APPENDIX VI
CURRENT INFORMATION REGARDING GROUND WATER FLOW AND RADIONUCLIDE TRANSPORT IN THE UNSATURATED AND SATURATED ZONES

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VI.1 UNSATURATED ZONE

VI.1.1 Unsaturated Zone Hydrology Model

The unsaturated-zone (UZ) flow analysis of Yucca Mountain comprises four components (climate, infiltration, mountain-scale UZ flow, and seepage into drifts) that are believed to play an important role in the performance of the potential repository. Climate and infiltration influence the amount of water percolating toward the repository. Subsequently, water seeping into the drifts and onto the waste packages can accelerate waste-package degradation, and rapid pathways from the repository to the water table via fractures can decrease the transit time of radionuclides to the accessible environment. Prediction of these events relies on process models of UZ flow that have been tested or calibrated against available data at Yucca Mountain. This section describes the development of these models and the important processes and relevant parameters used in the TSPA-VA.

The TSPA-VA is the most recent TSPA analysis conducted by DOE that has undergone thorough external review by outside parties (NRC, TRB, etc.). The more recent TSPA for Site Recommendation (TSPA-SR) has been release very recently. Changes in the treatment of flow phenomena in the TSPA-SR are changed minimally from those in the TSPA-VA, so the current discussion will focus on the more heavily reviewed of the two.

VI.1.1.1 Synopsis of TSPA-VA Treatment and Changes from Prior Efforts

A primary difference in the treatment of UZ flow between TSPA-VA and previous TSPAs is the use of a fully three-dimensional UZ flow model developed at LBNL by Bodvarsson et al. (BOD97). Their goal was to synthesize all of the available data into a coherent, predictive model of water and air flow in the UZ using the dual-permeability continuum formulation or fracture and matrix flow and interaction. The numerical formulation of the model is implemented with the TOUGH2 computer code (PRU91). Model calibration is performed using an inverse method implemented in ITOUGH2 (FIN93) to optimize the model parameters against available data. A new feature of the current LBNL model (BOD97) is that a fracture-matrix coupling parameter, related to the wetted contact area between fractures and matrix, can be used as an inversion parameter in each hydrogeologic unit. The use of the three-dimensional UZ flow model precludes the need for simplified or abstracted flow fields, as has been required in previous TSPAs. However, because of the size and computational requirements of the three-dimensional UZ flow model, the emphasis in TSPA-VA has been on using selected conceptual models and parameter sets that span the range of uncertainty in UZ flow modeling, rather than randomly sampling large combinations of parameters.

VI.1.1.2 Infiltration

The ultimate source of water in the unsaturated zone at Yucca Mountain is precipitation on the mountain. The spatial and temporal relationships between infiltration and recharge are complex, because of the hydrogeologic variability of Yucca Mountain. Some water that infiltrates returns to the surface by interflow; another part is returned to the atmosphere by evapotranspiration. A small quantity that is not evaporated, or discharged as interflow, percolates deep into the unsaturated zone and becomes net infiltration or percolation. The terms “infiltration” and “percolation” are used frequently, sometimes interchangeably, in literature about the Yucca Mountain unsaturated zone. For the purposes of this report, “infiltration” is used to describe the amount of water which enters Yucca Mountain at the ground surface, while “percolation” is used to describe the amount of water which actually penetrates deep enough into the mountain to reach the repository horizon and below. The difference between the two terms lies mainly in the partitioning of part of the infiltration flux into the vapor phase, which may then be recirculated to the atmosphere.

At Yucca Mountain, the infiltration rate is both spatially and temporally variable. Because the quantity of net infiltration that percolates through different paths is quite variable, estimated average recharge rates do not represent percolation rates through specific flow paths. Spatial variations of infiltration depend mostly on variations in the properties of surficial units, topography, the intersection of faults with the surface, and the presence of local fracturing. Temporal variations in infiltration rate are related to the seasonality and relatively infrequent precipitation events in the arid climate of Yucca Mountain. Temporal variations in the infiltration rate have also occurred over a much larger time span, reflecting long-term climate changes.

Knowing the temporal and spatial variability of the percolation rates is crucial to modeling efforts because of the importance of the relationship of infiltration rate to horizontal and vertical permeabilities of the various units and the effect this has on whether or not significant lateral flow occurs in the unsaturated zone. The higher the actual infiltration rate, the lesser the likelihood of significant lateral flow. Such lateral flow could result from a combination of two factors. The first factor is that infiltrating water may encounter zones of lower relative permeability as it moves downward. The second factor is that in many of the units, the relative permeability is far greater in the direction parallel to bedding than the direction perpendicular to it. The anisotropic permeability may cause lateral flow of mounded water away from the area in which it accumulates. Lateral flow is important because it could transmit water to structural features which would then move the water downward, possibly acting as a conduit to divert large amounts of water flowing downward through a small area. Such flow paths could direct water into and through the repository or away from it.

The actual quantity of net infiltration or percolation beneath the surface of Yucca Mountain has not been accurately determined. The percolation flux is a difficult parameter to determine for low flux regions such as Yucca Mountain. There are currently no reliable direct measurements that can be made to determine this important parameter (LBL96). Existing estimates have been obtained from a mixture of indirect methods involving field testing and modeling of various processes at different scales. Data exist to suggest that the flux reaching the repository horizon through the matrix is relatively small. Relatively low matrix saturations measured in the upper portion of the TSw suggest that much of the moisture which infiltrates into the TCw does not reach the TSw (LBL96). Data from the ESF show that no weeping fractures were found, even in the region where perched water exists in boreholes. It should be noted, however, that because of ventilation equipment inside the ESF, much of any such moisture might be removed from the ESF as water vapor. Furthermore, no moisture was observed infiltrating into the radial boreholes of Alcove 1 of the ESF after storm events, even though the boreholes are located close to the land surface in the highly fractured and broken TCw formation (LBL96). However, other data suggest that the percolation flux may reach the repository level mainly through episodic fracture flow. These data include observation and testing of extensive bodies of perched water located below the repository horizon, as well as measurements of bomb-pulse isotope levels from atmospheric nuclear testing which show that some water in the unsaturated zone is relatively young (LBL96).

Estimates of net infiltration vary from slightly negative (net loss of moisture from the mountain) to about 10 mm/yr (LBL96). It is reported in USG84 that net infiltration flux probably ranges from 0.5 to 4.5 mm/year, based on estimates of earlier workers for various localities in the Yucca

Mountain area. Flint and Flint (FLI94) provide preliminary estimates of spatial infiltration rates that range from 0.02 mm/yr, where the welded Tiva Canyon unit outcrops, to 13.4 mm/yr in areas where the Paintbrush nonwelded unit outcrops. The bulk of the area above the repository block is underlain principally by the Tiva Canyon member. The DOE's 1995 Total System Performance Assessment concludes that, if the predominant flow direction is vertical, then the average infiltration through the repository block, using the average infiltration rates of Flint and Flint (FLI94), would be 0.02 mm/yr. If, on the other hand, the predominant flow direction has a significant lateral component due to material property heterogeneity and/or anisotropy and the sloping nature of the hydrostratigraphic unit contacts, then the average net infiltration rate over the repository block could be as high as some weighted average of the infiltration rates inferred from FLI94. The 1995 TSPA (DOE95) also reports that the average, spatially-integrated infiltration rate is about 1.2 mm/yr; most of this infiltration occurs along the Paintbrush outcrop in the washes north of the repository block.

Recently, several lines of evidence have converged to alter the prevailing view regarding the magnitude of infiltration/percolation rates beneath Yucca Mountain, with the most recent estimates being revised upward from previous work. The newer estimates of percolation are around five mm/yr, with a range of one to 10 mm/yr (LBL96). Recent isotopic analyses of rock samples from the ESF are consistent with a percolation rate of five mm/yr (LAN96, LBL96). Profiles of temperature versus depth of water in boreholes are consistent with a range of infiltration rates from one to 10 mm/yr (LBL96). Three-dimensional modeling results of the percolation flux at the repository horizon using the latest available spatially varying infiltration map indicate percolation fluxes on the order of five to 10 mm/yr. The UZ expert elicitation panel estimates for mean infiltration rates range from 3.9 to 12.7 mm/y (GEO97). The effect of uncertainty in infiltration and percolation flux rates is presented in the TSPA-VA.

The conceptual model used in infiltration studies defines the physical processes determining net infiltration, and is based on evidence provided from field studies at Yucca Mountain combined with established concepts in soil physics and hydrology (FRE79, HOR33, HIL80, FLI96). The overall framework of the conceptual model is provided by the hydrologic cycle, which includes all the processes on the surface and in the shallow subsurface (0 to 6 m beneath the ground surface) that affect net infiltration. These processes include precipitation, infiltration, run-off and run-on, evapotranspiration, and the redistribution of moisture in the shallow subsurface. Precipitation is the dominant hydrologic process at the site because it is the source of all moisture for the surface and shallow subsurface (there are no permanent streams or bodies of surface water affecting the site), excluding water introduced to the site by human activity (dust-control, drilling, waste water). Precipitation is dependent mostly on meteorological factors, but geographic location, elevation, and physiography are also important. Evapotranspiration is the second most dominant hydrologic process (in terms of the total volume of water involved) at Yucca Mountain and is dependent on vegetation, the distribution of available moisture stored in the shallow subsurface, and potential evapotranspiration, which is determined by an energy balance. Redistribution of moisture in the shallow subsurface occurs in response to gravity and matric potentials and is strongly dependent on soil and bedrock properties. The removal of water through evapotranspiration is dynamically integrated with the redistribution of moisture in the shallow subsurface. The generation of run-off is dependent on a combination of soil depth, soil porosity, soil permeability, bedrock permeability, and ground surface slope. Run-on and the routing of surface flow are dependent mostly on surficial material properties, topography, and channel geometry.

The conceptual model of net infiltration has been developed from analysis of an 11-year record of neutron logs from 99 boreholes on Yucca Mountain (FLI95). Relative changes in water content profiles were compared against precipitation records and estimates of evapotranspiration (HEV94). The measured changes in water content were also compared to physiographic setting, bedrock geology, and soil cover. In general, field studies indicated that saturated soils are established primarily during the winter in response to a series of medium to large storm events which tend to occur more frequently during periods associated with an active El Nino Southern Oscillation. The timing, intensity, and duration of precipitation, the storage capacity of the soil, and evapotranspiration determine the availability of water for net infiltration. In the upland areas of Yucca Mountain where the soil cover is shallow, the lower the effective conductivity of the underlying bedrock, the longer moisture from precipitation is held in the soil profile where it is potentially available for evapotranspiration. During winter, when potential evapotranspiration is at a minimum, smaller amounts of precipitation are needed for developing and maintaining saturated conditions at the soil-bedrock contact. When the storage capacity of the soil and the effective conductivity of the underlying bedrock are exceeded, or when precipitation intensity exceeds the infiltration capacity of the soil, runoff is generated and water is available for routing down slopes and into channels. The significance of net infiltration beneath channels in washes relative to sideslopes and ridgetops depends on the frequency and magnitude of runoff events.

In the current conceptual model, net infiltration at Yucca Mountain is characterized as an episodic, transient process depending primarily on the length of time saturated or near-saturated conditions are maintained at the soil-bedrock interface, or, at a depth of 6 m in deep alluvium, and the effective conductivity of the underlying bedrock or alluvium. Net infiltration is determined as the rate of water percolation into bedrock or below a depth of 6 m in alluvium, and is limited by the effective permeability of the bedrock or alluvium. Evapotranspiration is assumed to be negligible in bedrock or below a depth of 6 m because no evidence of plant roots have been found beyond a 5 m depth. The potential for saturating the soil-bedrock interface is determined by the timing, frequency and intensity of precipitation: the depth, field capacity, and porosity of the soil cover; potential evapotranspiration, actual evapotranspiration (which is a function of the available moisture in the soil profile), and the lateral re-distribution of surface water. Lateral redistribution of soil moisture is assumed to be negligible because tho moisture-retention potential in the soil to divert flow laterally is relatively small. A detailed description of the actual determination of net infiltration is given in FLI96.

VI.1.1.3 Unsaturated Zone Flow

The most important data for understanding unsaturated zone flow come from several surface-based drill holes and from the ESF, which is an 8-km-long tunnel through Yucca Mountain. Considerable amounts of data are available on rock-matrix saturations, water potentials, and temperatures; on chemical composition and isotopic abundances of ground water and mineral deposits; on air permeability and air-pressure fluctuations; on rock types and mineralogy; on fault locations and offsets; on fracture density and orientations; and on matrix permeability and saturation/desaturation parameters. In addition, there is information on the upper boundary condition (i.e..infiltration) from a series of weather stations and shallow drill holes instrumented with neutron probes, and there is information on climatic effects from a variety of paleoclimate studies and from analogues such as present-day Ranier Mesa.

The first detailed conceptual model of unsaturated zone flow at Yucca Mountain was proposed in USG84. Since then, the majority of the data collected has been in general agreement with these ideas and concepts (LBL96). Most subsequent conceptualizations of unsaturated zone behavior are largely refinements of this model, revised to accommodate newly-acquired data. Newly-acquired data include isotopic analyses, concentration ratios of ions dissolved in matrix rocks and perched water zones, calcite fracture fillings, and thermal modeling of vertical temperature gradients. Perhaps the most significant change from early conceptual models has been the recent acquisition of new isotopic data which indicate the presence of “fast paths” for water moving through the unsaturated zone. This topic is discussed in more detail in a subsequent section.

The following presentation of the unsaturated zone flow conceptual model is taken primarily from USG84. Where appropriate, the published literature is referenced when describing refinements or revisions that have been made to the USG84 model. The conceptual model is presented as if it were an established physical reality. One must bear in mind, however, that the proposed model is probably not the only reasonable description that could be made of the system. Following the description of the conceptual model is a discussion of critical unknowns, their effects on unsaturated zone flow, and results of numerical modeling studies.

Percolation of infiltrated water through the exposed fractures of the Tiva Canyon welded unit is relatively rapid because of the large fracture permeability and small effective porosity of this unit compared to the alluvial material. Therefore, a large proportion of the infiltrated water normally is percolated sufficiently deep within the fractured tuff to be unaffected by the evaporation potential that exists near the surface. Depending on the intensity of the infiltration, percolation downward through the Tiva Canyon welded unit may occur without a significant change in rate. A small proportion of the water percolating through the fractures slowly diffuses into the matrix of the Tiva Canyon welded unit. Downward flow in the matrix is very slow because of the small effective hydraulic conductivity of the matrix. During dry periods, some of the diffused water flows back into the fractures and probably reaches the land surface by vapor diffusion. The mass of water involved during this process is likely to be negligible compared to the mass of percolating water.

The densely fractured Tiva Canyon unit, with small matrix porosity and permeability, overlies the very porous, sparsely fractured Paintbrush unit. A marked contrast in material properties exists at the contact between these two units; depending on the magnitude of the infiltration flux, this contrast could impart a significant lateral component of flow. Flow of water through fractures of the Tiva Canyon unit occurs rapidly until it reaches the contact. At this point, the velocity is significantly decreased because of the greater effective porosity and lesser hydraulic conductivity of the Paintbrush unit. As a result, lateral, unsaturated flow of water above this contact can occur. Perched water may occur above this unit if displacement along faults has created significant differences in permeability on opposite sides of the fault.

Although the conceptual model of Montazer and Wilson (MON84) hypothesized that perched water may occur at the contact between the Tiva Canyon welded (TCw) unit and the Paintbrush nonwelded (PTn) unit, no such occurrences have been observed in either surface-based boreholes (ROU99, p. 170-174; BOD97, Chapter13) or in the Exploratory Studies Facility (ESF). Based on field observations in boreholes and in the ESF, the existence of perched water above the repository horizon is believed by DOE to be unlikely (DOE98). In addition, three-dimensional modeling of flow in the unsaturated zone beneath Yucca Mountain resulted in no formation of perched water at this contact or within any lithostratigraphic interval above the repository horizon (BOD97). Although contrasting matrix properties at the TCw/PTn contact result in high matrix saturations (FLI98, Table 7), the permeability of the PTn is sufficiently high to allow downward drainage of water without perching. Furthermore, three-dimensional simulation of ground water flow using the base-case parameter set and base-case infiltration indicates that little lateral movement occurs as water travels from the mountain surface to the repository horizon (BOD97, Chapter 20).

Additional relevant information with respect to the likelihood of whether significant lateral flow may be occurring is also tied to the conceptual model of Montazer and Wilson (MON84). Although their conceptual model hypothesized that the ratio of horizontal to vertical hydraulic conductivity of the Paintbrush nonwelded (PTn) unit was 10 to 100, subsequent laboratory analysis of core samples and field-scale air-injection tests indicate that the PTn is not as strongly anisotropic as first envisioned. Comparison of air-injection permeability values (LEC97) with laboratory core values (FLI98, Table 7) indicates that although greater, the air-permeability values for the PTn fall in the upper range of the core values or differ by no more than a factor of ten (CRW98, Section 5.3.3.1.2.3). This similarity between the field air-injection and laboratory core permeability values indicates that the permeability of the PTn is much more isotropic at the two scales than that of the welded units and that the PTn has some fracture permeability (LEC97, p. 29). Further, the similarity of air-permeability values for the PTn from both air-injection testing and pneumatic monitoring (CRW98, Section 5.3.3.1.2.4) indicates that the PTn is not strongly anisotropic. Taken together, these data, as well as other available data, indicate that the tendency for lateral flow in the PTn is not as strong as envisioned in the 1984 conceptual model (ROU99, p. 123-124). This conclusion is supported by three-dimensional simulation of flow using base-case parameter sets in conjunction with base-case infiltration, which, as mentioned above, resulted in little lateral movement as water flows from the mountain surface to the repository horizon (BOD97, Chapter 20). Therefore, the DOE assumes that steady-state vertical percolation into the Topopah Spring welded unit is essentially the same as vertical percolation into and through the PTn.

The saturated hydraulic conductivity of the Paintbrush nonwelded unit in the direction of dip is 10 to 100 times greater than saturated hydraulic conductivity in the direction normal to the bedding plane. The combination of dipping beds and differences in directional permeability creates a downdip component of flow. The magnitude of this component depends on the magnitude of the principal hydraulic conductivity ratio. The permeability contrast may be sufficient to decrease vertical percolation into the underlying Topopah Spring welded unit to almost zero. In this case, water would flow laterally downdip until structural features are encountered that create perching conditions or provide pathways for vertical flow.

As water moves downward through the PTn, the effect of high porosity and low fracture density progressively moves water from fractures into the matrix. Except for areas where fast paths may exist (such as faults), beyond a certain depth in the PTn, flow may be almost entirely in the matrix. Travel times through the matrix of the PTn are thought to be relatively long because the matrix of this unit appears to act as a "sponge" which dampens out episodic infiltration pulses.

Although the 1984 conceptual model of Montazer and Wilson implied that slow, matrix flow would dominate in the Topopah Spring welded (TSw) unit, DOE believes that subsequent data collection and analysis have demonstrated this not to be the case. For example, in situ measurements of water potential and core measurements of water potential and saturation indicate a deep percolation environment that is generally conducive to sustaining deep fracture flow (ROU99). Water potentials throughout most of the PTn and TSw are very high [greater than -0.3 megapascals (MPa)] and are nearly depth invariant. Thus, the imbibition capacity of the densely welded rocks, at least near fractures, is very small because of low matrix permeabilities and low water-potential gradients across the fracture-matrix interface. In addition, pneumatic data indicate that fracture permeabilities of the densely welded rocks are very high, several orders of magnitude greater than those of the host matrix. The pneumatic data also indicate that the fracture network is globally interconnected throughout the TSw, thus providing a vertically interconnected system of openings to sustain downward liquid flow. Furthermore, three-dimensional simulation of flow in the unsaturated zone beneath Yucca Mountain using the base-case parameter set and base-case infiltration indicates that 80 percent of the percolation flux at the repository horizon occurs as fracture flow (BOD97).

The nature of flow at the contact between the Topopah Spring welded unit and the Calico Hills nonwelded unit depends on whether the vitric or zeolitic facies of the Calico Hills unit is present. The permeability and effective porosity of the vitric facies are much greater than those of the matrix of the Topopah Spring unit, which may result in a capillary barrier where those units are in contact. Conversely, the permeability of the zeolitic facies is about the same as for the matrix of the Topopah Spring unit, resulting in continuity of matrix flux across such a contact.

Flux within the Calico Hills unit may occur with some lateral component of downdip flux, because of the existence of layers with contrasting hydraulic conductivity in the unit. A large scale anisotropy probably is caused by intercalation of tuffs with alternately large and small permeability and by compaction.

Water that flows downdip along the top of the Calico Hills unit slowly percolates into this unit and slowly diffuses downward. Fracture flow is known to occur near the uppermost layers of the Calico Hills unit, but diffusion into the matrix may remove the water from the fractures deeper in the unit and thereby limit flow mostly to within the matrix, except along the structural flowpaths. It is possible, however, that fractures provide significant avenues for rapid flow through this unit. Beneath the southern part of the block, the Crater Flat unit occurs between the Calico Hills unit and the water table. This includes the welded part and underlying nonwelded part of the Bullfrog Member of the Crater Flat Tuff.

Fluxes along many structural flowpaths are probably larger than within the units they intersect. The Calico Hills unit is more ductile than the overlying Topopah Spring unit, which may give the Calico Hills unit fracture sealing properties. In addition, because of the lesser shear strength of this unit compared to that of the Topopah Spring, gouge formation along faults and shear zones is more common. These properties may result in a smaller fracture conductivity in the Calico Hills unit. In the case where the structural flowpaths are hydraulically continuous across the upper contact of the Calico Hills unit, water would be more likely to flow downward without a significant change in its path until it reaches the water table. In cases where the structural flow paths are discontinuous across the upper contact, flow may be diverted downdip along this boundary. Intermediate conditions between the two extreme cases are also possible. Recent numerical modeling (LBL96, ROB96) of flow through the unsaturated zone has provided important insights into the possible characteristics of flow in each subunit of the unsaturated zone. Some of these insights are discussed in the following paragraphs.

Several conceptual models of unsaturated-zone flow at Yucca Mountain have been considered for TSPA-VA. Past TSPAs have focused on the use of equivalent continuum models (ECMs). The strength of the ECM is that it can describe observed matrix saturations at Yucca Mountain. Two problems with ECM are (1) the forced-pressure equilibrium causes capillarity of the small pores to overwhelm gravity-driven flow in the fractures, leading to inaccurate descriptions of disequilibrium situations; and (2) it is computationally inefficient in solving time-variable flows. The generalized-equivalent continuum model (GECM) is very similar to the ECM except that a matrix saturation value less than one is prescribed to increase flow through the fractures. The GECM solves the first ECM problem to some extent, but it suffers from lack of data to define the fracture-flow threshold and the DOE indicates that it is not clear whether it is valid under hydrothermal conditions.

The Weeps model, used in TSPA-93 (WIL94) is a simplified stochastic discrete fracture model that only considers flow through fractures (similar to the discrete fracture conceptual model). It apparently predicted the fast paths observed in the ECF (as indicated by elevated $^{36}C1/Cl$ occurrences) and can describe observed flow-channel spacing at Rainier Mesa (CRW96).

