . The third scenario for a cold repository, Scenario 11 (Figure 44), begins with the arrival of water in fractures at the stress-altered region around the drift. "Fracture Flow to the Stress-Altered Region" could just as well be replaced by "Locally Saturated Flow." Recent work (Moreno and Tsang, 1994; Chesnut, 1994a, 1994b) has raised the possibility of rapid and possibly voluminous flow paths existing through the unsaturated zone because of the extent of heterogeneity of the rock. How water available from the surface is partitioned between fractures and locally saturated flow paths is an important question for modeling. In any case locally saturated flow reaches the containers



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Figure 41. Cold Repository, Scenario 9.



 $x_{1} \in \mathbb{R}^{n}$ 

Figure 42. Seepage around cylindrical cavities (from Philip et al., 1989). The diagram illustrates critical points and regions of the flow field, including the upstream and downstream stagnation points, retarded region, the boundary layer, the roof-drip lobes, and the dry shadow.  $\vartheta > 1$  everywhere outside the dry shadow, i.e., the presence of the cavity increases the moisture content.



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Figure 43. Cold Repository, Scenario 10.

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Figure 44. Cold Repository, Scenario 11.

in sufficient volume to cause local flooding or ponding of water. Corrosion due to this water completes the collapse of the waste container and exposes the waste. The tree presumes contaminant dissolution; however, as mentioned earlier, how the contaminants are distributed between solute and colloids depends on temperature, waste form, container materials, etc., and needs to be determined experimentally before analyses can proceed with any confidence.

The scenario continues with the assumption that the basal vitrophyre has been so altered that its top forms an intact and continuous layer of clay and zeolites that form a barrier to continued vertical flow. The carrier plume and contaminants perch on this layer. The topographic structure of the top of the basal vitrophyre diverts the flow elsewhere to reach the altered tuff aquifer. In this scenario both primary and secondary porosities are presumed plugged; transport therefore occurs in fractures too large to be plugged. Such an assumption puts a premium on determination of the sorption properties of fractures in the tuff aquifer.

Cold Repository, Scenario 12: time >  $2T_2$ . The final scenario for a cold repository, Scenario 12 (Figure 45), starts with the arrival of an unsaturated flow plume from the surface to interact with the repository. The unsaturated flow reaches the drifts through the altered region around them.

As the temperature of the rock declines, thermal compression diminishes and the stressed region around the drifts relaxes into the openings. This relaxation, along with any structural weaknesses produced by mineralogical phase changes during heating, causes localized collapse of the liner and surrounding rock into the drifts (Figure 46). The tree shows two alternatives for the water reaching the containers, "Unsaturated Flow to Containers" and "Philip's Drip onto Containers." Figure 7, which shows collapse of liner and rock in contact with a container, illustrates the difficulty of unsaturated flow of any importance reaching the container. For that reason, this alternative depends on substantial collapse of rock and liner into the drifts to provide good contact with waste containers or with the residual debris from collapsed containers.

Unsaturated flow to the container eventually produces container breach or collapse if it has not already occurred. Liquid water reactions are assumed to occur with the waste, producing colloids for transport. Because water entered the drift at a low rate, the scenario continues with unsaturated flow and transport through and around the invert and through the liner. The colloids are then transported down fractures. Contaminants are released from the colloids in the fractures—in effect a distributed source is formed in the rock.

Transport continues to the basal vitrophyre in an unsaturated carrier plume. By this time the basal vitrophyre has been altered extensively, and the unsaturated carrier plume is assumed to move through this altered basal vitrophyre. Experimentally derived characteristic curves and sorption data are required for the basal vitrophyre in order to model unsaturated flow and transport. The scenario continues with unsaturated transport through the Calico Hills units and arrival of the contaminants at the water table. We suspect there is sufficient rock fall to start this scenario only late in the lifetime of the repository, at which time there should have been enough flow in the saturated zone to start redissolving the precipitates that plugged primary and secondary porosity. Therefore, modeling of the final event, "Transport



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Figure 45. Cold Repository, Scenario 12.



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Figure 46. Collapse of the liner and rock into the drift, with attendant unsaturated flow reaching the waste container through this material.

in Large Fractures," should consider the possibility that the permeability of the tuff aquifer is reverting to its original state.