The DOE cites two problems with the Weeps model: (1) it ignores the rock matrix and thus any potential performance impact of flow in the matrix, and (2) much of the data that it requires have not been collected and might be difficult or even impossible to collect. This model was not used in TSPA-VA because the DOE favored a process-based model that could the calibrated to available site data such as borehole data and perched water data.

Another important flow conceptualization is the dual-permeability model (DKM). The DKM allows computation of flow in pressure disequilibrium in matrix and fracture continua, and the DOE believes it to be a reasonable compromise between the ECM and Weeps models. The DKM conceptual model has the flexibility to represent almost the entire range of possible flow behavior though variation of the fracture-matrix coupling parameter, allowing its behavior to change continuously from the ECM (which is dominated by matrix flow) to a Weeps-type flow almost entirely within the fracture network. Because of its flexibility and ability to model a broader range of unsaturated flow problems, the DKM conceptual model was used in TSPA-VA. However, the DOE points out that the DKM has its own problems, including (1) less computational efficiency than the ECM, and (2) lack of data describing the coupling term between matrix and fractures.

In addition to the conceptual model for fracture-matrix partitioning, the TSPA-VA conceptual model of flow in the UZ at Yucca Mountain includes an extensive perched water zone located between the repository horizon and the water table. The perched water exists because of a low permeability region that diverts flow laterally around the perched water region. Faults are also incorporated into the conceptual model of unsaturated flow and are believed to be pathways of fast flow from the surface down to the water table, giving rise to observed "bomb pulse" near faults in the ESF.

VI.1.1.4 TSPA-VA Abstraction Approach and Implementation

The DOE notes that the abstraction approach and implementation of UZ flow models for TSPA-VA were motivated by components and issues of UZ flow and UZ-flow modeling that have been identified as potentially important to PA calculations of Yucca Mountain. As noted previously, important issues addressed in the abstraction and testing analyses fall into four areas: (1) climate, (2) infiltration, (3) mountain-scale UZ flow, and (4) drift-scale seepage.

For TSPA-VA, uncertainty in future climates was represented by including uncertainty in the infiltration rates. DOE used the UZ flow model to calculate flow fields, using the expected present-day infiltration map, as well as to calculate variations on the expected map. The present-day infiltration map was multiplied and divided by three in the base case to include uncertainty in the infiltration values. The infiltration maps corresponding to the long term average and superpluvial climates were similarly divided and multiplied by three in the base case to develop lower-bound and upper-bound infiltration rates. The UZ flow model was used to generate flow fields for these cases, and sampling of these flow fields in TSPA-VA calculations was weighted the same as for the present-climate flow fields. Sensitivity studies also considered increased uncertainty in the infiltration maps by using factors of five instead of three.

Because of the time scales involved, a measure of uncertainty in mean climate precipitation is not presently available; in TSPA-VA, interannual precipitation variability is used as an estimate of climate precipitation uncertainty. Interannual variability (defined as one standard deviation from the mean) in precipitation in the State of Nevada over the last 100 years has been between 20% and 30% (DEW93). Arid and semi-arid regions can have interannual variability of 50% DEW93). A value of 50% uncertainty in mean climate precipitation was assumed for TSPA-VA. Therefore, although the mean precipitation for the long term average climate is estimated to be 300 mm/yr, it could be as low as 150 mm/yr (0.5 x 300 = 150) and as high as 450 mm/yr (1.5 x 300 = 450). In TSPA-VA, the estimated range of uncertainty in mean precipitation is relatively consistent with the estimated range of uncertainty in infiltration rate.

A quantitative characterization of the spatial and temporal distribution of net infiltration is needed for defining upper boundary conditions for site-scale, UZ ground water flow models in TSPA-VA. Net infiltration is defined as the downward rate of water percolation immediately below the zone of evapotranspiration; it is not necessarily equivalent to the rate of recharge to the underlying SZ. A site-scale net infiltration model was developed to provide temporally and spatially detailed estimates of net infiltration rates over the area of Yucca Mountain (BOD97).

The net infiltration model is primarily a deterministic model of surface and near-surface hydrologic processes, although climatic input involves both deterministic and stochastic processes. All major components of the water balance are solved in daily time increments. Daily results are provided for specified locations for analyzing the temporal distribution of net infiltration. Estimates of present-day and potential future net-infiltration rates are provided as detailed mappings of temporally and spatially varying time-averaged fluxes, which can then be applied to define upper-boundary conditions for the UZ.

VI.1.1.5 Model Calibration

The initial version of the infiltration model was calibrated using the 1984-1995 record of measured water-content profiles from approximately 80 neutron access boreholes and a developed record of daily precipitation for 1980-1995 (FLI96). Records from boreholes identified as potentially problematic because of the accelerated downward percolation of water along the annular space were excluded. Model calibration consisted of both qualitative and quantitative comparisons of measured versus simulated water-content changes for the soil profile.

VI.1.1.6 Unsaturated Zone Flow

The DOE would have preferred not to have had to abstract a model from the unsaturated zone process level model (BOD97). The DOE initially expected that the model would be simplified probably by reduction to two-dimensional or even one-dimensional geometry. The site-characterization investigators and modelers strongly recommended that three dimensions were important to represent Yucca Mountain flow adequately. This recommendation was based primarily on the flow below the potential repository, where the DOE believes there is significant nonvertical flow because of heterogeneity in the locations of the zeolitic layers and perched water. With the direct use of the process flow model, there is no need for testing of abstractions against the process model. The models are tested directly against the data as part of the calibration procedure (i.e., each case must be calibrated).

An important consequence of using a complex three-dimensional flow model is that the number of different cases that can be run is limited by computer-processing time, but even more so by the time needed for analysts to make necessary adjustments by hand for each case (to ensure proper model calibration). However, the DOE's current approach uses several select conceptual models and parameter sets that were determined (by sensitivity analyses) to have a significant impact on performance in order to encompass the range of uncertainty in UZ flow. The DOE has found that aqueous travel times between the repository and water table can vary by several orders of magnitude between different conceptual models.

The three-dimensional process flow model inherently contains several specific assumptions and issues that are listed below:

- Dual-permeability flow modeling (i.e., coupled matrix and fracture continua) is adequate. The DKM is capable of representing a large range of potential UZ-flow behaviors (e.g., fracture-matrix interaction, fracture and flow-channel spacing and geometry effective fracture apertures, and fracture- and matrix-flow velocities all vary greatly as the model parameters vary). In future work, the DOE may consider alternative models (e.g., discrete fractures, fractal fractures, etc.) to complement dual-permeability models, but alternatives were not considered for TSPA-VA.

- Steady-state flow modeling is adequate. Climate changes have been included by using a series of steady states; because of that, the flow could be said to be quasi-steady state rather than steady state. Perturbations to flow caused by repository heating were neglected. Such thermohydrologic perturbations were considered only in sensitivity cases because the waste packages are expected to last through the period when flow is strongly perturbed.

- Hydraulic properties of the matrix can be represented by the range of laboratory measurements. In some cases matrix properties were adjusted to get better fits to matrix-saturation measurements or other data.

- Fracture hydraulic properties can be derived from air permeabilities, fracture frequencies, and fracture orientations measured in drill holes and in the ESF. In some cases, the inferred fracture properties (van Genuchten alpha) were adjusted significantly in order to get better fits to matrix-saturation measurements or other data.

- The van Genuchten/Maulem functional form is satisfactory for use to represent the saturation/desaturation behavior of both matrix and fractures.

- The fracture-matrix connection area (i.e. area available for flow between fractures and matrix) is reduced below the geometric area implied by the fracture spacings used. Physically, this reduction represents effects of channelization of flow in fractures. The amount of reduction was chosen to optimize the fit to matrix-saturation measurements or other data.

- Heterogeneity within a unit does not need to be included. Hydrogeologic units are homogeneous.

- Infiltration at the surface is spatially variable, with the variability given by data in FLI96. Sensitivity to infiltration was investigated by multiplying the infiltration distribution by a constant factor keeping the same spatial variability.

- The lower boundary of the model is at the water table, which is fixed by drill-hole observations. For future climates, the water-table elevation is increased by prescribed amounts.

VI.1.1.7 Base-Case Hydrologic Properties Used in TSPA-VA

Model calibration allowed the DOE to develop what they believed to be the most reasonable estimate of parameters to be used with the UZ model for both liquid and gas flow. It was a combination of the "matrix" and "fracture" parameter sets and was named the "preliminary base case."

The base-case parameter sets used fracture-matrix multipliers that were calibrated to global classifications of welded, nonwelded, and zeolitic stratigraphic units. Together with the variations in present-day infiltration and ranges in fracture parameters, the base case consisted of five calibrated parameter sets:

- Base infiltration ÷ 3 and the van Genuchten air-entry parameter at a minimum for each layer

- Base infiltration + 3 and the van Genuchten air-entry parameter at a maximum for each layer

- Base infiltration and the van Genuchten air-entry parameter at the nominal "best estimate for each layer

- Base infiltration x 3 and the van Genuchten air-entry parameter at a minimum for each layer

- Base infiltration x 3 and the van Genuchten air-entry parameter at a maximum for each layer

VI.1.1.8 Recommendations for Development of Future Parameters

One of the DOE's contractors (LBNL) recommends that the project pursue three-dimensional inversions using available parallel-processing capabilities to minimize the number of assumptions in the inversions (such as the use of one-dimensional submodels that do not capture the perched-water effects). The contractor also recommends that the three-dimensional inversions add data, such as temperature and geochemical measurements, to explicitly constrain infiltration rates, fracture/matrix equilibrium and travel times during the three-dimensional inversions. Use of these three-dimensional inversions would increase the defensibility of the current calibration process. In addition, the creation of a heterogeneous property set should take advantage of the considerable data concerning parameter uncertainties developed in the one-dimensional models and with the heterogeneous distributions provided by Rautman and McKenna (RAU97) to generate a stochastic representation of the parameter fields in the site-scale UZ model.

VI.1.1.9 Sensitivity Studies for Determining Important Hydrologic Properties

The DOE performed a series of UZ simulations to examine the sensitivity of water flow to matrix and fracture permeabilities and van Genuchten properties in a one-dimensional, dual-permeability system. These studies, in part, formed the basis for the DOE's choice of parameters that were used in the base case, as described in a previous section. These simulations are divided into two sets. In the first set, ranges in property values were defined using the properties and mean and standard-deviation values determined from inverse modeling done at LBNL (BOD97). Results from these simulations show that, for the ranges of values considered, the fraction of infiltrating water that travels downward through the fracture continuum is primarily controlled by fracture alpha and to a lesser extent by fracture permeability. In this first set of simulations, the range of fracture alpha values considered was quite large relative to other property ranges and, as a result, its impact on flow behavior was most significant. To reduce the uncertainty in fracture-alpha values, the DOE conducted a subsequent study to derive more reasonable ranges of fracture alpha values. For this study, the DOE relied on published fracture permeability and fracture frequency data.

A second set of simulations based on the new fracture-alpha ranges was then performed. In this set of simulations only two properties, fracture alpha and fracture permeability, were varied over their ranges. There were two important differences between this set and the first set of simulations: (1) a Weeps formulation was used; that is, the matrix-fracture conductance area was reduced by the fracture relative permeability to water, and (2) in addition to using the new fracture-alpha values, different minimum and maximum values of fracture permeability that are consistent with the new fracture-alpha values were also used. Results of this study show that, for the ranges of fracture permeability and fracture alpha values considered, the fraction of infiltrating water that travels downward in the fracture continuum is controlled primarily by fracture permeability.

VI.1.1.10 Fracture-Matrix Interactions

Dual permeability models have been used to explicitly model unsaturated ground water flow and heat through both fractures and matrix. In the DKM, the fractures and matrix are treated as separate discrete continua. Heat, gas, and liquid are allowed to flow between the fractures and matrix, as well as through each continuum. While the DKM is generally more applicable to a wider range of problems than the ECM (e.g., transient flows, high infiltration boundaries), the DKM requires additional information about the coupling between the fracture and matrix continua.

VI.1.1.11 Analysis of Perched Water

Incorporation of perched water data is an important aspect of the UZ-flow-model calibration. The presence of perched-water bodies implies that vertical water fluxes locally exceed the saturated hydraulic conductivities of the perching layers. In order to capture the perched-water phenomena, the UZ-flow model must have a representative geologic/conceptual/trapping model, fracture/matrix properties, and sufficient net infiltration. The resulting model should reproduce hydraulic responses in pumping rests and remain consistent with geochemical data and the areal extent of the perched body.

Perched water can be defined as a SZ not directly connected to the static water table (FRE79). Two criteria must be met for the model to accurately reproduce perched water at Yucca Mountain. The first is that water saturation within a perched-water zone must be sufficiently high to initiate substantial fracture flow (if any fractures are present). The second is that water pressure within the perched-water volume must have values higher than the static atmospheric gas pressure that would be expected at the same elevation. Under these conditions, water will flow freely into a borehole intersecting a perched-water body. Perched water may accumulate where large contrasts in hydraulic conductivity exist between adjacent formation units, where a permeable layer overlies a relatively impermeable layer, or where a well-connected fractured unit overlies a locally unfractured or poorly connected fractured unit. Relative fracture density and fracture permeability have a strong influence on the accumulation of perched water. Perched water may also exist against a fault along a dipping horizontal plane if the fault acts as a barrier to downdip water flow.

As the DOE points out, one of the implications of an existing perched-water body is that the flow path may not be vertical through the UZ to the water table, but rather the water may be diverted laterally to a fault zone or other type of higher permeability channel in order to reach the water table. As a result, a nonuniform recharge rate to the water table is expected. The DOE notes that this has important implications for waste isolation at Yucca Mountain. Existence of perched-water zones along the base of the Topopah Spring welded unit implies that water may partially bypass the underlying zeolitic unit, and consequently some radionuclides may not be retarded by the highly sorbing zeolites.

Bodvarsson et al. (BOD97) detail how the field observed, perched-water data at the Yucca Mountain site were compiled, analyzed, and incorporated into the thee-dimensional UZ flow model. A conceptual model of occurrences of perched water was discussed, and a series of comprehensive computer modeling studies on perched water at the site was completed. A three-dimensional UZ perched-water flow model was then developed to investigate the perched-water phenomena at Yucca Mountain.

VI.1.1.12 Geochemical Analyses

Bodvarsson et al (ibid.) discuss the efforts made in calibrating the flow model to geochemical data. These analyses also provide methods of developing bounds and ranges for percolation flux and infiltration.

VI.1.1.13 Interface Between Unsaturated Zone Flow and Unsaturated Zone Transport

TOUGH2 (PRU91) and FEHM (ZYV97) are two prominent codes for evaluating flow and transport in the UZ for performance assessments. The application of TOUGH2 has focused on site-scale UZ hydrology (BOD97), while the use of FEHM has focused on fluid flow and radionuclide transport (ROB97) at Yucca Mountain. Both UZ hydrology and radionuclide transport are critical components in performance assessment calculations, and methods of coupling these components were investigated for TSPA-VA.

The DOE considered two methods to transfer the UZ flow results to the UZ radionuclide transport model, which was chosen to be the particle-tracking method in the computer program FEHM (ZYV97): (1) use the UZ flow fields calculated by TOUGH2 directly as input to the FEHM particle tracker, or (2) take the stratigraphy and calibrated hydrologic parameters and use them as inputs to a combined flow and transport calculation within FEHM. According to the DOE, the primary advantages of the first option are that preservation of the UZ-flow calibration is assured, and it is not necessary to recalculate the flow and recheck the calibration. The primary advantages of the second option are that the FEHM particle tracker is already set up to use flow fields calculated by FEHM (the first option requires development of a linking program to take TOUGH2 output and generate FEHM input), and there is additional flexibility to refine the computational grid to make the transport calculations more accurate. The first option (flow fields calculated with TOUGH2, radionuclide transport calculated with FEHM), has been implemented in TSPA-VA.

The particle-tracking method used in FEHM is a cell-based model in which particles are routed from grid block to grid block in a manner that preserves the overall residence time through any portion of the model and probabilistically reproduces the migration of a solute through the domain (ROB97). Flow calculation is based on a control volume in which fluid-flow rates into and out of each cell are computed. Since TOUGH2 is an integrated, finite-difference code and FEHM employs a control-volume, finite-element technique, the two codes are compatible from the standpoint of implementation of the particle-tracking technique. The required inputs for FEHM to use an externally developed flow field are: (1) grid-connectivity information and cell volumes; (2) fluid-state variables for computing density, fluid saturation, and rock porosity at each grid point; (3) internodal fluid-mass-flow rate for every connection in the numerical grid; and (4) fluid source and sink flow rates for each grid block.

VI.1.1.14 Grid and Model Domain for Three-Dimensional Site-Scale Unsaturated Zone Flow Model

Design of the three-dimensional grids was based on a geological framework model. The three-dimensional numerical grids were designed in two steps: (1) using all available surface information to create a horizontal, two-dimensional grid, and (2) integrating data from isopach maps of hydrogeological units to vertically develop the horizontal grid between the ground surface and the water table. This model was a further update of the existing three-dimensional UZ model first developed by Wittwer et al. (WIT92), which was later updated in 1996 (BOD96). The development of this new model, like the old one, started with the definition of the grid block centers that defined a single two-dimensional horizontal grid to use in all the three-dimensional vertical layer sections. After all the nodal points had been located, a numerical grid generator AMESH was used to develop the two-dimensional horizontal grid. These two-dimensional horizontal grids and the sub-layering criteria were used to develop a new three-dimensional numerical grid of the UZ at Yucca Mountain.

New boundaries for the site-scale model were developed as an update to the 1996 three-dimensional LBNL UZ model. These boundaries were based on revised fault maps, the observed shift in water level across the Solitario Canyon, the new infiltration and alluvium thickness maps, the observed pneumatic signals that were observed during the construction of the ESF Tunnel, and the requirements for thermal loading studies. The new boundaries take into account the extensive high-gradient SZ to the north of G-2 and explicitly include the Solitario Canyon Fault in the west by extending the model boundaries to about 1 km west of Solitario Canyon fault. The Bow Ridge fault forms the eastern boundary. The model extends from borehole G-3 in the south to about 1.5 km north of G-2 in the north. These boundaries enclose most of the existing and planned hydrology wells and the wells in which extensive moisture tension data and lithology are used as calibration points for formation properties. The 1997 site-scale model was based on the fault map that provided explicit offsets on Solitario Canyon Fault, Ghost Dance Fault, Iron Ridge, and the Dune Wash Fault, defined by the base of the Tiva Canyon.

One primary objective in the selection of grid boundaries was to minimize boundary effects resulting from thermal loading at the repository horizon, while investigating the influence of the major faults on the hydrological and thermal-hydrological response of the UZ at ambient conditions and during thermal loading. The modeled area covers nearly 43 km^2 and is bounded by Bow Ridge fault on the east; extends 1 km west of Solitario Canyon; is bounded by the plateau of high pressure gradient about 1.5 km north of G-2; and extends about 1 km south of the ESF south ramp. In this grid, the “East Block Repository” area is modeled as a locally refined area with an average grid of 100 x 100 m and accounts for proposed extension of the potential repository to the north. The resulting two-dimensional grid contains a maximum of 1,470 aerial grid-block nodes in each layer. The two-dimensional grid extends about 1 km west of the Solitario Canyon in order to explicitly model both the Solitario Canyon Fault and its associated

Iron Ridge fault branch to the south. Explicit modeling of the area west of the Solitario Canyon also allows for specification of the 40-m shift in the water table west of this fault. This grid was used to perform general site-scale UZ modeling and for detailed studies related to thermal loading of the repository.

VI.1.1.15 DOE Recommendations for Future Work

The DOE asserts that there is a need to harmonize the differences between the grids based on the USGS geological framework model and the geological model in order to select a single geological model for designing future numerical grids. Work is currently underway to integrate the ISM 3.0 geological-framework model into the site-scale UZ-flow model. Integration of the ISM 3.0 geological-framework model with the site-scale UZ-flow model will increase the defensibility of the UZ modeling effort.

VI.1.1.16 Summary of Implementation of the Base-Case Unsaturated Zone-Flow Model in TSPA-VA

The previous sections have detailed the development of the UZ-flow model used in TSPA-VA calculations. Sensitivity analyses have been performed to provide basis for parameters and divided by 3 and multiplied by 3 to yield three present-day infiltration scenarios. In addition, the DOE combined these present-day infiltration scenarios with variations of the fracture air-entry parameter to yield five base-case parameter sets. For each set, two future-climate scenarios were considered by using long-term average infiltration maps. These were either divided by 3 or multiplied by 3 to correspond to the value used in the present-day infiltration scenario. For all UZ ground water flow simulations, the EOS9 module of TOUGH2 has been used. This module implements Richards' equation and assumes that the gas phase is passive.

Once the flow fields have reached steady state, as indicated by a global mass balance within 1% error, the flow fields are used for mountain-scale transport calculations and near-field seepage studies. All developed data that are fed to other TSPA components are submitted to the Technical Data Base. These components are integrated for TSPA-VA calculations using the RIP code.

VI.1.1.17 Sensitivity to Mesh Resolution

All simulations aside from the mesh resolution study use a grid discretization of 0.5 m on a side (i.e., the numerical flow grid has the same resolution as the generated geostatistical permeability field). To study the sensitivity of the simulation results to the numerical grid resolution, the DOE performed additional simulations, with refined grids for a two-dimensional vertical cross section perpendicular to the drift center line. The original 0.5-rn x 0.5-rn discretization is refined by dividing each grid block first into 4 sub-blocks and then into 9 sub-blocks. The sub-blocks are assigned the same permeability value as the original grid block (i.e., the heterogeneity structure remains unchanged). Results indicate that there is some sensitivity to the grid design, as the derived seepage rates increase when using a finer grid resolution. The DOE believes that this is mainly because the gradients between elements of different permeability are steeper in a simulation with fine sub-gridding, while a simulation with the original grid—identical resolution of heterogeneity field and simulation grid—has smoother transitions as a result of the harmonic weighting of the two neighboring permeability values at element interfaces. The DOE notes that consideration must be given to the fact that an assumed step-change of permeability in the generated random fields is only an approximation of the more smooth transition in natural domains. Therefore, the DOE believes that the original grid design may actually allow for a reasonable representation of natural heterogeneity. The DOE further asserts that if the permeability values for the refined grids were derived by interpolation from the underlying random field to smooth out the strong step-changes, the impact of the mesh refinement would probably be small. DOE also notes that more work along this line will be performed in future studies.

VI.1.1.18 Summary

Following is DOE's summary of important points from the base-case seepage model.

A. Heterogeneity in the flow domain is critical for the calculation of seepage. It causes channelized flow and local ponding, so that the probability of seepage is much larger, and the time required for seepage into the drift is much shorter, than for the case where the flow domain is assumed to be homogenous.

B. The conceptual model for the interaction between fractures and matrix (i.e., X_{fm}) is important for transient flow in the case of episodic percolation events. Field-scale studies like the niche experiment can provide information on the "effective X_{fm}"

value; however, in considering long-term climate changes, the primary interest is seepage under steady-state conditions, so that fracture-matrix interaction need not be considered.

C. In general, seepage time decreases and seepage rate increases with an increase in percolation rate. The relationship between seepage and percolation is not linear, because of the many nonlinear processes involved.

D. Variation among geostatistical realizations is significant (though within the same order of magnitude) and dependent on details of local heterogeneity around the drift. Since such details are not known, a stochastic approach is necessary.

E. Comparison between two-dimensional and three-dimensional runs indicates that the probability of seepage and the seepage-initiation times are similar. The relative seepage rate, however, appears to be different in the three-dimensional runs, due to the possibility of flow in the third dimension.

F. The three-dimensional runs offer the opportunity for evaluating the possible spatial distribution of seepage along emplacement drifts, which cannot be achieved using two-dimensional vertical cross sections. The spacing of seepage locations is dependent on the correlation lengths of spatial heterogeneity.

G. Seepage is insensitive to the van Genuchten β parameter of the fractures. Seepage is sensitive to fracture α and permeability. For steady state, seepage is not sensitive to the matrix hydrologic properties. For transient problems, and for percolation rates lower than those considered here, matrix properties may be more important.

H. There are important questions about the effects of the discrete nature of fracture flow especially the possible role of fractures that dead-end at the drift wall. The preliminary niche-test results appear to fit the base-case conceptual model well, but more analysis (and testing) is needed.

VI.1.1.19 Recommendations

This chapter has detailed the DOE's development of four major components of UZ flow: (1) climate, (2) infiltration, (3) mountain-scale UZ flow, and (4) drift-scale seepage. Issues associated with each component have been presented, along with DOE's abstraction/testing plans that address these issues. The following sections summarize each of the four major UZ-flow components. The impact of each component on performance, along with the DOE's guidance and recommendations for the license application, are also provided.

Climate

The primary purpose of climate modeling was to provide precipitation rates and water table elevations that varied as a function of future climates. Future climate was modeled in TSPA-VA as a sequence of discrete steady states. Only three discrete climate states were considered for TSPA-VA: present-day, long-term average, and superpluvial. Present climate represented relatively dry, interglacial conditions, while the long-term average represented an average pluvial period at Yucca Mountain. The superpluvial represented periods of extreme wetness. The mean annual precipitation (MAP) rates for the present, long-term average, and superpluvial climates were estimated to be 150, 300, and 450 mm/yr, respectfully. These values were used by infiltration modelers to determine appropriate analog sites that had average precipitation rates that were commensurate with the predicted future climate values. The water-table rise from the present-day level (~730 m) was estimated to be 80 m and 120 m for the long-term average and superpluvial climates, respectively. Sensitivity analyses have shown that the overall performance is not sensitive to the duration of the climate cycles. The most significant impact was found to be the abrupt changes in water-table elevation and ground water flow rates that occurred at the transition between climates.

Climate models strongly impact performance through their influence on precipitation and evapotranspiration. These factors, in turn, influence the predicted infiltration in the UZ flow model. Therefore, the magnitude and timing of the prescribed climate states is important to performance.

The DOE believes that additional work is needed to understand the natural variability of current and future climates for Yucca Mountain. In particular the DOE feels that the adequacy of three distinct climate states needs to be addressed further. If distinct climate states are used in future analyses, their number, timing, duration, and the abruptness of the transition between them need better support. Additional modeling is needed to determine how the dose-rate pulses depend on the time of transition between climates, and whether noninstantaneous transitions would lead to lower peak doses. Appropriate climate analogs need to be defined, based on temperature and other factors in addition to precipitation. The superpluvial climate, especially, needs better definition.

Infiltration

Infiltration modeling provides the spatial and temporal distribution of net infiltration as an upper boundary for site-scale UZ-flow models in TSPA-VA. Distributed net infiltration rates were determined for each of the three climate states using the YMP infiltration model. The infiltration model simulated water movement at the ground surface by solving water mass balances using precipitation, a model for evapotranspiration, and available water in the soil profile. Also considered in the model were ground surface elevation, slope, bedrock geology, soil type, soil depth, and geomorphology. The primary driver for the infiltration model was precipitation, which was input using available records or, in some cases, a stochastic model. Daily precipitation records from different locations were used to define the present-day, long-term average, and superpluvial climates in the infiltration model. The sites were chosen based on how well their MAP values matched the estimated values associated with each climate. General results of the infiltration model are as follows:

- The modeled infiltration is highly heterogeneous and clearly correlated with topographic features.
- The highest net infiltration occurs along Yucca Crest.
- Net infiltration is lower in washes.

The spatially distributed infiltration maps were then upscaled to the site-scale UZ-flow model by averaging the simulated infiltration values over each surface element in the UZ-flow model. The DOE used average infiltration for each climate over the UZ-flow model domain of 4.9, 32.5, and 118 mm/yr, respectively.

Sensitivity analyses were also conducted to determine the effects of episodic infiltration on the percolation at the repository horizon. Results showed that the PTn unit effectively damped episodic pulses that were simulated on a yearly cycle, preventing the transient pulses from significantly impacting the percolation at the repository horizon.

Additional sensitivities that used infiltration to estimate the temperature profile in a borehole indicated that infiltration rates that were greater than three times the average present-day infiltration rate did not allow good matches with observed borehole temperatures because of increased advective heat transfer. Therefore, DOE used a factor of three as the upper and lower bounds for the range of infiltrations considered in each climate scenario.

Infiltration strongly affects repository performance because of its influence on mountain-scale unsaturated-zone flow and seepage into drifts (which subsequently affects waste-package-degradation models). The infiltration rates used in TSPA-VA are significantly higher than in past TSPAs. Higher infiltration rates, in general, tend to adversely impact performance. However, the increased infiltration must be considered in conjunction with other TSPA components such as seepage to understand the overall impact on performance assessment.

The DOE believes that the greatest need for improvement in infiltration modeling is explicit inclusion of processes that should be different for future climates, including effects of temperature, cloudiness, vegetation type, surface water runoff/run-on, and snow cover. Even for current conditions, some experts on the UZ expert elicitation panel suggested that runoff and run-on might be more important than is assumed in the infiltration model.

To provide a more quantitative basis for the uncertainty distribution for infiltration, the DOE notes that the infiltration model should be run in a stochastic mode (e.g., Monte Carlo simulation) to derive the infiltration uncertainty from the uncertainties in the input parameters of the model.

Finally, the DOE asserts that analogues with known infiltration, such as Rainier Mesa and Apache Leap, should be used to test and improve the infiltration models and methods.

Unsaturated Zone Flow

The three-dimensional UZ-flow model has been used to calculate unsaturated-ground water flow at Yucca Mountain for TSPA-VA. The model implements the dual-permeability formulation for fracture-matrix interactions and consists of nearly 80,000 elements. Hydrologic properties were determined using both direct measurements and calibration with field data, which included core samples, borehole log data, in situ water potential and temperature measurements, fracture measurements from the ESF, in situ pneumatic data, air permeability tests, and geochemistry data. A great deal of information on the calibration and details of the UZ-flow model development was taken from Bodvarsson et al. (BOD97). In the calibration approach, a number of vertical one-dimensional submodels that corresponded to borehole locations were extracted from the three-dimensional model. The code ITOUGH2 was used to perform simultaneous inverse simulations with these one-dimensional models to optimize hydrologic parameters by matching predicted and observed matrix saturations and moisture potentials. The selection of hydrologic parameters that were estimated by inverse modeling was influenced by sensitivity studies that determined important parameters to UZ flow, including the fracture air-entry parameter, and the fracture-matrix interaction parameter. The properties that were calibrated in one dimension were then used in the three-dimensional site-scale model, which included calibrations for perched water. Additional tests using geochemical data, infiltration data, and alternative weighting schemes were also performed to improve the three-dimensional model and increase confidence in the methods being used.

Results show that the flow through the UZ is predominantly in the fractures for the welded units and predominantly in the matrix for the nonwelded units. High infiltrations resulting from climate changes significantly increased the percolation flux in the vicinity of the repository and decreased the travel time between the repository and the water table. Travel times between the repository and the water table ranged from several days to hundreds of thousands of years. The fastest transit times resulted from flow through-fractures, whereas the matrix contributed to particle breakthrough at the water table at significantly longer times. Perched water, which has been calibrated in the three-dimensional flow model, diverted vertical flow laterally in the three-dimensional model, especially in the northern part of the repository. However, the total travel time of the diverted water was not significantly altered due to the fast flow path through the fractures. Sensitivity results using increased infiltration confirmed the importance of infiltration rates in determining travel times between the repository and the water table. In addition, sensitivity results using the DKM/Weeps alternative model showed that there was more significant fracture flow than in the base case, contributing to faster travel times. Finally, sensitivity studies of the zeolitic matrix permeability showed that increased matrix permeability can result in slower travel times due to increased flow through the matrix. However, decreased matrix permeabilities did not result in significant changes from the base case.

The DOE believes that a significant result of the current TSPA-VA UZ flow calculations relative to earlier TSPAs is that the higher estimates of current and future infiltrations can cause percolation fluxes to be significantly greater and travel times to be significantly shorter. While these effects have a negative impact on performance, the impact of UZ flow in general on the performance calculations must be determined collectively with other system components. For example, high infiltrations are thought to be adverse to performance, but performance calculations have shown that for a period of time, the high infiltration scenarios show a decrease in dose. This counter-intuitive result occurs because the temperatures around the waste package are reduced by the increased infiltration, and the corrosion of the waste packages is reduced. The use of the DKM/Weeps model produced significantly shorter travel times between the repository and water table because of increased partitioning of flow through fractures. As demonstrated in PA calculations, the decreased travel times increase dose rates for periods less than 10,000 years, but for longer times (100,000 and 1,000,000 years), the rapid transport does not significantly impact performance. At these later times, the travel time becomes small relative to the total simulation time, and the decreased travel in the DKM/Weeps model is less important. However, colloid-facilitated transport can be enhanced by increased flow and partitioning in fractures.

The uncertainty in matrix permeability in the zeolitic units resulted in travel times that could differ by several thousand years. Sorbing tracers traveling through the zeolitic matrix were retarded more if the permeability was increased, but little difference was observed if the permeability was decreased. Because the matrix permeabilities in low-permeability units is likely to be less than the reported values because of excluded "nondetect" values, the uncertainty associated with matrix permeabilities may not significantly impact overall performance.

The DOE believes that the most important need in the mountain-scale, UZ flow modeling is a better representation of localized channeling of flow, and in particular, the effects of flow in discrete fractures. The current approach uses continuum models with very coarse spatial discretization, and the adequacy of this approach is not fully established. There are indications from geochemical and isotopic tracers (chloride concentration, $^{36}C1$-to-chlorine ratio and ^{14}C-to-carbon ratio) that channeling of flow might be important. In addition, geochemical, isotopic and temperature data should be integrated into be calibration procedure because such data provide important information about flow through fractures.

The DOE also believes that more information is needed about the role of perched water in UZ flow. The current model assumes that the water is perched on a very-low-permeability underlying layer and flow is forced to go around it. The DOE notes that other interpretations are possible, such as mixing within the perched water and matrix flow out the bottom.

Thermal alterations of flow and thermal hydrology (TH)-chemical or TH-mechanical alterations of hydrologic properties are potentially important. In the current TSPA structure, these effects fall under the TH-component, but it is necessary to determine whether there should be a coupling of TH effects on mountain-scale, UZ flow and transport.

The DOE technical recommendations for improvement of the current mountain-scale UZ-flow model include the following:

- Incorporation of the most recent version of the integrated site model (site geologic framework model)
- More refined numerical grid
- Additional data to gain better estimates of fracture-hydrologic parameters
- Additional inhibition tests of hydrologic properties of the matrix
- Additional measurements of permeability of the zeolitic hydrogeologic units and properties of faults
- Additional studies to better characterize and understand the effects of perched-water
- Creation of heterogeneous property sets that take advantage of the heterogeneous distributions provided by Rautman and McKenna (RAU97) and a stochastic representation of the parameter fields in the site-scale UZ model

Fracture-flow processes should be further investigated with alternative conceptual models and additional field studies, such as niche and alcove studies, the planned east-west cross drift, and the Busted Butte transport study. Other flow processes that need to be further characterized include flow through faults, flow between disparate units (such as at the Paintbrush nonwelded—Topopah Spring welded and Calico Hills vitric—Calico Hills zeolitic interfaces), and fracture/matrix interactions. Finally, the process of model calibration can be further improved by developing two-dimensional and three-dimensional calibrations against field data, which may require using parallel computing techniques.

Seepage

The abstracted base-case seepage model was based on a large number of three-dimensional process-model calculations. The process model consisted of a three-dimensional heterogeneous fracture-continuum field. Three blocks of dimensions 20-m high,15-m wide and 16.5-m long were evaluated independently within this continuum. The drift was represented by a horizontal open cylinder of diameter 5 m at the center of the lower part of the block. Simulation grid cells were defined to be 0.5 x 0.5 x 0.5 m. Fracture properties were obtained from air-permeability tests of the DST in the ESF Thermal Test Alcove 5 and from evaluation of fracture surveys in the ESF. As a conservative estimate, matrix flow was neglected in seepage simulations used for TSPA-VA, and sensitivity studies were performed to evaluate the effects of fracture-matrix interactions. Sensitivity studies were also performed to determine the effects of episodic pulses, variations to hydrologic properties, and grid refinement.

The process-model results were abstracted by fitting the calculated seepage-fraction and seep-flow-rate distributions with beta probability distributions for which the mean and standard deviation are functions of percolation flux in the fractures. The seepage process model has been tested against recent preliminary data from the ESF niche liquid-release tests, and appears to fit them reasonably well. Finally, seepage sensitivity studies were performed to investigate reduced variance of fracture properties and variations to the fracture aperture.

Seepage into the drifts has a significant impact on performance for several reasons. Seepage controls waste-package degradation because the waste-package corrosion resistance material (Alloy 22) corrodes only in the presence of liquid water. Following the creation of openings through the waste package wall, the seepage volume controls the amount of water that can enter the waste package and dissolve the waste form. The flux of water into and through the waste package in turn controls the release rate of the solubility-limited radionuclides from the waste package. The impact of seepage on overall performance has been found to be important for periods ranging from 10,000 years to 1 million years.

The DOE has identified a number of additional studies that can be addressed in the near future (or are already underway) that the DOE believes will produce realistic and useful results for TSPA-LA. They are listed below:

- One of the key factors that control the spacing between drip seepage locations is the correlation lengths of spatial heterogeneity of the rock unit. The DOE recommends that a further careful study of the fracture distribution along the ESF should be made to provide estimates of these parameters. Field data from the ESF niche study can also yield important information related to this factor.

- The DOE indicates that a more comprehensive parameter-sensitivity study should be made, including sensitivity of drift seepage to the width of the permeability probability distribution function and the spatial correlation lengths of the heterogeneous fields. The occurrence of special features, such as long fractures intercepting the drift, should also be studied. The range of situations and property values used should be representative of the three stratigraphic units in which the potential repository will reside.

For reliable results, the DOE believes that the study needs to be performed with more realizations in the sense of a stochastic analysis and with potentially finer grids. Previous sensitivity studies have indicated that seepage may increase with finer grids.

- Gravity-driven flux in near-field discrete fractures close to the drift wall may increase the probability of drift seepage. Additional study of this possibility is needed.

- The DOE recommends that further study on successive percolation pulses should be carried out, especially since the current calculations seem to indicate that the time frame for the system to recover to its original initial state after the first pulse is very long, perhaps as long as hundreds of years.

The ESF niche test is an important first step in verifying seepage models, but the DOE notes that it is primarily a test of the overall conceptual model of the drift opening acting as a capillary barrier. The test offers little validation of the calculated values of seepage fraction, which the TSPA results show to be the most important aspect of seepage—indeed, the most important aspect of repository performance. Seepage fraction, or the fraction of waste packages contacted by seepage water, is related to the average spacing of seeps along the drift, which is presumably related to quantities such as fracture and fault spacing, permeability distribution, and permeability correlation length. Data on these quantities are needed, but the DOE notes that field data relating them to seep spacing are required in order to gain confidence in the model.

Even more so than for mountain-scale flow, seepage into drifts is potentially strongly affected by channeling of flow and discrete fracture effects. The DOE believes that the adequacy of the current fracture continuum model to represent these effects must be examined, and the DOE further asserts that the only real way to assess its adequacy is by testing it against field data. The DOE suggests that the model could be tested against observed seep spacing at analogue sites such as Rainier Mesa or Apache Leap. The DOE also recommends that additional niche tests should be conducted in all three repository hydrogeologic units--Topopah Spring, Lower Lithophysal, Topopah Spring Lower Nonlithophysal, and Topopah Spring Middle Nonlithophysal (where the first niche test was conducted)--in the east-west cross drift. The main

ESF tunnel does not go through the Topopah Spring Lower Nonlithophysal, but the east-west cross drift is designed to go through all three hydrogeologic units of the repository.

A potentially important issue identified by the DOE that was not addressed is the stability of seep locations over time. In the present models, seeps are assumed to occur at the same locations indefinitely, so that a fraction of the waste packages is always wet (the seepage fraction) and the rest are always dry. If seep locations change with time, more waste packages would be contacted by seeps, but only for a fraction of the time. This effect could result in more waste packages failing, but over a longer period of time, which could be important for performance. Thus, the DOE believes that the consequences of seep movement should be investigated.

Additional needs identified by the DOE are assessments of the effects of episodic percolation pulses, the potential increase in seepage during drainage of thermally mobilized water, the effects of chemical or mechanical alterations in hydrologic properties around the drifts, and the effects of drift collapse or emplacement of backfill.

VI.1.1.20 Unsaturated Zone Transport

Transport from a potential repository source is affected by the sorptive interactions with the rock and the degree of contact between radionuclides and the rock matrix. Some radionuclides, such as ^{99}Tc, do not sorb. Other radionuclides, such as ^{237}Np, move at a slower rate than a nonreactive tracer due to moderate sorptive interaction with various rock types. Still others, such as aqueous ^{242}Pu are found to strongly interact with all rock and, therefore, are relatively immobile. Nevertheless, sorptive interaction is only one part of the mechanism needed to retard the movement of radionuclides. Radionuclides that are transported through fractures cannot sorb onto the rock matrix without some mechanism that allows the radionuclides to contact the rock matrix. (Although the DOE believes that sorption onto minerals along fracture surfaces is likely, difficulty in characterization of this sorption mechanism has lead to the conservative assumption used for the TSPA-VA of no sorption in the fractures.) For example, many radionuclides have been found to strongly sorb to zeolitic rock. However, highly zeolitized rock generally has low matrix permeability, and in some cases, low fracture permeability as well. The low-permeability character will lead to transport pathways that bypass the zeolitic minerals, due to lateral diversion or transport through fractures, severely limiting the degree of contact between radionuclides and zeolitic minerals. Therefore, low levels of zeolitic alteration in the CHn vitric, which do not severely reduce matrix permeability, are found to have more influence on the transport of sorbing radionuclides. The effects of lateral diversion and focused flow in certain regions of the potential repository also tend to reduce the degree of contact between radionuclides and both the CHn vitric and zeolitic rocks. The more evenly distributed percolation flux in the TSw allows for more intimate contact of radionuclides with rock matrix, through matrix diffusion and advection, despite the low matrix permeabilities of the TSw.

Sorptive interactions may enhance radionuclide transport if the aqueous species sorbs to mobile colloids. Colloid-facilitated transport enhances the movement of the aqueous species because the sorptive interaction with matrix is reduced (hence reducing retardation in transport) and colloids may tend to move preferentially through the higher-velocity fracture pathways. In addition to reversible, sorptive type interactions with colloids, radionuclides may also be irreversibly attached to colloids (e.g., coprecipitation during colloid formation). Isotopes of Pu have been identified as radionuclides that are likely to be affected by colloid-facilitated radionuclide transport.

Radionuclides that have little or no sorptive interaction with the welded tuff matrix are expected to migrate through the TSw relatively quickly due to advective transport along fractures. The nonsorbing radionuclides travel primarily through fractures except for transport through the CHn vitric, where matrix flow and transport is expected to dominate. Therefore, transport times to the water table for nonsorbing radionuclides such as ^{99}Tc, and ^{129}I are primarily governed by transport in the CHn vitric.

Another factor that affects travel time to the water table is the lateral diversion of flow above the CHn. Although the lateral diversion increases the transport path length to the water table, the transport pathways are primarily fracture pathways. The diverted percolating flow eventually finds some pathway to the water table. Therefore, lateral diversion can lead to zones of focused flow to the water table, where the flow rates may be locally magnified well beyond the flow rates anticipated for uniform vertical percolation. The travel times for radionuclides transported through a focused percolation zone will tend to be relatively short, including transport through the CHn vitric.

The separation of UZ radionuclide transport from UZ flow is a process abstraction used by the DOE for sensitivity studies and development of the TSPA-VA UZ radionuclide transport model. The DOE combined the two processes in TSPA-VA calculations by using a set of pre-calculated, three-dimensional, UZ flow fields computed with the site-scale UZ flow model. These flow fields are incorporated directly into the 3-D, UZ radionuclide transport model for TSPA-VA.

The waste heat released in the potential repository influences UZ flow and temperature behavior. As for UZ flow, the separation of thermal hydrology and UZ radionuclide transport is a process abstraction. Since the DOE assumes that the thermal-hydrologic effects of the repository do not result in any permanent changes to the mineralogic or hydrogeologic conditions of the UZ, then the effects of the UZ temperature processes on radionuclide transport are assumed to the minor. The DOE's modeling of this process suggests that the time period during which the temperature and flow fields are significantly perturbed occurs prior to the release of most of the radionuclides. Therefore, the DOE has assumed that the thermal-hydrologic effects on the UZ temperature and flow fields have a negligible influence on radionuclide transport. However, the DOE points out that the effects of thermal-hydrology are still important for defining the behavior of the waste package and radionuclide releases from the engineered barrier system. Therefore, thermal-hydrology is included for these subsystem models.

The DOE also notes that the effects of thermal perturbations can also potentially have long-term consequences relative to minerals in the UZ and change both hydrogeologic and transport properties of the system. These types of thermal-hydrologic changes to the system may affect long-term radionuclide transport in the UZ. Although the DOE indicates that their present evaluation of these coupled processes is not complete, they have conducted sensitivity calculations concerning off-normal behavior to address this coupling.

The waste form mobilization process provides the radionuclide fluxes at the emplacement drift boundary for UZ radionuclide transport calculations. The emplacement drift boundary represents a spatial-domain abstraction interface between processes that affect radionuclide transport inside the emplacement drift and radionuclide transport in the UZ. Therefore, the radionuclide fluxes calculated at the emplacement drift wall are a source term for UZ radionuclide transport calculations. The DOE expects this source term to provide radionuclide fluxes at the emplacement drift boundary that will vary as a function of the location in the repository and time.

Saturated zone flow and radionuclide transport calculations use the results of the UZ radionuclide transport calculation to assess the migration to the accessible environment. The water table in the vicinity of the potential repository represents a spatial-domain abstraction interface between processes that affect radionuclide transport in the UZ and SZ. The radionuclide fluxes calculated at the water table due to UZ radionuclide transport are a source term for SZ radionuclide calculations. This source term is expected to provide radionuclide fluxes at the water table that will vary as a function of position on the water table and time. Although the DOE has used no feedback mechanisms between SZ radionuclide transport and UZ radionuclide transport, the position of the water table is recognized as a feedback from SZ flow to UZ radionuclide flow and transport.