## Summary

The nominal-flow report (Barr et al., 1995) identified approximately 130 scenarios for consideration in performance-assessment modeling for the Yucca Mountain Site Characterization Project. The level of detail in these scenarios anticipated the results of research that is likely to require the next decade for completion. From the large number of scenarios that resulted, we have extracted 12 reference scenarios that we think are most likely to include the physical phenomena necessary to understand the evolution of the repository. The repository is not guaranteed to evolve in accordance with the scenarios in this memo; however, resolution of the descriptions and behavior of the key phenomena included in the reference scenarios (e.g., container failure, heat-pipe behavior, alteration of the basal vitrophyre, and so on) will be applicable to many scenarios. Providing a basis for experimentation and modeling to support such resolution is the point of reference scenarios.

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## Appendix

1

This appendix connects expansions of trees that appear in Figures 8 through 22 with the trees of the nominal-flow report (Barr et al., 1995). Two figures from the nominal-flow report, Tree Segments 1a and 1b, provide the connection. Tree Segment 1b shows an overview of where each part of the tree being discussed fits into the flow system.

In the text we defer any discussion of the entry of new water into Yucca Mountain to the distribution function derived by Flint and Flint (1994) and begin with the interaction of water with the repository. As a result, Tree Segment 1b serves as a stand-in for all the scenarios in the nominal-flow report: there each tree segment begins with one or another pathway for the entry of water. The discussion here mentions each expanded subtree (from Figures 8 through 22) and refers to the place in Tree Segment 1a where that expansion fits.

Figure 8, "Interaction of water with the condensation cap at a hot repository, saturated flow," expands the element "2-Phase Convection with Condensation Cap." This expansion first recognizes that the structure of a condensation cap may be determined by how the containers are loaded and by their thermal output. It presumes a saturated return based on the structure of the condensation cap.

Figure 9, "Water enters drift to interact with containers as vapor or as liquid flow," develops the element "Saturated Return" on Path 1.1 below "2-Phase Convection with Condensation Cap."

Figure 10, "Container failure and waste mobilization in a hot repository," expands "Degradation of EBS" in Path 1.1, allowing for variation of chemical response (e.g., speciation) as a function of temperature and mentions criticality for reference only.

Figure 11, "Mobilization and exit from a drift," expands "Saturated Mobilization of Contaminants in Path 1.1 and continues in the following figure, Figure 12.

Figure 12, "Transport of colloids in a carrier plume," is a continuation of the previous figure. It introduces both the complexity of colloid transport and the idea of the carrier plume into mobilization of contaminants.

The nominal-flow report made no attempt to explicitly account for transport in the saturated zone; scenarios ended with arrival of contaminants at the water table. Figure 13, "Saturated-zone flow," attempts to continue scenarios to include repository-induced changes in the water table (tuff) aquifer.

Figure 14, "Influence of the liner," develops "Saturated Mobilization of Contaminants" from Path 1.1, for the case that a liner is emplaced in the drifts. It is not certain that a liner will be used; however, it must be included as part of mobilization of contaminants because it affects chemistry of the carrier plume and interaction with the basal vitrophyre.



A .....

Tree Segment 1a (from Barr et al., 1995).



Tree Segment 1b (from Barr et al., 1995).

Figure 15, "Transport through the liner," is a piece of Figure 14. It was given a separate identity because it was used in discussing unsaturated flow in reference scenarios.

Figure 16, "Interaction of water with the condensation cap at a hot repository, unsaturated return," is Figure 8 altered to allow "Unsaturated Return" flow from the condensation cap, as in Path 1.2, Tree Segment 1a.

Figure 17, "Water enters drift to interact with containers as vapor or as unsaturated flow," develops the elements "Unsaturated Return" and "Degradation of EBS" of Path 1.2.

Figure 18, "Mobilization and unsaturated flow exit from drift," expands "Unsaturated Mobilization of Contaminants," Path 1.2.

In Tree Segment 1a, one option for the behavior of a hot repository is formation of heat pipes. Figure 19, "Development of heat-pipes," expands the development of heat-pipes by considering whether they form singly or multiply and whether they evolve (and seal themselves) or continue until they no longer generate sufficient heat to drive two-phase circulation. This development is summarized as "2-Phase Convection with Heat-pipe" in Path 1.4.

Figure 20, "Liquid water enters drift - saturated flow," expands the elements "Saturated Return" and "Degradation of EBS" in Path 1.4.

Figure 21, "Arrival of water at a cold repository," expands the "Cold Repository" branches, Paths 1.5 and 1.6. It introduces specific mechanisms by which flow can reach containers in a primarily unsaturated system. In particular a mechanism for producing locally saturated flow from unsaturated flow at a mined opening (Philip et al., 1989) is discussed.

Figure 22, "Container failure and waste mobilization for a cold repository," addresses "Degradation of the EBS" for the cold repository, Paths 1.5 and 1.6.