Advection

Advection is the movement of dissolved or colloidal material because of the bulk flow of a fluid, which in this case is water. This key transport mechanism can carry radionuclides through the approximately 300 m of unsaturated rock between the potential repository and the water table. Advection is also an important mechanism for radionuclide movement between fractures and rock matrix. In many of the hydrogeologic units, advection through fractures is expected to dominate transport behavior, primarily because the expected flow rates through these systems exceed the matrix flow capacity under a unit gravitational gradient. Advection through fractures is fast because of high permeability and low porosity, with few opportunities for radionuclides to contact rock matrix. A few of the hydrogeologic units have much larger matrix permeability and are expected to capture most of the fracture flow by advection from the fractures to the matrix, causing much slower transport velocities and closer contact of the radionuclides with the matrix. Advective transport pathways result from and therefore follow the flow pathways, which are predominately downward. However, lateral diversion is expected along hydrogeologic unit contacts having strong contrasts in rock properties, particularly in areas of perched water. Flow that is diverted laterally ultimately finds a pathway to the water table through more permeable zones which may be faults.

The detailed geometry of fractures and matrix pore spaces at Yucca Mountain is far too complex to be modeled explicitly. On the other hand, it is important to capture the larger-scale spatial variability, such as differences between welded and nonwelded hydrogeologic units, and the differences in fracture and matrix properties at the local scale. To show this variability, the DOE uses a dual-permeability model for fractured rock. In the dual-permeability model, the fractures and matrix are distinct interacting continua that coexist at every point in the modeling domain. Each continuum is assigned its own hydrologic properties such as permeability and porosity, which may also vary spatially. In general, the fractures are modeled as a highly permeable continuum having low porosity while the matrix is modeled as a much less permeable continuum having higher porosity. The dual-permeability model offers a bimodal approximation to the true spectrum of fracture and matrix properties. More importantly, the dual-permeability model can capture the effects of fast pathways for radionuclide transport from the repository to the water table. This feature is an important improvement over single-continuum models.

The conceptual model for UZ transport is strongly tied to the conceptual model for UZ flow. As described above, advective transport because of flow is the main transport mechanism that can move radionuclides from the repository to the water table. Conceptual models for UZ flow are commonly based on a continuum relationship, known as Darcy's law, which relates volumetric flow rate and the gradient in hydraulic potential. In the case of fractured, porous rock such as the volcanic rock that constitutes Yucca Mountain, these continuum relationships are extended to embrace two coexisting continua, fractures and rock matrix, that interact according to the same constitutive relationships that govern flow in a single continuum. From the standpoint of UZ transport, the need for explicit and separate representation of fracture and matrix flow is because of the extreme disparity in transport velocities that can occur in the two continua. Travel times for radionuclides transported to the water table exclusively in fractures are expected to be about 10,000 times faster than travel times for radionuclides moving exclusively in the matrix. In addition, the transport velocities in the fractures may be sufficiently rapid that radionuclide concentrations in the fractures are in disequilibrium with the matrix. For example, a high concentration of radionuclides entering fractures at the repository may penetrate the entire UZ before establishing a uniform, equilibrated concentration in the rock matrix. Therefore, an explicit and dynamic model of transport through fractures and matrix, as well as exchange between the fractures and matrix, is needed to represent the system. The dual-permeability model provides the necessary level of detail to capture the important differences between transport through fractures and matrix. There are other possible approaches to modeling flow in fractures and matrix rock. However, these other models either do not recognize the important dynamic coupling between fractures and matrix, such as the ECM, or are impractical to implement at the field scale, such as the discrete fracture model (particularly for systems with advective transport in the fractures and matrix, such as a dual permeability system). For these reasons, the flow and transport models for the UZ are based on dual permeability.

In general, flow in the UZ is time dependent or transient. One mechanism responsible for this time dependence is the time variations in the infiltration flux at the surface. The time variation of the infiltration flux may be approximated as occurring over short intervals characterized by changes in weather, resulting in episodic transient flows, or over much longer time periods corresponding to climate changes. Existing information concerning episodic transient flow seems to indicate that such flow may not be able to frequently penetrate through the UZ to the level of the repository because of the dampening influence of the PTn hydrogeologic unit. Episodic transient flow propagating through fractures tends to be absorbed by the PTn unit, resulting in much slower drainage of the episodic flows in lower hydrogeologic units at and below the repository level (ROB97, Section 6.13). For these reasons, the DOE has not incorporated episodic transient flows into the TSPA-VA calculations.

Changes in unsaturated flow because of longer-term changes in climate have a more pronounced influence on UZ flow than episodic transient flow. Sustained changes in infiltration associated with climate change ultimately impact the entire flow field in the UZ. The actual transient period during which the UZ flow responds to a climate change, however, has been found to be less significant (ibid.). The reason is that the change in flow in the fractures, which dominates the flux in most hydrogeologic units, responds relatively quickly to a change in infiltration. Therefore, the quasi-steady flow model was used to estimate the effects of climate change on radionuclide transport. In this model, infiltration rate is assumed to change abruptly when climate changes from one steady flow field to another. Transport calculations simply re-start when climate changes. A distributed source of radionuclides throughout the UZ is derived from transport calculations using the flow field for the previous climate, and a new steady state flow field is selected based on the new climate.

In addition to the change in the UZ flow field, the location of the water table is also assumed to change abruptly at the time of climate change. The three climate states—present day, long-term average, and super pluvial—have successively higher water table elevations to response to the increasing infiltration. If the water table rises with the climate change, the radionuclides in the UZ between the previous and new water table elevations are immediately available for transport. In the TSPA-VA model, water table elevations change by 80 m from present-day to long-term-average climates and by 120 m from present-day to super-pluvial climates.

The dominant flow direction is expected to be mainly downward over large scales. However, local flow field variations are expected to be three dimensional. The importance of these variations lies primarily in the kinds of rock units and fracture characteristics that dominate along the 3-D flow paths. A secondary consideration is that 3-D flow paths from the repository to the water table will necessarily be longer than strictly vertical flow paths. 3-D flow patterns are expected along rock unit contacts with contrasting properties, particularly in zones where these contrasts are believed to be features that create perched water. To capture these effects, the DOE has used three dimensions to model the flow and transport. Spatial variability is captured in the 3-D relationships of the hydrogeologic units and structural features, for example, faults, and in the variations in hydrogeologic and transport properties assigned to the hydrogeologic units.

Matrix Diffusion

Diffusion is the movement of dissolved or colloidal material because of random molecular motion. It is not an effective mechanism for transport between the repository and the water table because of the large distance involved (about 300 m). However, diffusion can play an important role in radionuclide exchange between fractures and rock matrix. In this case, molecular diffusion affects the persistence of a dissolved ion in the fracture flow stream. The relative influence of this mechanism on overall transport through the UZ depends on the rate of movement through fractures as well as the degree of fracture/matrix contact.

Bulk diffusive flux occurs when concentration gradients are present because diffusion is driven by random molecular motion. In addition, the matrix diffusion coefficient is a function of the free water diffusion coefficient, temperature, radionuclide mass, atomic or molecular dimensions and charge, as well as the matrix pore structure and water saturation. The temperature variations are expected to be small over the time period for radionuclide releases to the UZ. The effects of pore structure and water saturation have been shown to depend primarily on the volumetric water content of the rock (ROB97). For rock in the UZ, the water content is relatively uniform spatially. Therefore, as a simplification, variations in the matrix diffusion coefficient are assumed to be primarily dependent upon the radionuclide type, that is, mass, size, and charge. In this case, measurements indicate that the primary difference is between cationic and anionic radionuclides (TRI97). Anionic radionuclides have lower matrix diffusion coefficients than cationic radionuclides; that is, they are transported more slowly by diffusion. Lower coefficients for anionic radionuclides are believed to be a result of size and charge exclusion of the anionic radionuclides from a portion of the pore structure. The surfaces of the pore minerals are generally negatively charged under the chemical conditions of the undisturbed environment.

In general, the direction of radionuclide transport by matrix diffusion between the fracture continuum and the matrix continuum depends on the direction of the concentration gradient. However, the most important influence of matrix diffusion is expected to be on radionuclide transport through fractures. Radionuclides traveling through fractures are always near the matrix relative to the fracture spacing. This proximity is a result of the fracture and matrix geometry where the ratio of fracture aperture to fracture spacing is small. Also, diffusive penetration of the matrix is proportional to the square root of the fracture transport time. Because of relatively fast transport through fractures, most radionuclides diffusing from fractures into the matrix do not penetrate far, relative to the fracture spacing. For this reason, the DOE expects the effects of fracture spacing on matrix diffusion to be negligible, and ignores the effects of finite fracture spacing. Similarly, because of the relatively small fraction of matrix affected by matrix diffusion (that is, diffusive movement from fractures into the matrix is relatively slow), the DOE makes an approximate representation for fracture transport, including matrix diffusion, separately from the advection of radionuclides through the matrix.

Dispersion

Dispersion is a transport mechanism caused by localized variations in flow velocity. These variations cause dispersion of the radionuclides both along and transverse to the average flow direction. Variations in both the magnitude and direction of the velocity contribute to the overall dispersion. This dispersion, under certain limiting conditions, can act in a manner analogous to diffusion, in which mass flux is proportional to the concentration gradient. Dispersion is most important where concentration gradients are the largest—near the front of a propagating plume or along the lateral edges of the concentration field. Dispersion smears sharp concentration gradients and can reduce the breakthrough time, or arrival time at a specific point, for low concentration levels of an advancing concentration front.

Dispersion is included in the transport conceptual model using a standard relationship based on Fick's law between mass flux and concentration gradient (ROB97). The dispersion coefficient in the Fickian relationship is expressed as the product of the mixing length scale or dispersivity, and the average linear velocity. Dispersion is independently represented in both the fracture and matrix continua. However, the DOE does not expect dispersion to play an important role in the UZ transport. The repository emplacement area is very broad, relative to the distance to the water table, and this geometrical arrangement tends to suppress dispersion effects. Longitudinal dispersion becomes secondary to the explicitly modeled variations in transport velocities across the repository because of variations in infiltration. Lateral dispersion is limited by the short transport path from the repository to the water table compared with the size of the source. Also, the explicitly modeled variations in transport velocity caused by the fracture/matrix system tend to dominate dispersion.

Radionuclide Sorption

Sorption is the general term for describing a combination of chemical interactions between the dissolved radionuclides and the solid phases (that is, either the immobile rock matrix or colloids). Any given sorptive interaction is caused by a set of specific chemical interactions such as surface adsorption, precipitation, and ion exchange. However, the sorption approach does not require identifying the specific underlying interactions. Instead, batch sorption experiments are used to identify the overall partitioning between the aqueous and solid phase, characterized as a "sorption" or distribution coefficient (K_d). The strength of the sorptive behavior is a function of the chemical element, the rock type involved in the interaction, and the geochemical properties of the water contacting the rock. Sorption reduces the rate of advance of a concentration front in advective and diffusive transport, and amplifies the diffusive flux of radionuclides from the fractures to the rock matrix through its influence on the concentration gradient.

Numerous rock-water chemical interactions may influence radionuclide transport (TRI97):

- *Ion adsorption* —metal cations sticking to mineral surfaces due to London-van der Waals forces and hydrogen bonding
- *Ion exchange* —substitution of an aqueous cation for the anion in a mineral structure
- *Surface complexation* —coordination of an aqueous cation with a deprotonized metal hydroxide at the mineral surface
- *Precipitation*—generation of a bulk solid phase

The nature and strength of these rock-water interactions are highly dependent on the chemical composition of both the aqueous and solid phases. The conceptual model used to capture all these interactions and sensitivities is the minimum K_d model. This model bounds the distribution of radionuclides between the mobile, or dissolved in the aqueous phase, and immobile, or attached to the solid phase, using a linear, infinite-capacity partitioning model. In this model, the sorbed, or immobile, concentration is equal to the aqueous concentration times the partitioning coefficient. Because of the numerous mechanisms and dependencies known to influence sorption, using a linear partitioning model with a single coefficient provides only a minimum bound for K_d, and hence the immobilized fraction.

Colloid Facilitated Transport

Colloids are potentially mobile in water flowing though the UZ. Since colloids are small solids they can interact with radionuclides through sorption mechanisms. Unlike sorption of radionuclides to the rock matrix, however, radionuclides sorbed on colloids are potentially mobile. Therefore, colloidally-sorbed radionuclides can be transported through the UZ at a faster rate than the aqueous species without colloids. Another form of colloidal radionuclide movement occurs when the radionuclide is an integral component of the colloid structure. In this case, the radionuclide is irreversibly bound to the colloid, as compared to the typically reversible sorption mechanism. The different types of colloids considered in the performance assessment model are clay colloids, iron oxy-hydroxy colloids, spent fuel waste form colloids, and glass waste form colloids.

Thermal-Hydrologic, Thermochemical, and Thermomechanical Processes

The potential repository will perturb the natural system due to the introduction of waste heat and foreign materials. Thermo-hydrologic modeling is done for TSPA-VA to better define the temperature, humidity, and water contact conditions that will affect waste package corrosion, waste form dissolution, and radionuclide releases from the engineered barrier system. The thermal-hydrologic conditions also affect the flow field, and hence the radionuclide transport, through the UZ. However, the thermal-hydrologic process is most significant over the first 2,000 to 3,000 years following waste replacement. Sensitivity studies indicate that most of the radionuclide transport through the UZ will take place after thermal-hydrologic activity has subsided. Thermal-hydrologic processes are not expected to substantially alter UZ radionuclide transport as compared to transport through the undisturbed system. Therefore, the DOE has not incorporated the effects of thermal-hydrologic processes in the UZ radionuclide transport model.

TSPA-VA Approach

Unsaturated zone radionuclide transport calculations are computed using the particle tracking method available in the unsaturated flow and transport code FEHM. This computational method for UZ radionuclide transport is dynamically linked with the TSPA's RIP code for these calculations. A 3-D, dual-permeability model is used for computing radionuclide transport in a fracture/matrix system. Three-dimensional, steady, UZ flow fields, computed with the unsaturated flow code, TOUGH2, are used for the particle tracking transport calculations.

Changes in the flow field due to climate change are accounted for through a quasi-steady flow and transport approximation. The transport model includes the effects of fracture/matrix interaction driven by advective and diffusive exchange between the fracture and matrix continua. The transport model includes the effects of radionuclide sorption in the rock matrix using a bounding, minimum K_d modeling approach. Colloids are included as a mechanism for the transport of plutonium. The model for aqueous plutonium transport allows for reversible sorption of plutonium on colloids. Plutonium releases from the EBS also include a fraction plutonium irreversibly sorbed to colloids.

Radionuclide mass flux at the EBS boundary is provided by RIP for the UZ radionuclide transport calculations. The radionuclide mass flux from any source within a potential repository region is distributed uniformly over the computational grids for fracture nodes in the transport model that lie within the region. Radionuclide mass flux at the water table from the fracture and matrix continua are mixed in a RIP cell and provided to the SZ radionuclide transport model.

The model for unsaturated radionuclide transport incorporates several assumptions. The primary conservative modeling assumptions are no fracture sorption and no colloid filtration. These assumptions clearly result in model predictions having more rapid migration of radionuclides through the unsaturated zone. Assumptions about the influence of thermal-hydrologic-chemical processes, fracture spacing in the matrix diffusion model, and fracture/matrix contact in the matrix diffusion model, are potentially nonconservative.

Long-term Transient Flow and Climate Change

An approximate method was developed for computing UZ radionuclide transport under the long-term transient flow conditions associated with climate change. The approximation was developed due to the computational burden associated with the complete transient flow and transport calculation. The method is based on a quasi-steady flow approximation, in which the flow fields instantaneously change from one steady flow field to another in response to changing infiltration rates caused by climate change. The transport calculations restart upon change in climate using the new flow and water saturation distributions. Radionuclides present in the UZ at the time of climate change are also restarted as a distributed source of radionuclide mass in the UZ flow and transport grid. The method is shown to provide an excellent approximation to the complete unsaturated transient flow and transport problem resulting from climate change.

Colloid-Facilitated Radionuclide Transport

An approximate computational method was developed to treat the effects of radionuclide interactions with colloids. This method is applied in the TSPA-VA calculations to the problem of plutonium transport. Previous TSPA analyses did not include the effects of colloid-facilitated radionuclide transport. The treatment addresses two types of colloidal interactions with plutonium: reversible sorption between aqueous and colloidal plutonium and plutonium irreversibly attached to colloids. For reversibly sorbed plutonium, the approximate colloid facilitated transport method assumes linear, equilibrium partitioning of aqueous and colloidally-sorbed fractions. Colloid movement is represented by advective transport in fractures or matrix with no diffusion of colloids between fractures and matrix, and no colloid filtration.

Unsaturated Zone Radionuclide Transport Sensitivity Investigations

The DOE performed additional sensitivity studies to provide a better understanding of transport parameter sensitivity, identify the range of conditions under which a K_d sorption model may be used to bound geochemical interactions, investigate the effects of episodic transient flow on radionuclide transport, and investigate the effects of fine-scale mineralogic heterogeneity.

DOE Conclusions

The results of investigations into radionuclide transport through the UZ lead the DOE to conclude the following:

- For present-day climate, the average travel time for nonsorbing radionuclides released from the northern portion of the repository is on the order of a thousand years, but for the wetter long-term average climate, the average travel times are tens of years.

- For present-day climate, the average travel time for nonsorbing radionuclides released from the southern portion of the repository is several thousand years, but for the wetter long-term average climate, the average travel time is hundreds of years.

- For most of the mass of strongly sorbing radionuclides, such as plutonium, arrival at the water table is delayed tens to hundreds of thousands of years. Radionuclides that reversibly sorb onto colloids are also delayed; however, irreversibly bound radionuclides may behave as nonsorbing radionuclides.

- Matrix diffusion has little effect on transport of nonsorbing radionuclides. However, combining matrix diffusion with sorption significantly retards radionuclides compared with sorption and no matrix diffusion.

- The TSw unit is the primary barrier to radionuclide transport because of slower fracture transport in this unit compared with the Calico Hills zeolitic unit, and its greater thickness and continuity compared with the Calico Hills vitric unit.

- Alternative flow models like the dual-permeability model with Weeps modeling, which have smaller coupling strengths for effective fracture/matrix contact area, increase fracture-dominated transport, particularly for sorbing radionuclides. However, the magnitude of this effect is not large for weakly sorbing radionuclides.

The following items are viewed by the DOE as the areas where additional work would provide the greatest improvements in the comprehensiveness and credibility of the radionuclide transport model in the UZ:

- Effects of Thermal, Hydrologic-Chemical Alteration—The current model does not account for alteration of the UZ because of thermal alteration of minerals, chemical interactions of repository materials, mineral dissolution, and precipitation. These effects are potentially important to transport behavior in the UZ and need to be addressed. Thermal-chemical alteration could cause reduced matrix sorption and fracture-matrix interaction. These effects could cause increased release rates from the UZ for base case transport results; however, it is expected that existing sensitivity studies bound most of these potentially nonconservative interactions.

- Colloid Filtration—The ability of colloids to facilitate radionuclide transport is a function of their ability to migrate over large distances without being "filtered out" by the host rock. This filtration effect was not included in the TSPA because of inadequate information to bound the mechanism. The filtration effect is particularly important for the fraction of radionuclides that are irreversibly bound to colloids. However, the assumption that there is no colloid filtration is conservative for transport in the UZ .

- Fracture Sorption—The effects of higher infiltration determined in the TSPA-VA guarantee that transport will be fracture-dominated in many of the unsaturated-zone units. Minerals that line fractures are known to sorb radionuclides, but more information is needed to define the distribution and character of the fracture materials so that sorption on fracture surfaces may be included. However, the assumption that radionuclides do not sorb onto fracture surfaces is conservative for transport in the UZ. Although the present sensitivity studies have found that transport is not highly sensitive to fracture sorption, this result requires further investigation to better define the appropriate range of parameters for fracture sorption.

VI.1.1.21 Expert Elicitation and Peer Review Panel

The Yucca Mountain project conducted a UZ Flow Model Expert Elicitation, in which project data and models were presented to a group of experts (mostly from outside the project) so that they could provide an evaluation of the work being done (CRW97). Particular emphasis was placed on estimates of surface infiltration, deep percolation, and the uncertainties associated with each. Each expert estimated probability density functions (PDFs) of infiltration. The mean values of their estimated net infiltration ranged from 3.9 mm/yr to 12.7 mm/yr, and the mean values of their estimated percolation flux at the repository horizon ranged from 3.9 mm/yr to 21.1 mm/yr. These values are commensurate with the simulated average present-day infiltration over the modeled repository (~8 mm/yr) and the simulated average percolation fluxes within the six prescribed repository subregions for the present-day base case (3.9 mm/yr to 11 mm/yr) of TSPA-VA.

Additional topics that were covered during the expert elicitation included spatial variability of net infiltration and percolation flux, temporal variability of infiltration and percolation flux, lateral diversion above the repository, partitioning of fracture and matrix flow, seepage into drifts, modeling issues, and additional data and work requirements. The experts generally agreed that the infiltration map that was used in TSPA-VA captures the general spatial variability of infiltration, but several suggested that more infiltration could occur beneath washes with thin alluvial cover. The experts also agreed that temporal behavior of net infiltration was characterized by episodic events associated with major storm events, but that most of the transient flux was attenuated within the system. With regard to lateral diversion above the repository, most of the expert agreed that contrasts in the hydrologic properties between units would likely cause lateral flow, particularly in the Tiva Canyon welded unit - Paintbrush Turf nonwelded unit contact, but that the amount of diversion was limited to scales of several meters to tens of meters. This is consistent with the results of the TSPA-VA UZ-flow simulations, which show nearly vertical flow above the repository. The experts did not address the issue of lateral diversion caused by perched water below the repository. The experts also estimated that, based on the low matrix permeabilities in the Topopah Spring welded unit, partitioning of flow in the TSw was predominantly in the fractures. Also, the fast-flow component likely represents only a small part of the total flux. This is consistent with simulated results in TSPA-VA. With regard to seepage into drifts, the experts agreed that a capillary barrier will exist around the drifts, diverting a majority of the water around the area of the drifts. This behavior is also consistent with the TSPA-VA simulations for seepage. Finally, the experts recommended a number of additional modeling and data-collection activities that address estimates of infiltration, percolation, and seepage.

In addition to the expert elicitation, the TSPA-VA Peer Review Panel provided input to the UZ flow activities. They recognized the use of environmental tracers (^{36}C1) as evidence of fast flow paths between the surface and the repository and recommended its use in supporting the conceptual models of UZ flow. The Peer Review Panel also recommended studies to better understand fracture-matrix interaction. Finally, the Peer Review Panel emphasized the need to better understand seepage into drifts.

VI.2 SATURATED ZONE

VI.2.1 Saturated Zone Modeling

VI.2.1.1 Saturated Zone Flow Model Construction

The transport of radionuclides in the saturated zone away from a repository depends on a wide variety of factors including, but not limited to, ground water and host rock geochemistry; advective ground water velocities; radionuclide concentrations and retardation properties; flux rates of radionuclides from the unsaturated zone; the presence of sorbing materials such as zeolites and clays; rock fracture density; fracture-matrix interaction; future climate changes; and anthropogenic influences. Knowledge of the transport properties in the site-scale and regional flow systems would allow researchers to more completely address four of the most important questions surrounding repository performance and regional ground water flow issues in the area around Yucca Mountain:

- What path would radionuclides from the repository follow?
- How fast and how far would radionuclides travel in the saturated zone?
- Where would radionuclides become accessible to the biosphere?

- What will the concentrations of radionuclides be when they become accessible to the biosphere?

The answer to all of these questions is uncertain. The ability to know or predict the answers to these questions depends on performing sufficient scientific investigations over the study area in order to reduce the associated uncertainties to acceptable levels. Some level of uncertainty will always remain, as it is not possible to completely characterize any underground system.

In order to address these issues, the DOE has performed modeling of the saturated zone at Yucca Mountain at a number of different scales, including: regional, site, and sub-site. The ground water flow modeling activities that are most closely linked to the TSPA-VA are a regional scale model that was developed by D'Agnese et al. (DAG97a), a site-scale model formulated by Zyvoloski et al., (ZYV97), and a sub-site scale model that was completed by Cohen, et. al. (COH97).

The regional-scale 3-D flow model was developed by D'Agnese et al. (DAG97a) to characterize the conditions of the present day ground water flow in the Death Valley region. The modeled area is 244 km long and 229 km wide. The numerical code used for the regional flow model was MODFLOWP (HIL92). MODFLOWP is an adaptation of the U.S. Geological Survey 3-D, finite-difference modular ground water flow model, MODFLOW (MCD88).

A smaller site-scale TSPA three-dimensional flow model was formulated by Zyvoloski et al., (ZYV97) to determine the flowpath from the repository footprint, or outline, at the water table to a distance 20 km downgradient, the approximate distance to the nearest domestic well where ground water is extracted. The computer code FEHM (ZYV83) was used to model an area of 20 by 36 km. Originally, it was intended that the regional scale model be used to provide the boundary conditions for the site scale model. Apparently, the authors of the site-scale modeling (COH97), however, did not believe that the calibration of the regional model was sufficient to provide reliable boundary conditions. Therefore, the regional modeling, from the perspective of the TSPA-VA, was used primarily to determine a ground water flux multiplier for the long-term average and superpluvial climate conditions assumed for the base-case TSPA-VA analysis as will be discussed later in this section.

The sub-site scale model constructed by Cohen et. al. (COH97) was also performed in order to assess the effectiveness of the saturated zone as a barrier to radionuclide transport. However, the sub-site-scale model more accurately captures the faulted and variable-thickness stratigraphy than either the regional or site-scale modeling. Thus, allowing for more detailed modeling of processes that cannot be obtained from larger scale models. As will be discussed later in this section, the sub-site scale model was not as explicitly integrated into the TSPA-VA as the larger-scale models.

Conceptual Model of Saturated Zone Flow

Regional Scale Conceptual Model

The current state of knowledge suggests that ground water beneath the proposed repository moves laterally downgradient until the volcanic aquifer pinches out, at which point it discharges laterally into the alluvial aquifer. Radionuclides dissolved in ground water would potentially follow a similar path. Much of the ground water that enters the alluvial aquifer currently moves southward to the primary discharge location at Alkali Flat. Other actual or potential points of discharge for the system include water wells in the Amargosa Desert and springs in the Furnace Creek Ranch area of Death Valley.

Ground water travel times to any of these locations are not well known. Estimates of ground water travel times can be developed by simple calculations or by more sophisticated numerical modeling. In either case, travel time calculations are based on hydraulic gradient, hydraulic conductivity, and effective porosity of the formation through which the water is flowing. Of these three parameters, hydraulic gradients are probably the best known and most easily measured.

D'Agnese et al. (DAG97a) formulated a conceptual model of the Death Valley regional ground water flow system by integrating interpretations of flow system components. Their discussion of the flow system dynamics includes a description of regional, subregional and sub-basin boundaries, as well as the source, occurrence, and movement of ground water in the system. The most pertinent aspects of that discussion are summarized below.

Flow System Boundaries. The Death Valley regional flow system consists of ground water moving through a three-dimensional body of consolidated and unconsolidated materials. The flow system boundaries may be either physical boundaries, caused by changes in bedrock conditions, or hydraulic boundaries, caused by potentiometric surface configurations. The upper boundary of the flow system is the water table. The lower boundary of the flow system is located at a depth where ground water flow is dominantly horizontal and moves with such small velocities that the volumes of water involved do not significantly impact regional flow estimates. The lateral limits of the regional flow system may be either no-flow or flow boundaries. No-flow conditions exist where ground water movement across the boundary is prevented by physical barriers or divergence of ground water flow paths. Flow boundaries exist where ground water potentiometric gradients permit flow across a boundary through fractures or higher permeability zones.

Regional Boundaries. The lateral boundaries selected for the flow system were modified from those described by Waddell et. al. (WAD84). Most system boundaries are no-flow boundaries that result from the presence of low-permeability bedrock. Flow boundaries occur where bedrock has a high enough permeability to allow significant ground water fluxes to enter the system and where a hydraulic gradient exists across the boundary. Faulting and fracturing most frequently cause the enhanced permeability, and ground water flow may occur at various depths through open regional fracture zones. Based on potentiometric and hydrogeologic framework data, areas where inflow may occur from are Pahranagat Valley, Sand Spring Valley, Railroad Valley, Stone Cabin Valley, Ralston Valley, Fish Lake and Eureka Valleys, Saline Valley, Panamint Valley, Pilot Knob Valley, and Soda Lake Valley. Good estimates of flow across these lateral flux boundaries do not exist except for Pahranagat Valley, which has been estimated by Winograd and Friedman (WIN72) to be approximately 20,000 m^3/d. The remaining areas have very little data required to estimate flux volumes; however, the authors (DAG97a) believe that flux across these boundaries should not be dismissed without further investigation.

The flow system boundary in northern Las Vegas Valley near Corn Creek Springs results from the presence of a ground water divide. Ground water recharging from the Sheep and Spring Mountains forms a ground water divide that extends across the valley and separates flow that moves southeast toward Las Vegas Valley from flow that moves to the northwest toward Ash Meadows in the Amargosa Valley.

For numerical simulation, the flow system was subdivided into three subregions that represent the areas where regional ground water flow moves from recharge areas in Nevada toward Death Valley saltpan, the ultimate terminus of the system. Local recharge along the southern boundary of the system and subsurface inflows along parts of the southeastern and southern boundary of the system were not included in the simulation. These model boundaries are based on previously defined flow system boundaries, the potentiometric surface developed for their modeling study, and the hydrogeologic framework. The authors (DAG97a) comment that few data exist that would allow a precise definition of the western and southern extent of the flow system. The western boundary of the flow system is placed to coincide with the eastern edge of the Death Valley saltpan, which is interpreted as the terminal sink of the flow system. Although some ground water that originates on the west side of Death Valley may discharge into the saltpan, this discharge is mostly at Mesquite Flat and is a small volume compared to the contribution from the east (PRU93).

Subregional Boundaries. To define the subregional boundaries, the Death Valley regional ground water flow system was divided into three major subregional flow systems. The names of the subregions reflect the part of Death Valley into which each discharges. For example, the Northern Death Valley subregion discharges into the northern part of Death Valley at Grapevine and Staininger Springs and Mesquite Flats. The Central Death Valley subregion predominantly discharges into the Saratoga Springs area at the southern terminus of Death Valley.

Ground water is thought to flow across the subregional boundaries in three places: (1) across the southeast border of the Central Death Valley subregion from the Amargosa Desert into the Lower Amargosa Valley in the Southern Death Valley subregion; (2) from the Northern Death Valley subregion across a boundary at Salt Creek Springs (just south of Mesquite Flat) into the Central Death Valley subregion; and (3) at the southern end of Death Valley, ground water that has not discharged in the Saratoga Springs area may continue to flow northward from the Southern Death Valley subregion across the subregion boundary to discharge at Badwater Basin in the Central Death Valley subregion.

Numerical Modeling Difficulties and Simplifying Assumptions. The authors (DAG97a) pointed out that previous studies by Prudic et. al. (PRU93) and Waddell (WAD82) showed that it is difficult to utilize computer models to effectively describe ground water flow in an area as geographically large and geologically complicated as the Death Valley region. Prudic et. al. (PRU93) reiterated that many arguments can be invoked concerning the validity of the assumptions and hydrologic values used in simulating ground water flow when such complex geology and hydrology are involved.

In any modeling investigation, it is inevitable that simplifications and assumptions must be used to adapt the complex conceptual model for numerical simulation. The assumptions and simplifications used to develop the Death Valley Regional Flow System (DVRFS) model include the following:

- Ground water in the region flows through fractured volcanic and carbonate rocks, as well as in porous valley-fill alluvium. However, fracture flow simulation is impractical at a regional scale, and, therefore, a porous medium simulation is used. Zones of high hydraulic conductivity are used to account for highly faulted and fractured regions.

- Hydraulic conductivities within each model cell are assumed to be homogeneous and horizontally isotropic. Thus, features smaller than the grid cells are not represented. The authors (DAG97a) believe that this approach is likely to produce reasonable approximations to large-scale flow patterns. Small-scale flow paths, however, are not represented.

- The system can be represented adequately as steady state. Four conditions exist that may violate this assumption. First, the regional flow system still may be undergoing a drying-out sequence following a wetter climate cycle related to the late Pleistocene (PRU93). As a result, current ground water levels and discharge rates may not be in equilibrium with present-day recharge and interbasinal flux rates. Second, and perhaps more important, ground water withdrawals by wells for domestic, municipal, mining and irrigation uses are imposing new stresses on the present-day system. This pumpage is derived initially from ground water, from storage, and subsequently from capture of natural discharge. Incorporating pumping in a steady-state model omits the possibility of deriving water from storage, so that water flowing to wells must be offset by capture of natural discharge, that is, reductions in discharge or induced inflow. Although a transient simulation beginning at predevelopment conditions would avoid this assumption, additional assumptions would be needed to define historic pumping levels. In addition, some current water-level data and some spring-flow rates already reflect changes to the system resulting from development, suggesting that the DVRFS may have already adapted to these changes. For example, the springs at Pahrump Valley, including Manse and Bennetts Spring, have ceased to flow in historic time. Third, the flow system experiences seasonal fluctuations that are not simulated. A resulting annual average condition is simulated. Fourth, hydraulic-head, spring-flow and other data used in model calibration were collected over an interval of many years, and these data are affected by seasonal and yearly changes to the ground water flow system.

Site-Scale Conceptual Model

The major components of the site-scale conceptual model (ZYV97) are presented below.

Geologic Setting. The conceptualization of the geologic setting by Zyvoloski et al., (ZYV97) which, briefly summarized, is that Yucca Mountain is located in the Great Basin section of the Basin and Range physiographic province, and consists of a group of north-south-trending block-faulted ridges that are composed of volcanic rocks of Tertiary age that may be several kilometers thick. The basin to the west of Yucca Mountain is Crater Flat, which is comprised of a thick sequence (about 2,000 m) of Tertiary volcanic rocks, Tertiary and Quaternary alluvium, and small basaltic lava flows of Quaternary age. Crater Flat is separated from Yucca Mountain by the Solitario Canyon Fault. West of Crater Flat is Bare Mountain, which is comprised of Paleozoic and Precambrian rocks. Fortymile Wash, a structural trough, delimits the eastern extent of Yucca Mountain. East of Yucca Mountain are the Calico Hills, a mottled assemblage of Tertiary volcanic rocks and Paleozoic rocks. Yucca Mountain terminates to the south in the Amargosa Desert, which consists of interbedded Quaternary and Tertiary alluvial, paludal, and tuffaceous sediments.

These rocks and deposits in the vicinity of Yucca Mountain were classified by the authors (ZYV97) into hydrogeologic units based on hydraulic properties. Where possible, hydrogeologic units identified by previous investigators (LUC96, WIN75) were used. Many of the units are not present in the model area and/or are not expressed at the land surface. In all, sixteen hydrogeologic units are present in the model area.

In general, the hydrogeologic units at Yucca Mountain form a series of alternating volcanic aquifers and confining units overlaying the regional carbonate aquifer. The volcanic aquifers and confining units interbed with undifferentiated valley-fill and the valley-fill aquifer to the south, while structural features delimit the eastern and western edges of Yucca Mountain.

Hydrogeologic Setting. The hydrogeologic framework briefly described by the authors (ZYV97) is that Yucca Mountain is centrally located within the Death Valley ground water basin and also is centrally located within the Alkali Flat (Franklin Lake playa)-Furnace Creek subbasin. The subbasin is assumed to receive water from areal recharge within its boundaries and the authors (ZYV97) believe that it probably also receives water as underflow from adjoining subbasins. Depths to water range from about 3 m beneath Alkali Flat (Franklin Lake playa) to about 750 m beneath Yucca Mountain. Ground water beneath Yucca Mountain flows generally toward the south through fractured volcanic rocks which interfingers with Quaternary and Tertiary valley-fill in the Amargosa Desert.

The climate is arid to semiarid, with Yucca Mountain receiving annual precipitation between 150 mm to 200 mm (HEV92). As a result, stream flow is infrequent and occurs following intense precipitation events which can be very localized. There are no perennial streams.

Vertical Gradients. As is discussed later in this section, the ability to reproduce and understand the vertical flow gradients between hydrostratigraphic units will be an important aspect of model calibration. Therefore, the authors (ZYV97) believe it is important to include them as an explicit component of the conceptual model. The authors (ZYV97) remark that Luckey et. al. (LUC96) examined the vertical relationship of hydraulic head at Yucca Mountain, and found "no unambiguous areal patterns in the distribution of vertical hydraulic gradient around Yucca Mountain." However, they also make the following generalizations as to the distribution of potentiometric levels in the lower sections of the volcanic rocks. Potentiometric levels in the middle volcanic confining unit are relatively high (altitude greater than 750 m) in the western and northern parts of Yucca Mountain and are relatively low (altitude about 730 m) in the eastern part of Yucca Mountain. Based on potentiometric levels that were measured in borehole UE-25 p#1, the potentiometric levels in the middle volcanic confining unit in boreholes USW H-l, USW H-3, USW H-5, and USW H-6 may reflect the potentiometric level in the carbonate aquifer. It is also noted that boreholes UE-25 b#1 and USW H-4 do not seem to fit the pattern established by the other boreholes. Potentiometric levels generally are higher in the lower intervals of the volcanic rocks than in the upper intervals, indicating a potential for upward ground water movement. However, for unknown reasons, at four boreholes (USW G-4, USW H-1, USW H-6, and UE-25 b#1) potentiometric levels in the volcanic rocks are higher in the uppermost intervals than in the next lower intervals.

The potentiometric levels in the Paleozoic carbonate aquifer at borehole UE-25 p#1 are about 21 m higher than in the overlying volcanics. Therefore, a potential for upward ground water movement from the Paleozoic rocks to the volcanic rocks is indicated. Because of the large difference in potentiometric levels in these two aquifers, Luckey et. al. (LUC96) conclude that they seem to be hydraulically separate. This conclusion appears to be supported by hydrochemical data. However, some of the analyses of hydraulic-test data at the C-hole complex indicate a possible hydraulic connection between the volcanics and the carbonate aquifer at the C-hole complex (GEL96). Hence, the vertical hydraulic gradients represent a complex three-dimensional flow system that is not completely understood. Little information is available for vertical gradients away from Yucca Mountain. A more detailed discussion of data limitations and modeling needs will be presented later in this section.

Steady-state Conditions. A comprehensive analysis of water levels from all observation wells at Yucca Mountain (GRA97) shows the fluctuations of water levels for the period 1985 to 1995. The authors (ZYV97) concluded that, in general, most wells at Yucca Mountain show less than 1 meter difference between the maximum and minimum values of water-level altitude during this period. The authors (ZYV97) further conclude that the preponderance of wells with small water level changes and the small fractional changes in saturated thickness at wells with greater changes indicates that assuming that the flow system is at steady state at Yucca Mountain is a reasonable approximation. It should be noted that the modelers simulating the regional scale model (DAG97a) expressed some concern with assuming that the system is or would remain at steady state, and outlined four conditions that exist which may violate this assumption.

Zyvoloski et al., (ZYV97) do discuss, however, that water-level changes have declined by as much as about 10 m (KIL91) in the Amargosa Farms area (southwest comer of the site model) resulting from ground water withdrawals for irrigation. The modelers made no attempt to reconstruct the potentiometric surface for conditions prior to these ground water withdrawals. The potentiometric data dictate a complex three-dimensional flow system, but the authors (ZYV97) have made the following generalizations. There appears to be a general upward gradient from the regional carbonate aquifer into the volcanic rocks. In general, this upward gradient persists in the volcanic rocks. Furthermore, the potentiometric data indicate that most of the flow system is essentially at steady state.

Potentiometric Surface. Because the potentiometric data dictate a complex three-dimensional flow system, a number of different conceptual models of the flow system are possible. In particular, the different conceptual models may result in different potentiometric surfaces. Although the boreholes are open at different depths below the hydraulic head and are open to different geologic zones, water levels in most of the wells appear to represent a laterally continuous aquifer system. The well-connected system may result from the presence of many faults and fractures (TUC95), and, at the scale of the site model, the authors (ZYV97) believe that the ground water flow system may behave as a porous medium. Flow in the volcanic rocks occurs primarily in fractures and secondarily in the matrix of the rock. Therefore, the uppermost aquifer may be unconfined or confined depending upon the areal location of the point being measured (TUC95).

Most of the wells only partially penetrate the hydrogeologic units. This can be important during model calibration because it can lead to significant errors if vertical gradients are large. No attempt was made by the modelers to segregate and analyze water-level measurements associated with specific hydrogeologic units or fracture zones. The authors (ZYV97) believe, however, that the potentiometric surface is probably a reasonable representation of the water table for the following reasons: (1) At Yucca Mountain, water levels at most wells were obtained from the uppermost part of the saturated zone (GRA97); (2) south of Yucca Mountain, wells penetrate a significant thickness of the saturated zone, but in this area most ground water flow is believed to be horizontal and all available data indicate that the vertical-head gradients are negligible; (3) for the case of wells having multiple piezometers, only water levels from the uppermost saturated interval were used in the construction of the potentiometric-surface map.

Large Hydraulic Gradient. Possible differences in conceptual models of the flow system pertain to the representation of an apparent large hydraulic gradient (LHG) on the north end of Yucca Mountain, an area where the altitude of the potentiometric surface appears to change by about 300 meters over a lateral distance of 2 kilometers (CZA94, CZA95). Prior to the construction of borehole USW G-2 in 1981, no water-level data existed at Yucca Mountain on which to base the LHG. As more boreholes were constructed at Yucca Mountain, particularly holes UE-25 WT#6 and UE-25 WT#16, a somewhat better definition of the LHG developed.

On a regional basis, other large hydraulic gradients are associated with a contact in the Paleozoic rocks between clastic rocks and regional carbonate aquifer; however, the cause and nature of the LHG near Yucca Mountain is not clear. Proposed explanations include: (1) faults that contain nontransmissive fault gouge (CZA84); (2) faults that juxtapose transmissive tuff against non-transmissive tuff (CZA84); (3) the presence of a different type of lithology that is less subject to fracturing (CZA84); (4) a change in the direction of the regional stress field and a resultant change in the intensity, interconnectedness, and orientation of open fractures on either side of the area with the LHG (CZA84); or (5) the apparent large gradient actually represents a disconnected, perched or semi-perched water body so that the high water-level altitudes are caused by local hydraulic conditions and are not part of the saturated-zone flow system (CZA94, ERV94). Fridrich et. al. (FRI94) suggest two hydrogeologic explanations for the LHG: (1) a highly permeable buried fault that drains water from tuff units into a deeper regional carbonate aquifer, or (2) a buried fault that forms a “spillway” in the volcanic rocks. Their second explanation, in effect, juxtaposes transmissive tuff against non-transmissive tuff, and is therefore the same as (2) above. Explanation (5) differs from the others in that it does not require a permeability contrast to represent the large gradient, because the LHG is absent, and actually represents a disconnected, perched or semi-perched water body.

For the site-scale model, explanation (1): faults that contain nontransmissive fault gouge was used to represent the LHG using reasonable permeability values by imposing a vertical barrier to horizontal ground water flow. Several of the other alternatives were tested by the modelers but did not yield satisfactory results.

Hydraulic Properties. Knowledge of hydraulic properties is critical to understanding the hydrogeology of Yucca Mountain and is required for numerical models. The authors (ZYV97) obtained information on the hydraulic properties from the following sources: (1) previously published hydraulic analyses for wells at Yucca Mountain conducted during the 1980s; (2) published hydraulic properties for hydrogeologic units obtained beyond the immediate Yucca Mountain area; and (3) recent (1995-97) hydraulic analysis of wells USW WT-10, UE-25 WT#12, and USW SD-7 (OBR97), UE-25 c#1, UE-25 c#2, UE-25 c#3, and USW G-2.

Aquifer tests. Several aquifer tests were conducted in Yucca Mountain boreholes during 1995 and 1996. Single borehole, composite interval tests resulted in transmissivity (i.e., hydraulic conductivity multiplied by thickness) estimates in boreholes USW WT#10, UE-25 WT#12, and USW G-2. The middle volcanic aquifer was the primary hydrogeologic unit tested in boreholes USW WT#10 and UE-25 WT#12. Transmissivity in these boreholes ranged from 7 to 1,800 m^2/day (OBR97). The upper volcanic confining unit was tested in USW G-2 and the mean transmissivity was 9.4 m^2/day. Transmissivity was reported for these boreholes because composite intervals were tested and the thickness of water-producing intervals was unknown. Hydraulic-conductivity estimates obtained from these transmissivity estimates would probably understate the actual hydraulic conductivity because the entire interval thickness does not contribute water to the borehole. Hydraulic properties obtained from single-borehole aquifer tests generally represent flow conditions within tens of meters of the borehole. Given the large degree of heterogeneity in the Yucca Mountain area, individual single-borehole aquifer-test results are not directly appropriate for the scale represented by the site model (kilometers).

Preliminary aquifer tests were conducted at the C-well complex during 1984. Horizontal hydraulic conductivity was about 0.15 m/d in the upper volcanic confining unit and ranged from 3 to 30 m/d within the middle volcanic aquifer (GEL96). Cross-hole aquifer tests during 1995-96 in the C-well complex also resulted in transmissivity and hydraulic-conductivity estimates. During these tests borehole UE-25 c#3 was pumped and boreholes UE-25 c#1, UE-25 c#2, UE-25 ONC-1, USW H-4, and UE-25 WT#3 were used as observation wells. The lower Bullfrog Tuff is the most transmissive interval within the middle volcanic aquifer and hydraulic conductivity range from approximately $1x10^{-5}$ to $7x10^{-4}$ meters per second in the observation boreholes (GEL97).

Hydraulic properties obtained from the cross-borehole aquifer tests at the C-hole complex represent flow properties between the tested boreholes. As such, they may be more appropriate for the scale of the site model than those obtained from single-hole tests. There is evidence that this area has extensive fractures that enhance the transmissive properties of the aquifer system. Northerly and northwesterly trending high angle faults such as the Paintbrush Canyon, Midway Valley, and Bow Ridge Faults have brecciated, offset, and tilted the tuffaceous rocks in the vicinity of the C-hole complex. Extensive tectonic and cooling fractures have been identified in the C-hole complex boreholes (GEL96). The relatively high transmissive properties obtained from C-hole testing are probably due to the intensity of fracturing in this area and may not be representative of the entire Yucca Mountain area.

<u>Recharge</u>. The authors (ZYV97) assumed that recharge to the model area is from the following sources: (1) downward and possible lateral recharge from episodic flooding of Fortymile Wash; (2) throughflow from Pahute and Rainier Mesas, which is hypothesized to result in recharge along the northern border of the study area; (3) throughflow from the northwestern part of the Amargosa Desert; (4) minor recharge from episodic flooding of the Amargosa River channel; and (5) net infiltration from precipitation events. Fortymile Wash is a major southward-draining ephemeral channel located adjacent to Yucca Mountain and it is thought to contribute intermittent recharge to the saturated zone. Water levels in UE-29 a#1 and UE-29 a#2 are affected periodically by streamflow events in Fortymile Wash and Pah Canyon Wash. In various numerical ground water flow models (CZA84, RIC84, CZA85, SIN87), recharge had to be specified in Fortymile Wash to replicate potentiometric levels. Czarnecki and Waddell (CZA84) simulated a flux in Fortymile Wash of 22,140 m^3/d or 256 kg/s. Based on geomorphic/ distributed-parameter simulations, Osterkamp et. al. (OST94) estimated recharge along the entire 95-km length of Fortymile Wash to be about $4.22x10^6$ m^3/year or 134 kg/s. Based on field studies of stream loss, the total recharge in Fortymile Wash is estimated as 0.86 kg/s. Savard acknowledges that this estimate would represent a minimum value based on the inability to account for all reaches of Fortymile Wash, which may have received unobserved runoff and recharge, coupled with the minimum period of streamflow observations.

<u>Discharge</u>. The authors (ZYV97) believe that no natural discharge occurs within the model domain. The nearest natural discharge areas connected to the saturated-zone flow system

beneath Yucca Mountain are Franklin Lake playa (also known as Alkali Flat) and possibly the major springs at Furnace Creek Ranch and the valley floor of Death Valley. Although most models of the region (DAG97a, RIC84, CZA84) require a ground water flow path from Yucca Mountain to Death Valley, Czarnecki and Wilson (CZA91) postulate that a ground water flow path from Yucca Mountain to Death Valley (by way of the Amargosa Desert and the Funeral Mountains) was unsubstantiated (but not inconsistent with) with available data. They suggest that ground water from Yucca Mountain ultimately discharges at Franklin Lake playa through evapotranspiration (CZA90).

Discharge through ground water withdrawals occurs within the model domain in the Amargosa Desert for agricultural and domestic use. This discharge, which was estimated in the USGS regional flow model at about 6,300 m^3/d, occurs mostly in the southwestern corner of the model domain. The authors (ZYV97) believe that this discharge may be responsible for the southwestwardly oriented gradient which appears to have persisted since the 1950s (KIL91).

Numerical Modeling Difficulties and Simplifying Assumptions. In the site-scale modeling, the following assumptions are applicable (ZYV97):

- The hydrogeologic framework is an appropriate description of the principal hydrogeologic units and faults.
- Permeability is invariant within each hydrogeologic unit.
- Ground water flow occurs in three dimensions and within the rock mass (which includes both rock matrix and fractures).
- Ground water flow system is isothermal at 44°C (the effect of this assumption was tested by simulating the system at 20°C).
- Hydraulic heads of the potentiometric surface along the north, south, east, and west edges of the modeled area are an appropriate data set for specifying boundary conditions along the sides of the model.
- The system is at steady state so that ground water flow into and out of the flow domain is invariant with time.
- Volumes associated with the finite-element mesh are sufficiently large so as to exceed the representative elementary volume necessary to simulate fracture flow as porous-media flow.

- A no-flow boundary at the base of the model approximates hydrologic conditions.
- The large hydraulic gradient is part of the saturated zone and not an artifact of perched-water occurrence.
- Recharge is assumed to occur only at the top of the model along upper Fortymile Wash; all other nodes on the top of the model are specified as a no-flow boundary.

Assumptions 5 and 8 are not and have not been supported by field data. The authors (ZYV97) found, however, that they both represent an expedient means to assign boundary conditions, which may have affected model calibration. Additional discussion of the site-scale model calibration is presented later in this section.

Sub-Site Scale Conceptual Model

DOE's sub-site-scale conceptual model of the saturated zone at Yucca Mountain scale model also places the saturated zone within a sequence of dipping and faulted tertiary volcanic rocks, underlain by Paleozoic carbonates at depths greater than 1200 meters beneath the water table. The sub-site scale conceptual model, however, places considerably more emphasis on the effects that faults will have on ground water flow than either the regional or site-scale models, as discussed below.

The volcanic rock sequence is comprised of variable thickness tuffs, lava flows, and volcanic breccias. Water levels in boreholes in the immediate area around Yucca Mountain are generally either within or below the Topopah Spring Tuff. Borehole flow meter surveys show that discrete fractured zones are the dominant pathways for saturated zone flow. More than 90% of pumped flow commonly emanates from discrete zones within densely welded sections of tuff, typically located in the central section of a particular unit. Fluid originates from fault zones and other intervals in some boreholes. The high permeability of the densely welded tuff is due to the high density of cooling joints, which generally form a fractured zone subparallel to dip. The Prow Pass, Bullfrog, and Tram Tuff each exhibit moderate to densely welded mid-sections, and are the most permeable units within the saturated tuffs. Non-welded tuff has relatively few open fractures, and is therefore less permeable. These sections are situated above and below the more densely welded intervals within each geologic unit, thereby producing a layered permeability heterogeneity. In addition, the dipping and faulted hydrostratigraphic units produce a heterogeneous distribution of rock units at the water table. The fate of potential radionuclides reaching the water table is therefore a function of the infiltration source in addition to the flow within the saturated zone.

Faults that displace stratigraphic units are pervasive at Yucca Mountain (DAY96). The dominant fault set is composed of steeply dipping normal faults which have offsets on the order of hundreds of meters and which are laterally continuous for kilometers. These faults are north-trending and exhibit a surface spacing of approximately 1 km. When stratigraphic units are displaced by faults, abutment of high permeability intervals against lower permeability intervals can result. In this case, fluid pathways may diverge in three dimensions due to the presence of low permeability structures. If fault zones exist, due to the presence of brecciated rock, for example, they could provide the vertical pathways that link the displaced high permeability zones. Conversely, mineralization within a fault zone may create a flow barrier if a high permeability unit is not made discontinuous by the fault. In either case, fault displacements produce discontinuities in stratigraphic units, which produce large scale permeability heterogeneity. Northwesterly-striking faults with offsets on the order of meters to tens of meters may introduce similar, yet smaller heterogeneities within the blocks bounded by normal faults.

Fluid between faults may be effectively isolated and have travel times orders of magnitude larger than surrounding areas (flow stagnation), a feature suggested by some geochemical data. Such a phenomenon would enhance the storage capability of portions of the saturated zone. The very low horizontal gradient downstream of the repository may be the result of barrier faults or divergence of flow upstream. West of Solitario Canyon Fault water elevations range from 775-780 m above sea level and the hydraulic gradient ranges from 0.02-0.04 (TUC95). Ervin et al. (ERV94) interpreted water to be mounded against the west side of the fault and a splay of the fault. They attributed the influence of the fault to a low permeability fault gouge. However, faults that simply displace units and that do not possess internal permeability may also have considerable effect on flow geometry. Some fault zones may be infiltration sources at the water table, and thereby influence the potential source locations of radionuclides at the water table.

Several researchers have proposed that the high temperature anomalies observed at the water table near the Solitario Canyon and Paintbrush Canyon faults may be due to upwelling of warm water through permeable fault zones that extend into the Paleozoic formations (SZY89). This upwelling could result in dilution of radio nuclides because of the introduction of additional fluid into the tuff aquifer. Conversely, the upwelling could restrict vertical mixing. Vertical flows may also be caused by the large-scale geologic heterogeneity described above. Geologic units have different thermal conductivities, and these differences coupled with the faulted structure could also be a contributing factor to the observed water table temperature anomalies (COH97).

In general, the large-scale heterogeneity created by superposition of the multiple sub-horizonal flow zones, displacement of strata by faults of varying hydrologic properties, and variable thickness and dipping geologic units will result in a complex 3-dimensional flow geometry. Actual flow directions at depth are very likely different from those inferred from water table elevations. In summary, saturated zone flow is affected by (1) the presence of high- and low-permeability faults which offset hydrogeologic units sub-vertically; (2) the heterogeneous permeability distribution within geologic units; (3) the variation of dip and thickness of strata; (4) the heterogeneous permeability distribution at the water table; (5) the distribution of infiltration from the unsaturated zone; and (6) the three-dimensional channelization, hydrologic mixing and dilution produced by the above mechanisms. In addition, saturated zone flow could be affected by upwelling or convection in faults, if faults are connected hydraulically to the Paleozoic units.

Computer Code Selection

Regional Flow Model

The computer code selected by D'Agnese et. al. (DAG97a) to perform the regional flow modeling is MODFLOWP (HIL92). As documented by Hill (HIL92), MODFLOWP is an adaptation of the U.S. Geological Survey 3-D, finite-difference modular ground water flow model, MODFLOW (MCD88) in which nonlinear regression is used to estimate flow-model parameters that result in the best fit to measured hydraulic heads and flows.

MODFLOWP is a block-centered finite-difference code that views a 3-D flow system as a sequence of layers of porous material organized in a horizontal grid or array. The horizontal grid is generated by specifying array dimensions in the x and y dimensions.

Flow between cells in each model layer is controlled by user supplied transmissivity values. Similarly, flow between the layers is controlled by user supplied values of vertical transmission or leakage.

The remainder of the model inputs describing boundary conditions, recharge, evapotranspiration, spring flow and well discharge are specified using arrays or lists of row-column cell locations. The model calculates ground water heads based on the model boundary conditions, and transmissivities.

Site-Scale Flow Model

To model the saturated-zone flow system at the site scale at Yucca Mountain, several simulation capabilities were considered important, including the ability to: (1) simulate 3-D transient ground water flow and heat transport, including 3-D representation of spatially variable permeability, porosity, and thermal conductivity; (2) allow specification of constant pressure, constant hydraulic head, constant fluid and heat flux boundary conditions; (3) represent discontinuous, irregularly shaped 3-D hydrogeologic units; (4) permit specification of dual permeability and porosity representing both fracture and matrix flow; (5) represent hydraulic-head and temperature observation points where they occur in 3-D space; (6) calibrate the model with respect to observations of hydraulic head and temperature through the use of automated parameter estimation techniques; and (7) directly interface the resulting flow model with radionuclide transport models used in Performance Assessment of the Yucca Mountain site. This list includes features of the model not used in the present report, but important for anticipated modeling efforts. The FEHMN simulation code was selected because it possessed these capabilities when coupled with the mesh generation software, GEOMESH (described later in this report), and with the model-independent parameter estimation software, PEST (also described later in this report). The following section discusses the theory for many aspects of FEHMN.

The FEHMN (Finite Element Heat Mass Nuclear) computer code is capable of simulating flow and transport through both the unsaturated and saturated zones. FEHMN is a non-isothermal, multiphase flow and transport code. It can simulate the flow of water and air, and the transport of heat and contaminants, in 2- and 3-D saturated or partially saturated, heterogeneous porous media. The code includes comprehensive reactive geochemistry and transport modules and a particle tracking capability. Fractured media can be simulated using an equivalent continuum, discrete fracture, dual porosity or dual permeability approach. The basic conservation equations, constitutive relations and numerical methods are described in Zyvoloski (ZYV83), Zyvoloski (ZYV86), Zyvoloski and Dash (ZYV90), Reeves (REE94), and Zyvoloski et. al. (ZYV95).

Sub-Site-Scale Flow Model

Modeling at the sub-site scale uses the integral finite difference simulator TOUGH2 (PRU87). TOUGH2 can simulate non-isothermal flow and transport in single and dual-porosity media. TOUGH2 utilizes an integral finite difference formulation, which, in part, enables construction of a mesh with highly variable gridblock geometries that are necessary to properly represent the geologic structure.

Layering and Gridding

Regional Flow Model

DOE's regional flow model developed by D'Agnese et. al. (DAG97a) used 163 rows, 153 columns and 3 layers. The 78,817-cell model is oriented exactly north-south. Grid discretization along both rows and columns was set to 1,500 m. The three model layers represent hydrogeologic units at 0-500 m, 500-1,250 m, and 1,250-2,750 below the interpreted water table; which are 500, 750, and 1,500 m thick. The first and second model layers are interpreted as simulating local and subregional flow mostly within valley-fill alluvium, volcanic rocks and shallow carbonate rocks; the third layer is interpreted as simulating regional flow in the volcanic, carbonate and clastic rocks. The authors (DAG97a) also point out that the use of only one model layer to represent each of the local, subregional, and regional flow paths may potentially result in model error in areas of significant vertical flow, particularly if the vertical flow component is somewhat complicated.

Site-Scale Flow Model

The site model area is 1,350 km^2 and extends 30 km west to east, and 45 km north to south. The model used a detailed three-dimensional hydrogeologic framework model (HFM) to characterize the heterogeneous, porous, and fractured media beneath Yucca Mountain. This approach is different from the regional model in that rather than inserting hydraulic properties into directly into the numerical mesh, the HFM model was first developed so that it could be converted into a tetrahedral mesh, using GEOMESH (GAB96).

The site-scale finite-element mesh is spaced at 1,500 m and consist of 9,279 nodes. The authors (ZYV97) note that this is a very coarse resolution and is only suitable for initial calibration of a preliminary flow model. For example, the upper volcanic confining unit is much more extensive in the model than in reality. Because of the coarse grid increment, offsets across faults are also much less abrupt in reality.

The authors (ZYV97) indicate that a 250-m sampled mesh is planned for the future with improved error checking, which will improve the quality of both the framework model and the numerical grid based on the framework model.

Sub-Site-Scale Flow Model

The model extends 10 km eastward and 15 km northward. However, it covers an area of 108 km^2 because it is not a rectangle. The horizontal mesh has 1993 gridblocks. There are currently 23 model layers that define different hydrostratigraphic units. Including fault gridblocks, the total number of gridblocks is approximately 50,000. Gridblock sizes are highly variable, mostly ranging in size from approximately 50 to 500 m on a side; several approach 1 km^2 near model boundaries. The locations of boreholes correspond to the gridblock nodal points, making conditions at the particular borehole correspond directly to conditions in the gridblock. Horizontal dimensions of fault gridblocks are approximately 150 m x 150 m. These dimensions do not represent the actual fault zone width, but rather are the gridblock dimensions over which fault zone properties are averaged. (Note that for the pure displacement conceptualization of modeled faults, the fault zone is given properties corresponding to the hydrostratigraphic units on either side of the fault, and thus the fault effectively has no width whatsoever.)

The finely discretized region near the center of the sub-site-scale domain corresponds to the area near the C-hole complex, borehole P#1, and borehole ONC#1. This area was finely discretized because transient hydraulic tests can be simulated in this area to design future hydrologic tests and simulate smaller-scale flow processes and effects.

The northernmost model area corresponds to the location of the large hydraulic gradient (FRI94). Several conceptual models have been proposed to explain this feature (e.g., FRI94, BOD96). The hydrogeologic structure beneath the water table in this area is poorly understood, and the authors (COH97) believe that different hypothetical models should be tested by numerical simulation to more fully constrain the possible causes.

The water table defines the top of the model. Use of this surface assumes that the water level measurements in borehole G-2 and WT-6 represent a water table, although two- and three-dimensional simulations of flow geometry do not include the large gradient zone. By defining the top of the model by these water levels, the model can also be modified to simulate perched water in that area. The bottom of the model is defined by the base of the Lithic Ridge Tuff. This unit is a thick confining structure that separates the Crater Flat Tuff aquifer and the lower carbonate aquifer. The higher head anomaly observed in UE-25p#1 deemed indicative of the Paleozoic formation actually first appeared in the older unnamed tuffs just beneath the Lithic Ridge Tuff and above the Paleozoic carbonates (CRA84). The older tuffs lie beneath the Lithic Ridge Tuff. The isopachs (i.e., thickness) of units beneath the Lithic Ridge Tuff and lower carbonate aquifer are unknown, as only p#1 penetrates the carbonate aquifer. Therefore, an isopach cannot be constructed for these intervals. Using the base of the Lithic Ridge as a lower boundary preserves the lower confining structure and still enables consideration of a higher head boundary condition. In addition, Lithic Ridge is the lowermost unit for which an approximate isopach has been developed (CAR86).

Gridblocks are discretized in a manner that preserved the thickness, orientation, dip, and lateral continuity of strata. The vertical dimension of the model is composed of gridblock layers with variable thickness distributions, which are then concatenated to produce a sequence of layers that correspond to the actual vertical distribution of units observed in boreholes. The lateral continuity of hydrostratigraphic units is thus preserved, which is important since many strata exhibit densely welded, high permeability zones parallel to dip. Displacement by faults is also explicitly considered. The number of model layers in areas between faults remains constant at 23. Because not all geologic units are present beneath the water table, several thin layers are present at the top of the model everywhere and are assigned the properties of the unit at the water table at a particular location. All gridblock nodes in the model are connected vertically to the adjacent node(s) located directly on top and bottom of the same column of gridblocks. The nodes of gridblocks located in regions between faults are also connected laterally to adjacent nodes of the same layer. Fault gridblocks are connected differently, as described below.

The choice and rationale for representing particular faults for the model is described by the authors in a previous report (COH97), a brief summary of which is presented below. Day et al. (DAY96) divide the faults at Yucca Mountain into three main groups. The dominant set is composed of north-trending normal faults that have steep down-to-the-west displacement over most of their length. These faults generally have offsets on the order of hundreds of meters, and define the boundaries of the relatively intact blocks of east-dipping Miocene volcanic strata. They have therefore been termed block-bounding faults. The second set is composed of northwesterly striking strike-slip faults located in the northwest section of the model region. These faults have offsets on the order of meters to tens of meters only. Thirdly, intrablock faults are those not continuous on scales greater than the defined fault blocks and not connected with either set. There are very little data to indicate that the intrablock faults are present below the water table. The linearity and dip of faults with depth, occurrence of fault zones, and fault zone flow properties beneath the water table are mainly unknown. Given the inherent uncertainty of fault properties beneath the water table and the intended modeling objective of investigating the potential effects of the complex geologic structure on flow, only north-trending faults, which have the greatest displacement of any of the fault sets, are considered. Most of these are block-bounding faults. The location of faults comes from the surface location of faults as defined in ISM2.0 (CLA97). Most faults at Yucca Mountain have steep dips on the order of 80°; therefore the general fault structure in the model is preserved by assuming vertical faults.

All faults can be assigned a fault zone with particular flow properties or can simply be treated as displacement-only faults. The gridding scheme enables hydrostratigraphic unit displacement across the fault to be considered realistically, as described above.

Initial and Boundary Conditions

Regional Flow Model

Specified-head boundary conditions surrounding the entire model are based on interpolation of measured head data. The slope of the potentiometric surface toward the southwest may be indicative of ground water withdrawals that were not specified in the model. Discharge by pumping wells occurs in the Amargosa Desert in the southwest part of the model domain, but this pumping was not explicitly represented in the model. However, the influence of these well withdrawals is implicitly reflected in the specified-head lateral boundary conditions applied along the southern boundary of the model. No-flow boundary conditions were specified along the base of the model. Specifically, the model boundaries used for the regional study are the following:

- In layer one, all lateral boundaries were designated as no-flow except along the western boundary at Death Valley, where constant head boundaries are designated at Cottonball, Middle and Badwater Basins, and Saratoga Springs. Head values along this boundary were defined using the potentiometric-surface map developed for the modeling study and reflect the nearly perennial ponds supported by ground water flux out of the system.

- In layer two, all lateral boundaries were designated as no-flow because at these depths flow is believed not to cross the lateral boundaries.
- In layer three, the lateral boundaries were designated as no-flow except at flow locations along the northern and eastern boundaries. These were assigned constant-head values to reflect possible or perceived interconnections along buried high transmissivity structural features with regional flow paths in adjacent valleys outside the model domain. The head values were selected to correspond to measured water levels.

<u>Site-Scale Flow Model</u>

A key concern addressed in the site-scale flow modeling is the compatibility of the regional flow model and the site-scale flow model. Although, ideally, the output from the larger-scale regional model would be used as direct input for the boundary conditions to the site model, the authors (ZYV97) point out several factors, however, that make such an interface impractical. First, the geologic model is defined in more detail at the site scale, so an exact piecing together of the models is impossible. Second, the regional model, focusing on larger-scale issues, does not have a detailed representation of geology near the site and does not attempt to include features such as the large hydraulic gradient in the calibration. Because of these differences, the models are compared with each other for consistency, rather than coupled more directly.

Hydraulic-head data are considered to be more accurate than flux data within the site model, and for that reason were chosen for specifying boundary conditions for the model despite the influence that such a constant-head boundary is likely to have on a model being calibrated to hydraulic-head observations. Specified-head boundary conditions are based on the potentiometric surface that includes the large hydraulic gradient. However, no measured vertical head distributions at the boundaries of the model exist. The regional model (DAG97a) does provide coarse estimates of vertical hydraulic head, but these were not used in assigning the boundaries at the site model. An appropriate set of hydraulic-head values on the outside nodes of the model consistent with the potentiometric-surface data was computed for use in specifying constant hydraulic-head boundary conditions.

Improving the representation of the lateral boundary conditions is considered by the authors (ZYV97) to be of primary concern for future modeling efforts. Alternate ways to specify boundary conditions within the site model exist. These include but are not limited to: (1) specifying constant heads only along the top edge of the model (this was not done because no flow would be allowed at the remaining nodes along the sides); (2) specifying flux explicitly (this was not done because of the difficulties in redistributing flux from the regional model onto the

sides of the site model); or (3) projecting hydrostatic head from the top edge down the outside faces of the model (this was not selected because it forces flow to be horizontal).
As noted previously, one concern with specifying hydraulic heads on all model sides, while calibrating using hydraulic heads within the model, is that the specified heads are likely to dominate the simulated heads at the observation locations. The severity of this problem was tested in independent numerical experiments using a model developed by Sandia National Laboratory of a subdomain that included Yucca Mountain. The results indicated that specified pressure (constant head) boundary conditions could be applied while still observing changes in model simulated pressures as a result of changes in model permeability values. Because the site model covers a substantially larger area than that of the Sandia model, application of specified head boundary conditions was considered to be less of a constraint. However, the use of any specified-head boundary condition will have some constraint on model calibration. As a result, the fluxes in and out of the model will have to be checked against any available data.

Sub-Site-Scale Flow Model

The local-scale saturated zone model is situated such that the western and eastern sides are nearly perpendicular to the hydraulic gradient. Constant head boundary conditions are therefore placed along the western and eastern sides of the model. A uniform and constant head is assigned to the entire vertical column of gridblocks that underlay a particular gridblock at the water table. In addition, constant head conditions are assigned to gridblocks along the sides in the northwestern corner in the area of the large hydraulic gradient where the potentiometric contours are not perpendicular to the model sides. The latter condition assumes the high gradient area represents a water table gradient, and it maintains the observed high gradients along the sides of the high gradient area. Calibration still considers the high gradient area, however, since assignment of different permeabilities in this area will produce different fluxes and hence head profiles downstream. The northern side of the model immediately downgradient from the high gradient area and the full southern side of the model are no-flux boundaries. The relative difference in hydraulic head between gridblocks along head boundaries represents the relative elevation change between gridblocks.

Model Parameterization

Regional Flow Model

Flow Parameters. The regional model lumped aquifer properties into 10 hydrogeologic units. In reality, aquifer property variation is considerably greater; however, the properties were lumped into a limited number of categories to facilitate the simulations. The subsurface materials of the hydrogeologic framework model were initially classified into eight rock conductivity units (RCUs). Each RCU represents mean hydraulic conductivity of several subsurface materials whose interpreted characteristics, such as rock type, depth, and degree of fracturing resulted in very similar hydraulic conductivity values.

Because each of the three model layers contained several hydrogeologic framework model units, multiple RCUs were associated with each finite-difference model cell. The RCU occupying the largest volume in the finite-difference flow model cell was assigned to each cell. To reduce the number of parameters that would need to be estimated, the authors (COH97) reclassified the layer maps by combining the eight RCUs into four hydraulic-conductivity zones (K-zones) representing large (K1), moderate (K2), small (K3) and very small (K4) hydraulic-conductivity values. The resulting K-zones were not contiguous; each K-zone included cells distributed throughout the model. The 50th percentile K-value for each of the zones was used for the initial hydraulic conductivity values assigned to each K-zone. Transmissivity values for the model layers were calculated by multiplying the applicable K-zone values by layer thickness.

Evapotranspiration. The authors (DAG97a) expressed evapotranspiration (ET) in terms of a linear function based on three variables: (1) land-surface altitude, (2) extinction depth, and (3) maximum ET rate (MCD88). Each of these variables was specified from data sets including ET area maps. Extinction depths were assigned for each unique ET area based on information about plant type and ranged in value from 0 to 15 m. Each of these data sets was resampled to a 1,500 m grid. Since the Death Valley saltpan was simulated as a constant head boundary, it was not assigned an ET rate.

Recharge. To define ground water recharge, a recharge potential map was resampled to a 1,500 m grid and reclassified into an array for MODFLOWP containing four zones associated with high (RCH3), moderate (RCH2), low (RCH1), and no (RCH0) recharge potential parameters. Each parameter defines a percentage factor that represents the amount of average annual precipitation that infiltrates. Average annual precipitation is defined by a multiplication array in MODFLOWP. These zone and multiplication arrays, therefore, along with the parameter values, define the recharge distribution for the model area. In initial parameter-estimation runs, recharge rates based on fixed percentages were lumped into a single recharge parameter (RCU) for simplicity.

Springs. The regional springs data set was utilized to specify the row-column locations of spring nodes. All but three groups of springs were thought by the authors (DAG97a) to discharge from deep regional flow paths, and were, therefore, assigned to layer three. Sand Springs, Indian Springs and Cactus Springs are interpreted as discharging from more localized flow paths in model layer 2. Springs were specified using the general-head boundary package for which the altitude and conductance of spring orifice are assigned. Because the conductance term is poorly known, springs were grouped according to geographic location and a conductance parameter (GHB) assigned for each of the groups of springs.

Pumping Wells. The MODFLOWP well package was used to simulate the amount of ground water pumped from the system. Because most of the water pumped from the wells is relatively shallow ground water, all pumping wells were located in the first model layer. The water-use well data set was used to specify the grid-cell locations and approximate ground water volumes being removed from the model domain. The authors (DAG97a) believe that approximate pumpage rates probably exceed actual values, so they assigned two parameters to make it easy to modify simulated pumpage. The two parameters are multiplication factors representing the percentage of pumpage included in the simulation. WEL2 represents the parameter applied to the Pahrump Valley area, which bears the majority of ground water withdrawal in the region. WEL1 represents the parameter applied to the remainder of the model domain. Pumping rates were obtained from the regional model (DAG97a).

Observation Data. Measured hydraulic heads and spring discharges were used by MODFLOWP during parameter estimation (i.e., calibration) to provide values to define the objective function for the model simulation (i.e., to see how well the model results matched actual field measured values).

Faults and Geologic Structure. The regional model does not incorporate some structures explicitly. In the regional model, northeast-southwest trending regional structures are identified as zones of large permeability and northwest-south-east trending regional structures are identified as zones of small permeability. Because of the large-scale of the regional model, hydraulic properties of such features used in that model may not be appropriate at the scale of the site model. The area underlying Fortymile Wash was also identified as a zone of large permeability in the regional model. Because the site model does not explicitly consider many structural features, the hydraulic conductivity ranges for these hydrogeologic units are much larger than those defined for the regional flow model.

Site-Scale Flow Model

Potentiometric Data. Hydraulic-head values from eighty boreholes, located within the model area, were used in model construction. Twelve of the boreholes (USW H-1, USW H-5, UE-25b 1, USW H-6, USW H-4, USW H-3, UE-25p 1, UE-25c 1, UE-25c 2, UE-25c 3, and two unnamed boreholes) have multiple piezometers. Forty-five of the boreholes are either uncased or have fifty percent or more perforated casing. Twelve boreholes are cased, while the presence or absence of casing is unknown for eleven of the boreholes. Many of the boreholes are "dry" until a fracture zone is intercepted, at which point the water level in the borehole rises to a static level. Because of long open or perforated intervals, many boreholes intercept multiple permeable zones. As a result, the hydraulic head in many of the boreholes represents a composite head.

Permeability Zones. In FEHMN, nodes are grouped into zones in which rock and hydraulic properties, and boundary conditions may be specified. There are 16 zones used in the model that define nodes pertaining to hydrogeologic units with specific permeability and porosity values. Permeability values used in the model are considered preliminary. Only the nodes closest to Fortymile Wash and Solitario Canyon Fault are represented explicitly as fault or fracture zones. In the numerical model, Solitario Canyon is a separate permeability zone and forms a barrier to flow.

The permeability values used in the model are derived partly from a sequence of parameter-estimation simulations. Permeability specified for the middle volcanic aquifer (1.6×10^{-14} m^2) is about three orders of magnitude less than values reported by Geldon (GEL96, p. 70) for tests at the C-wells. The authors (ZYV97) provide a possible explanation for this discrepancy which is that the C-hole tests reflect hydraulic conditions in locally faulted and intensely fractured rock. The possibility of such a condition was tested to a limited extent by specifying a vertical zone, extending approximately 5 km southeast from the C-wells, with a larger permeability of 1×10^{-11} m^2. The small increase in the resultant sum of squared residuals (23,262 m^2) over that of simulation 40 (23,163 m^2) indicates that the model was insensitive to such a zone and that such a zone might be possible. This zone would be consistent with northwest-southeast oriented faults in the area. The small change could also be an artifact of the density of observation points near this zone of large permeability coupled with the small horizontal hydraulic gradient. However, because of the non-unique nature of the model, an overall large permeability (1×10^{-11} m^2) for the entire middle volcanic aquifer also is possible, but would require a considerably different combination of permeability values for the other hydrogeologic units to achieve calibration. Investigating the possibility of a zone of large permeability would be more appropriate using a more finely sampled hydrogeologic framework model and associated finite-element mesh.

Large Hydraulic Gradient Zone. To reproduce the LHG on the north end of Yucca Mountain, where the apparent water-table altitude changes about 300 meters in a distance of less than 2 km, an additional zone was defined within the model as an east-west barrier to flow. Large head residuals (i.e., errors during calibration) had occurred at the wells defining the LHG prior to the definition of this zone. Because no independent geologic evidence for a structure exists, and because the length of such a structure is in question, the coordinate defining the eastern extent of this zone was selected as a parameter and allowed to vary from the western limit of the zone to the eastern edge of the model during earlier scoping simulations. Model fit was best when the zone was extended to the eastern edge.

A single zone extends from the top of the water table to the bottom of the model, and is one node thick that, in essence, forms a 2-D plane. The present model zonation results in uniform permeability changes over the entirety of the upper volcanic aquifer, the upper volcanic confining unit, and the middle volcanic aquifer wherever they occur within the model.

The authors (ZYV97) note that an alternate approach to representing the LHG would be to further subdivide the zones defining the upper volcanic aquifer, the upper volcanic confining unit, and the middle volcanic confining unit along the east-west occurrence of the LHG. This subdivision would then allow reduction of the permeability of these units where they occur to the north of the gradient, producing a ‘spillway’ model (FRI94). The authors (ZYV97) also point out that a 250-m resolution mesh would better represent the large hydraulic gradient as well as the fault and hydrogeologic unit distribution, coincident with the LHG as portrayed by Fridrich et. al. (FRI94).

Solitario Canyon Fault Zone. Based on hydrologic and hydrochemical data, the Solitario Canyon fault appears to act as at least a partial barrier to ground water flow. Currently, the authors (ZYV97) have not specifically simulated the Solitario Canyon fault in the model. However, they have included a hydraulic conductivity zone to better reproduce the approximately 50-meter change in hydraulic head across the Solitario Canyon fault system. Its exact correlation with Solitario Canyon fault is approximate owing to the coarseness of the grid. This zone was introduced after initial attempts to simulate the 50-m change in head resulted in large hydraulic-head residual values (i.e., errors). No hydraulic-test data exist to provide information about the permeability of the Solitario Canyon fault zone.

Fortymile Wash Recharge Zone. Many lines of evidence indicate recharge occurs in upper Fortymile Wash. Therefore, the authors (ZYV97) placed a zone in this area to specify recharge in upper Fortymile Wash. The zone consists of seven nodes each with a uniform mass recharge rate of 0.22 kg/s.

Sub-Site-Scale Flow Model

Hydrogeologic Units. Permeabilities of the Topopah Spring units for the sub-site-scale model are derived from Bandurraga et al. (BAN97). These values are the averaged values from inversion of pneumatic data from the unsaturated zone. The sources of data are described in Bandurraga et al. (ibid.). The values shown are derived from analysis of fracture traces and results of air-injection tests.

Luckey et al. (LUC96) provide apparent hydraulic conductivity values for saturated zone units, as obtained from pumping and other hydrologic tests conducted in the 1980s. The authors (ZYV97) observe that no single value of permeability for each unit can be assigned, given the inherent heterogeneity in the system and general paucity of data. The values chosen by the authors (ibid.) for each unit fall within the range of values available, and also maintain the contrast in unit permeabilities due to their geologic structure. Thermal properties of each unit are derived from laboratory tests on rock core (BRO97), and from analysis of temperature profiles in boreholes (SAS88). These values are very well constrained relative to the hydrologic properties. Porosity values are representative of the fracture porosity. An effective fracture porosity has been difficult to determine for all flow models at Yucca Mountain, and simulations presented later in this section illustrate the highly variable flow estimates obtained using different porosities. The authors (ZYV97) apply a single-continuum model that considers fracture porosity for most units since fractures are the dominant fluid pathways in the saturated zone. The authors (ibid.) further believe that the fracture-dominated flow conceptualization is supported by two lines of evidence: (1) borehole tracejector surveys have consistently shown water derives from several discrete fractures or fractured zones (e.g., WAD84); and (2) permeability calculations from pumping tests are many orders of magnitude larger than matrix permeability (e.g., GEL96).

Drill-hole data for boreholes in the saturated zone were carefully reviewed by the authors (ZYV97) to establish correlations, note discrepancies, and delineate hydrostratigraphic units for the model. The geologic unit thickness values used to construct the model are defined by lithologic logs (CLA97). These may be an apparent thickness, since faults may intersect the borehole within a particular unit. For example, the thicknesses of the Tram Tuff and Lithic Ridge Tuff in borehole p#1 are very likely less than their true values because a fault observed in the borehole separates the units.

The Lithic Ridge Tuff located beneath the Tram Tuff and the lava flows and flow breccias situated between the Tram and Lithic Ridge units are included in the model. A layer of lava flow and flow breccias was penetrated in boreholes H 1, H 6, G-1, G-2, and H-5. The observed thicknesses are 119, 253, 118, 24, and at least 176 m, respectively. This unit is located between the Lithic Ridge and Tram Tuffs of the Crater Flat Tuff, which are adjacent in the rest of the model area. Most of the unit in each of these holes is altered to clays and zeolites (MAT96). The unit therefore is considered a confining unit (i.e., low permeability). The isopach (i.e., thickness) of the thin lava flows and breccias and the associated underlying thin bedded unit beneath was constructed using the observed thicknesses and zero thickness constraint imposed by nearby boreholes H-3, H-4, b-1, and WT-6, in which the unit was not observed (ZYV97).

The Lithic Ridge and lavas are lumped into a single lower confining structure due to their common low permeabilities. This confining structure exhibits large variations in its thickness over the model area, which may have implications for where large vertical gradients are observed.

In the remaining upper stratigraphic units, an important hydrogeologic feature results because of the intersection of the water table with the dipping units. Different units are located at the water table in different areas. In addition, the actual thickness of each unit beneath the water table will be less than its total thickness.

<u>Selection and Representation of Faults in Model</u>. Eleven (11) faults are modeled explicitly. The fault locations in the sub-site-scale model are generally preserved as they occur at the surface. Due to the disparity in scales between geologic mapping and model discretization, several

closely-spaced faults observed in the field are represented as one model fault, or one model fault accounts for the offset across two nearby faults.

Faults are represented as continuous gridblock bands, which preserve the natural continuity of faults. Fault displacement makes the contact area between different units on either side of the fault vary, depending on the fault offset. At large fault offsets, hydrostatigraphic units may be completely discontinuous at the fault and abut against different hydrostratigraphic units. Fault displacement also varies along strike.

The column of gridblocks located along fault traces uses a special node-connection scheme that enables proper representation of the large scale heterogeneity created by fault displacement. Due to fault displacement, hydrostratigraphic units partially to fully abut against other units on the adjacent fault side. The number of vertical gridblocks at fault traces is 46, which provides the additional nodes needed to account for the fractional contract area that connects a particular unit on one side of the fault to a unit on the other side. Both displacement-only faults and fault zones with particular permeabilities were modeled. The authors (ibid.) point out that a bulk fault zone property could later be modeled by setting the properties of fault gridblocks to different values. This is done when considering a fault as a zone of differing hydrologic character from that of the surrounding units.

Model Calibration

<u>Regional Flow Model</u>

Calibration of the regional model by strictly trial-and-error methods was judged by the authors (DAG97a) to be both ineffective and inefficient; therefore, nonlinear regression methods are used to estimate parameter values that produce the best fit to observed heads and flows.

<u>Conceptual Model Testing</u>. During calibration, a number of conceptual models were evaluated using the regression methods in MODFLOWP. A best fit to hydraulic-head and flow observations was calculated for each conceptual model. Evidence of model error or data problems were investigated after each model run. These analyses were used in conjunction with independent hydrogeologic data to modify, and hopefully improve, the existing conceptual model, observation data sets, and weighing. No modifications were made simply to improve

model fit; supporting independent hydrogeologic criteria were also needed before modifications were made.

To perform the conceptual model testing, the authors (DAG97a) adjusted the location and type of flow system boundaries in the north and northeast parts of the model area to test the premise that the regional flow system could be receiving interbasinal flux from adjacent basins. Although water-level data exist adjacent to the model boundaries, considerable uncertainty remains concerning the existence of such fluxes and their volumes.

Modification to the numerical model involved increasing or decreasing the size of the constant-head boundaries, moving the locations of the boundaries to different model layers, and adding new constant-head boundaries to the northeast. In general, these modifications provided very clear results. The optimal location for the constant-head boundaries used to simulate interbasinal flux conditions was the third layer. Locating the constant-head boundaries in the upper layers of the model often led to extremely large deviations from observed heads.

The most appropriate boundary conditions between Sand Spring Valley and Emigrant Valley were evaluated. Simulating a constant-head boundary in this region instead of a no-flow boundary resulted in extremely large residuals for heads (100 m too high) in the northern part of the model domain, and large residuals for spring flows (simulated flows 50 percent too large) at both Ash Meadows and Furnace Creek Ranch. As a result, this boundary was redefined as no flow boundary. The constant-head boundaries at Railroad, Stone Cabin and Ralston Valleys, however, were needed to simulate spring flows close to measured flow at both Grapevine Springs and Oasis Valley. The constant-head boundary at Pahranagat Valley was needed to match to the measured domain and spring flows at Ash Meadows.

Hydrogeologic Framework Testing. Four types of hydrogeologic framework variations were considered during calibration of the regional model. These include: (1) adjustment of hydraulic conductivity zones to improve numerical stability; (2) addition or refinement of hydraulic conductivity zones to better define hydrogeologic units or geologic structures included in the 3-D hydrogeologic framework model; (3) addition of hydraulic conductivity zones to better represent interpreted geologic structures that were not included in the hydrogeologic framework model; and (4) addition of new hydraulic conductivity zones required to better represent faulted terrains supplying ground water to springs and discharge area.

Recharge Distribution Determination. The initial distribution of recharge areas was changed during model calibration to determine the sensitivity to their extent and magnitude. Initially, a single multiplication array was used to describe the rate of recharge, and a single multiplication parameter defined to adjust this rate. Initial modeling indicated that the model results were very sensitive to this single recharge parameter. The large residual errors suggested that the use of a single recharge parameter was an oversimplification, and that parameters in multiple recharge areas would have to be estimated with the available data.

A detailed evaluation that had been conducted by the authors (DAG97a) to delineate various zones of recharge potential was used to divide the single recharge parameter into four zones. Each was assigned a parameter that represented a percent of average annual precipitation that infiltrates. In the final model, RCH0 and RCH1 were assigned values of 0 and 1 percent, RCH2 and RCH3 were estimated by regression and were variable, ranging from 1 to 10 percent and 10 to 30 percent, respectively.

Calibration Results. After calibration, the regional model was evaluated to assess the likely accuracy of simulated results. This is accomplished by comparing measured and expected quantities with simulated values. The quantities included in the comparisons are (1) hydraulic heads and spring flows, which were matched by the regression; (2) hydraulic conductivities, vertical anisotropy, and percent of precipitation that infiltrates, all of which were represented by parameters estimated in the regression; and (3) water budgets.

An advantage of calibrating the model using nonlinear regression is the existence of substantial methodology by which to evaluate model results. As will be demonstrated, these methods produce a more thorough evaluation than is normally accomplished and reported when calibrating using trial-and-error methods. The thorough analysis produces a good understanding of the strengths and weaknesses of the model, and the likely accuracy of simulated results and associated confidence intervals and other measures of parameter and prediction uncertainty.

The authors (DAG97a) believe that the model reproduces the measured hydraulic heads and estimated water-budget components reasonably accurately. They also believe that the estimated parameter values include all aspects of the system that are most important for steady-state simulation, and the parameter values that produce the best match between simulated and observed hydraulic heads and flows; that is, the parameter values estimated by the regression, are all reasonable.

Because the weighted residuals are not entirely random, some model error may be indicated. This is related to the occurrence of large positive weighted residuals for hydraulic heads and large negative weighted residuals for spring flows. In addition, weighted residuals are not normally distributed. The authors (DAG97a) believe that additional calibration may significantly improve model accuracy. They further conclude that the model is a reasonable representation of the physical system, but evidence of important model error exists.

One of the more apparent factors contributing to model error is the vertical discretization of the regional system into three layers. While a three-layer model is an improvement on previous 2-D and quasi-3-D models, simplification of the complex 3-D hydrogeologic framework into three layers inevitably results in model error, particularly in areas with significant vertical flow components. The introduced model error may translate into model bias in computed parameters and all quantities computed using them, particularly head and flux. Furthermore, this potential bias may be contributing to closeness of fit calculated for the model. The authors (DAG97a) believe that an evaluation of the extent of model error should be conducted. This evaluation may include a series of cross-sectional or subsystem models with varying degrees of vertical discretization. A comparison of the levels of detail in vertical discretization with the model fit and computed parameter values would give some indication of the potential for model error. They also indicate that the calibrated site-scale model has a flux of 465 kg/s from the south face versus 323 kg/s over the same region for the regional model. This agreement is acceptable considering the compatibility issue raised above. Furthermore, the recharge and discharge flux values themselves, as input into the regional-scale model, have uncertainties that are larger than the computed difference of these two models. Because the difference is within the range of uncertainty of the actual flux values, the authors (DAG97a) consider the two models to be, for all intents and purposes, in agreement with one another.

Site-Scale Flow Model

The calibration of this model was achieved through the use of the model independent parameter estimation software, PEST (WAT94). PEST uses nonlinear least-squares regression to estimate parameters. The benefits of using nonlinear regression include: (1) expedited determination of best-fit parameter values; (2) quantification of the quality of the calibration; (3) estimates of the confidence limits on parameter estimates; and (4) identification of the correlation among parameters.

PEST was selected because of the ability to couple it with FEHMN without significantly changing the FEHMN software. PEST is designed to be used with virtually any model, provided that one can identify: (1) model input files; (2) model output files; (3) commands that invoke the model; (4) observation data; and (5) model parameters. Each of the required input and output files needs to be in ASCII format.

PEST was used to run FEHMN and to vary user-specified model parameters prior to each run such that the weighted sum of the differences between observed and simulated values of pressure, hydraulic head, or temperature is minimized using nonlinear regression. The optimization is accomplished using the Gauss-Marquardt-Levenberg method. The strength of this method lies in the fact that it can generally estimate parameters using fewer model runs than any other estimation method, a definite advantage for large models whose run times may be considerable (WAT94).

As mentioned above, model calibration was attempted using nonlinear least-squares regression to estimate parameter values. Permeability values were modified to achieve a close match to 94 measured hydraulic heads, all of which were equally weighted. Fluxes at the specified-head nodes for the outside nodes were summed for each side of the model for comparison against regional model values. The authors (ZYV97) believed that it may be advantageous to compare flows for smaller parts of each side, but this was not done in the present work.

Several simulations using a pressure-based configuration instead of hydraulic heads, provided experience regarding which parameters tended to be highly correlated, a condition which indicates that the available data are not sufficient to estimate all parameters individually. Hydrogeologic units with similar permeabilities were combined or "lumped" as parameters to gain some insight about the hydrologic importance of areas of large and small permeability. For example, the permeability parameter of the middle volcanic aquifer (mva) was observed to be correlated to the upper volcanic aquifer (uva). Experience has shown that spatially connected hydrogeologic units with similar permeability which are oriented approximately parallel to the direction of ground water flow tend to be highly correlated, preventing independent estimates of their associated permeability values. An initial strategy of the modeling focused on optimizing permeability in those units that appeared to have sufficient information provided by hydraulic-head observation points. In addition, a determination of which potential model parameters were highly correlated was done using PEST by assigning as many model variables of permeability and flux as possible so that correlation among parameters could be evaluated. From these correlations, parameters either could be lumped with other correlated parameters, or set so that parameter estimation could be achieved.

Forty PEST parameter estimation runs were done for various combinations of fixed and estimated parameters. Fixed parameter values are not modified during a run; estimated parameter values are adjusted using nonlinear regression. In most of the runs, one or two parameter values are estimated; at most, five are estimated. Because so few parameters are estimated without a thorough evaluation showing that the other parameters are unimportant, the authors (ZYV97) believe that the regression runs need to be considered as very preliminary. The results of the PEST simulations include 95% confidence intervals for the adjustable parameters, which the authors (ibid.) indicate may or may not be meaningful, depending on many factors in the model construction and parameter estimation processes. A large range in the 95% confidence interval generally indicates that the data contain little information about the parameter. In many instances, minimum values of 95% confidence intervals were estimated as negative values. Use of a log transformation of such a parameter typically would result in a minimum value with a large negative exponent (or essentially a minimum value of zero), indicating that insufficient information was available to provide a good estimate of the parameter.

Sub-Site-Scale Flow Model

The sub-site model was calibrated to the observed water table. The high gradient area is conceptualized as a zone of uniform permeability. Initial simulations used a range of rock properties, and all fault zones were assigned a permeability of 10^{-13} m^2. Steady-state simulations using these parameters showed that the medium gradient across the Solitario Canyon Fault could not be sustained with the assigned fault permeability. Permeability values were adjusted manually and simulations were performed in an iterative manner. Subsequent simulations showed that the dominant areas that needed permeability adjustments were the Solitario Canyon and Iron Ridge faults. The authors (COH97) found that in order to reduce the simulated heads on the eastern side of the Solitario Canyon Fault, a permeability of 10^{-16} m^2 was needed. In order to reduce the heads east of the Iron Ridge Fault to their approximate measured values, the Iron Ridge Fault and neighboring fault to the west were adjusted to a permeability of 10^{-15} m^2. In parallel to fault permeability adjustments, the gradient conditions to the north were observed, and the authors (COH97) found that a permeability of 10^{-15} m^2 for the entire high gradient area enabled the lower heads immediately downgradient from this area to remain within observed bounds.

Water-level matches for boreholes are generally within 1 m, except for those boreholes that are situated immediately adjacent to the Solitario, Iron Ridge, and High Gradient areas. The measured heads are generally taken from Ervin et al. (ERV94). The large discrepancy between measured and simulated heads at borehole H-5 is due to the anomalously high head at H-5, which may be due to an intersection of a Solitario Canyon fault splay with this borehole (ERV94). The model does not consider this splay. The simulated gradient in the northwestern corner of the model is 0.12, compared to the measured gradient of 0.11 (ERV94). A head residual for borehole G-1 results because the low permeability zone within the high gradient area was not extended to this borehole. The authors (COH97) believe that a short extension of this zone will yield a closer match. Gradients calculated from actual field measurements is the low-gradient area range between 0.0003 and 0.0004 (ERV94). The simulated heads in the low-gradient area yield a gradient that ranges between approximately 0.0005 immediately downgradient from the repository, to as much as 0.003 in the area west of C-wells. The Midway and Paintbrush Canyon faults are located in this area, and their displacement results in the complete displacement of the Bullfrog Tuff, the most permeable unit in the model. This discontinuity creates this localized higher gradient. The authors (COH97) believe that such a gradient is possible, as it may occur between boreholes where measurements are not available. The 2-D and 3-D simulations described later in this section show how the Bullfrog abutment at these faults significantly alters the flow field, and reveal the possible fault effects in greater detail.

<u>Using Hydrochemical Data for Calibration</u>. The authors (COH97) reviewed the possibility of using hydrochemical data to facilitate model calibration and concluded that the ground water composition in the region around Yucca Mountain is heterogeneous at the kilometer scale. They also noted that separate domains define the ground water composition of Jackass Flats, Fortymile Wash, Crater Flat, and Yucca Mountain, but at the sub-site scale, it is difficult to distinguish separate domains. All water samples from Yucca Mountain itself plot in a relatively coherent region.

Another of their observations relates to the availability of data. Dozens of chemical analyses that include rare earth and trace elements are now available from springs that sample discharge waters (HOD96). These provide useful end components (although not end member compositions) to the history of ground waters. Similar analyses would be very useful for recharge waters and for wells in the Yucca Mountain area. Without additional samples at greater depths in the saturated zone, the authors (COH97) believe that this assumption can only be tested on the basis of mixing models using existing isotope data.

The authors (COH97) continued their discussion by outlining the data limitations with respect to the ground water chemistry and maintained that uncertainties regarding the saturated zone hydrochemistry abound due to the limited number of boreholes that penetrate the water table near Yucca Mountain and the uncertain quality of some of the existing data.

Predictive Simulations

Regional Flow Model

The predictive simulations of the regional model were all focused on determining the adequacy of the calibration and the appropriateness of the conceptual model(s). Calibration of the regional model using the techniques available in MODFLOWP allowed for estimation of a series of parameters that provide a best fit to observed hydraulic heads and flows. Numerous conceptual models were evaluated during calibration to test the validity of various interpretations about the flow system. Conceptual model evaluations focused on testing hypotheses concerning the (1) location and type of flow system boundaries; (2) extent and location of recharge areas; and (3) configuration of hydrogeologic framework features. For each hypothesis tested, a new set of parameters was estimated using MODFLOWP and the resulting new simulated heads and flows were compared to observed values. Only those conceptual model changes contributing to a significant improvement in model fit, as indicated by a reduction in the sum of squared errors, were retained in the final optimized model.

The final model was evaluated to assess the likely accuracy of simulated results. This was accomplished by comparing measured and expected quantities with simulated values. The quantities included in these comparisons are: (1) hydraulic heads and spring flows, which were matched by regression; (2) hydraulic conductivities, which were represented by parameters that were estimated in the regression; and (3) water budgets. Unweighted and weighted residuals for hydraulic heads show a very good model match with observed conditions in flat hydraulic gradient areas and a relatively good match in large hydraulic gradient areas. Weighted and unweighted residuals for spring flows show somewhat of a bias in that simulated spring flows are generally lower than observed. The difficulty in simulating these spring flows in previous models of this area without imposing discharge by using a specified flux, however, suggests that even the somewhat lower simulated discharges are an improved match with observed conditions. Estimated parameters were evaluated to determine if reasonable values of hydraulic conductivity, vertical anisotropy and recharge rates were obtained. All estimated parameter values are within expected ranges. The MODFLOWP-calculated linear confidence intervals also were well within the range of expected values. Water budgets were evaluated to determine if they were within the range of expected values. The authors (COH97) believe that even with the limited understanding of fluxes in and out of the regional ground water flow system, overall budgets are within the expected ranges for the flow system.

Site Scale Flow Model

In a fashion similar to the regional scale model, the primary objective of the site-scale modeling was also to achieve a calibrated model. Therefore, the predictive simulations are essentially an evaluation of how well the model is calibrated. The authors (ZYV97) used several criteria including how well the simulated hydraulic heads matched those observed in monitoring wells; and how closely estimates of flux from the site model match those determined in the regional modeling.

In general, the model fits the observation well data relatively closely in small gradient areas, but fits more poorly in larger gradient areas. With respect to the model fluxes, a comparison of the regional versus site model predictions indicates fairly large discrepancies. The authors (ibid.) believe, however, that it is more of a problem with the regional model conceptualization than with the site model.

Another flow issue addressed in the site-scale modeling is the effect of temperature on the flow field and on the prediction of flux through the site-scale model. An analysis performed with the site-scale model shows that the model calibration is not significantly affected by the selection of 20˚C for model calibration purposes. Computed heads differed by less than 1% between the system simulated assuming 40°C temperature and the system simulated assuming 20°C. The difference in computed flux out of the south end of the model was somewhat larger but still well within the range of uncertainty of the flux in the actual ground water system. Therefore, the authors (ibid.) conclude that the calibrated model at 20°C is acceptable for the present study but recommend that, in future modeling, a more appropriate mean temperature be used to alleviate this concern.

Sub-Site-Scale Flow Model

A number of different types of simulations were performed at the sub-site-scale; including both two- and three-dimensional analyses, simulating matrix diffusion effects, and attempts to match well pumping tests results at the C-hole complex with model predictions as discussed below.

Two-Dimensional Simulations. Two-dimensional cross-sections of the full model are used by the authors (COH97) to study specific scenarios such as the coupled effects of up welling, varying fault and hydrostratigraphic unit properties, and fracture-matrix interactions. Although the 2-D cross sections are a larger abstraction from the actual system then the full 3-D model, the results of 2-D simulations are often easier to understand. In addition, the faster execution time for 2-D simulations enables one to quickly investigate the effects of varying specific properties and thereby guide the design of full 3-D simulations.

Three-Dimensional Simulations. The area of the model corresponding to the small-gradient area was used as an investigative tool to explore and define saturated zone processes by way of hypothesis testing. By using this sub-area of the model only, biases that would be introduced by assuming the true cause of the large gradient zone are avoided. The western boundary of this sub-grid was defined by the 731 m water table contour. The full 3-D saturated zone model is used by the authors (COH97) as an investigative tool to explore and define saturated zone processes by way of hypothesis testing and calibration against hydrologic, thermal, and geochemical data. This approach yields answers to questions concerning the plausibility of various flow and transport scenarios. In addition, unanticipated saturated zone flow processes can be demonstrated and investigated. Three-dimensional simulation of hydraulic tests is also used for model calibration by way of matching pumping test results.

Single and Dual Continuum Models. Although flow in the saturated zone may be dominated by fractures, the interaction of fracture and matrix must be captured in order to understand dilution and mixing. To this end, the authors (COH97) developed two saturated zone grids: (1) single continuum; and (2) dual-porosity. Most of the simulations utilized the standard single continuum model, which represents an effective porous medium as a fracture-dominated system. The single continuum model is used for calibrating the model against measured water table elevations, and for investigation of steady-state flow geometry and flow visualization. The dual-porosity model is used to consider fracture-matrix interaction. The dual-continuum model enables simulation of pumping and tracer tests in dual-porosity media. Matrix properties are derived from unsaturated zone modeling analysis and fracture data.

Simulation of Long-Term Pumping at the C-Hole Complex. Although more than 150 individual aquifer tests have been conducted at 13 boreholes in the vicinity of Yucca Mountain, the C-hole complex is the only multi-hole complex in the saturated zone at Yucca Mountain. The C-wells were drilled to perform multi-well aquifer tests and tracer tests. The authors (COH97) used the sub-site-scale model to simulate a long-term pumping test at the C-wells in order to use C-hole data to calibrate and validate the model. The full three-dimensional model was used to study the drawdown behavior at the six observation wells for the long-term pumping test.

The model uses the regional hydraulic gradient observed for the Yucca Mountain site as an initial condition and the pumping test is then an additional stress on the system. Boundary conditions are constant pressure corresponding to the observed heads (ERV94). Pumping for a total period of 250 days is simulated and the final steady-state drawdowns are reported for the six observation wells.

The matching of the simulated drawdowns to the observed drawdowns was done by a manual trial and error process. A constant withdrawal rate of 9.46 l/s (150 gpm) was assigned to one element (Lower Bullfrog unit at UE-25 c#3). A fine discretization in the vicinity of the C-hole complex was judged by the authors (COH97) to provide sufficient resolution of the distance between the pumping well c#3 and the two neighboring observation wells, UE-25 c#1 and UE-25 c#2. However, the authors (ibid.) believe that a still finer discretization may be needed to fine-tune the performance of the simulation results to the observed transients in the two wells, UE-25 c#2 and UE-25 c#3.

These simulations were intended to show what effects the faulted structure has on pumping test results. This model capability is especially useful since the pumping test results at the C-hole are a function of heterogeneities at the scale of tens to thousands of meters, and it is at this scale that radionuclides may be dispersed within the immediate site area. Since the model has been calibrated by matching results of long-term pumping tests at the C-wells, simulations of pumping tests under different conditions and at different locations can show what data would be obtained, as well as what hydrogeologic signatures could be subject to analysis. Proper test designs for the proposed Second Testing Complex, for example, can also be determined by simulating different pumping test scenarios around faults using the model.

VI.2.1.2 Saturated Zone Transport Model Construction

The saturated-zone flow modeling performed for the Yucca Mountain Project has focused on the key controlling factors influencing the measured head distributions at the site. In this section, issues related to the transport of radionuclides in the saturated zone are presented, which in addition to flow issues, requires that processes specific to the migration of solutes be considered.

The saturated zone radionuclide transport model was constructed by Zyvoloski et. al., (ZYV97), and although the transport modeling was not used directly in the TSPA-VA, the findings of the modeling were used to guide the approach that was taken to address radionuclide transport in the TSPA-VA as discussed in later in this section.

Conceptual Model of Saturated Zone Transport

The site-scale ground water flow model provides the hydrologic framework for determining the direction and rate of movement of radionuclides that reach the saturated zone beneath Yucca Mountain. In addition to flow issues, the migration of radionuclides to the accessible environment depends on transport processes and parameters distinct from the flow model itself. This section presents the authors (ZYV97) conceptual model for transport that includes advective transport of radionuclides, dispersion, diffusion of radionuclides from fractures into the rock matrix and sorption. Within the fractured tuffs, the authors (ibid.) expect the migration of radionuclides to be primarily through regions with higher bulk fracture permeability. They also believe that flow within individual joints probably occurs through channels, rather than as sheet flow through parallel-plate fractures. The authors (ibid.) note that at more distant downstream locations, the migration is likely to be through alluvium, and a model for flow and transport through a porous continuum, rather than a fractured rock, is likely to apply.

Fluid Flow In Fractures

The hydrologic evidence to date strongly supports the model of fluid flow within fractures in the moderately to densely welded tuffs of the saturated zone (e.g., WAD84, WHI85). First, as expected, the hydraulic conductivities measured for core samples in the laboratory are orders of magnitude higher when the sample is fractured (PET84). Also, there is generally a positive correlation between fractures identified using the acoustic televiewer of a borehole television tool and the zones of high transmissivity.

Because the role of fractures is so important to the hydrology in the saturated zone, the permeability distribution and principal flow directions depend strongly on the spatial distribution and orientations of fractures. Karasaki et al. (KAR90), in an attempt to correlate the C-wells fracture data with transmissivity measurements, tentatively concluded that the regions of high transmissivity in the C-wells correlate with fractures oriented to the northeast, with the steeply dipping fractures contributing most to the transmissivity.

Matrix Diffusion - Laboratory and Field Evidence

Instead of simply traveling at the flow rate of the fluid in the saturated zone, radionuclides will potentially undergo physical and chemical interactions that must be characterized to predict large-scale transport behavior. These interactions include molecular diffusion into the rock matrix, sorption on the minerals along the fractures or within the rock matrix, or transport in colloidal form. These phenomena are described below.

When a dissolved species travels with the fluid within a fracture, it may potentially migrate by molecular diffusion into the stagnant fluid in the rock matrix. When a molecule enters the matrix, its velocity effectively goes to zero until the Brownian motion carries it back into the fracture or into an adjacent fracture. The result is a delay of the arrival of the solute at a downgradient location from what would be predicted if the solute had remained in the fracture. In hydrologic tests not involving tracers, the pore water velocity can often be estimated given assumptions about the fracture porosity. For interpreting hydrologic tests, the fracture porosity is usually the correct porosity value because aquifer properties (i.e., transmissivity) from pump testing is controlled by fracture flow. However, the ground water travel time is often computed by dividing the flow path length by this velocity. This estimate is potentially a severe underestimate of the time required for a water molecule to migrate along the flow path. A more accurate definition of travel time for the purpose of predicting transport behavior would take into account matrix diffusion.

There have been several theoretical, laboratory, and field studies performed to demonstrate the validity of the matrix-diffusion model. Grisak and Pickens (GRI80) and Neretnicks (NER80) first applied mathematical models to demonstrate the likely effect of matrix diffusion in flow in fractured media. In these studies, transport was idealized as plug flow within the fracture with diffusion into the surrounding rock matrix. Sudicky et al. (SUD85) applied a similar model to a laboratory experimental apparatus which tracer was injected into a thin sand layer with surrounding low permeability silt layers, showing that matrix diffusion was necessary to model the conservative tracer data. Neretnicks et al. (NER82) reached the same conclusion in their experiments of transport in natural fissures in granite. Rasmuson and Neretnicks (RAS86) extended the concept of matrix diffusion to examine the coupling between matrix diffusion and channel flow usually thought to occur within natural fractures.

Transport models incorporating matrix-diffusion concepts have also been proposed to explain the often conflicting ground water ages obtained from ^{14}C data compared to ages predicted from flow data. Sudicky and Frind (SUD81) developed a model of flow in an aquifer with diffusion into a surrounding aquitard to show that the movement of ^{14}C can be much slower than predicted if only movement with the flowing water is considered. Maloszewski and Zuber (MAL85, 91) reach a similar conclusion with a model for ^{14}C transport that consists of uniform flow through a network of equally spaced fractures with diffusion into the surrounding rock matrix between the joints. Their model also includes the effect of chemical exchange reactions in the matrix, which further slows the migration velocity. Maloszewski and Zuber (MAL85) also present analyses of several interwell tracer experiments that show that their matrix-diffusion model can be used to provide simulations of these tests that are consistent with the values of matrix porosity obtained in the laboratory and aperture values estimated from hydraulic tests. The results are, in all cases, superior to previous analyses that did not include matrix diffusion effects. Finally, of greatest relevance to the saturated zone beneath Yucca Mountain is the C-wells reactive tracer test (REI97), which demonstrates that models incorporating matrix diffusion provide more reasonable fits to the tracer-experiment data than those that assume a single continuum. They showed that a suite of tracers with different transport characteristics (diffusion coefficient, sorption coefficient) produced breakthrough curves that can be explained using a diffusion model that assumes diffusion of tracers into stagnant or near-stagnant water. Finally, Waddell (WAD97) recently reported a similar result for nonsorbing tracers with different diffusion coefficients in a fractured-tuff tracer experiment at the NTS.

Thus, the theory of matrix diffusion is generally thought to be based on sound physical principles, and demonstrations of its effect have been shown in both laboratory-sized specimens and interwell tracer tests. The effect on transport under ground water flow conditions could be extremely large and, thus, should be incorporated into any realistic radionuclide migration model. It is still unclear, however, how DOE will ultimately incorporate these processes (matrix diffusion) into the TSPA-LA since they are currently not considered in the TSPA-VA.

Dispersion. Dispersion is caused by heterogeneities at all scales from the pore scale to the scale of the thickness of individual strata and the length of structural features such as faults. The resulting spreading of radionuclides is important to performance in that it will lead to dilution and should be captured in transport models. As will be discussed later in this section, the TSPA-VA simply assigns a dilution factor, to account for dispersion, rather than modeling dispersion explicitly.

Only the largest heterogeneities are represented as property zone values in the site-scale model; all dispersion caused by smaller-scale features must be represented through the use of dispersion values input into the model. Numerous ground water transport studies have been conducted at a variety of scales, and the results are compiled using the dispersivity as the correlating parameter. It is well-known that dispersivity increases with the scale, or distance, for transport of a solute (NEU90). The only site-specific data comes from the C-wells reactive tracer experiment of Reimus and Turin (REI97) and accompanying tracer tests carried out by the USGS at the C-wells. These experiments yielded estimated dispersivity values that fall in the range of uncertainty of correlations to data collected and compiled at many sites. The authors (ZYV97) believe that this result provides credibility that the dispersivity values used in the field simulations are appropriate. Very little experimental information exists for assigning transverse dispersivity. In the site-scale modeling study, however, the "rule-of-thumb" value of one-tenth the longitudinal dispersivity is used for transverse dispersivity.

Other Transport Processes. Sorption of radionuclides on rock surfaces is another mechanism that will result in retardation. These radionuclide-rock interactions can potentially occur on the surfaces of fractures and within the rock matrix. This distinction is important because the surface-area to fluid-volume ratio and the mineral distributions are probably different in the fractures as compared to the matrix. The lithium tracer in the C-wells reactive tracer experiment was modeled by Reimus and Turin (REI97) using a matrix-diffusion model with the sorption coefficient as an additional adjustable parameter. The matrix sorption coefficient that fit the data agreed quite well with the value determined in laboratory sorption tests, thus providing an additional degree of confidence in the matrix-diffusion model. The fact that the early lithium response had the same timing as that of the nonsorbing tracers, but with a lower normalized peak concentration, is consistent with matrix-diffusion coupled with sorption in the matrix.

Transport of radionuclides on colloidal particles or in colloidal form is a third mechanism that may apply at the field scale. Colloidal particles have the potential to provide a direct pathway through fractures. Strongly sorbing radionuclides such as plutonium may adhere to these particles and move more rapidly than if the radionuclide were confined to the aqueous phase. The size of the colloids may minimize diffusion into the rock matrix, thereby reducing one possible retardation effect. On the other hand, filtration of colloidal material is likely to come into play, thereby potentially resulting in large retardation factors. The key uncertainties identified by the authors (ZYV97) in predicting colloid transport in the field are:

- Whether a continuous pathway exists with large enough pore size to facilitate transport over large distances without filtration or migration into stagnant fluid storage; and

- The uncertainty regarding the relative amount of radionuclide on colloid surfaces versus that in the aqueous phase.

For the first uncertainty, field demonstration of colloidal transport is necessary to prove that this mechanism is important at the field scale. Furthermore, given the complexities of the interactions of colloids with the surrounding rock and geochemical conditions, further laboratory work to characterize these effects is necessary. Other key uncertainties not discussed by the authors (ZYV97) include the relative stability of the colloid in various geochemical environments and potential chemical and physical (i.e., filtration) retardation of the colloid itself.

Summary of Conceptual Model

Summarizing the discussion of fluid flow behavior given above, the saturated-zone transport conceptual model is outlined below:

- Radionuclides enter the saturated zone via the fluid percolating through the unsaturated rock above the water table. The exact nature of this transport is not expected to exert a great effect on the subsequent saturated-zone model, and thus, the saturated-zone transport model can be developed independently from a transport model for the vadose zone, which acts as a boundary condition for the saturated-zone model. Of course, for detailed predictions of radionuclide migration, the spatial and temporal distributions of the input from the unsaturated zone are important.

- Flow occurs within the highly fractured portions of the tuffs near the water table. There is probably not a continuous zone of high permeability to the accessible environment. Assuming there is not a continuous zone, then the low-permeability regions will effectively act as large-scale heterogeneities that give rise to large-scale macroscopic dispersion due to the tortuous nature of flow over the scale of hundreds of meters to kilometers.

- Although the vertical matrix permeability is assumed to be small over the length scale of several hundreds of meters, within a fractured region, vertical permeabilities should be as large as the horizontal permeabilities. Thus, the radionuclide will spread vertically and be present within the entire thickness of a fractured zone. The thicknesses of these fractured zones are difficult to estimate from the present data. However, the extent of fracturing correlates reasonably well with the degree of welding, which is one of the criteria used to define the submembers within a lithologic unit. Therefore, it seems reasonable to assume that the heights of the fracture zones are on the order of the thicknesses of the individual lithologic members, namely 100 to 200 m. This possibility is in contrast to flow zones detected in individual boreholes, where measurements reflect the intersection of specific fractures with the well.

- Fluid flow occurs within the fracture with stagnant fluid residing in the rock matrix blocks. All fractures have large contact areas due to the *in situ* stresses exerted on them at these depths. The conductivity of an individual fracture is probably not a strong function of its orientation because all are on the flat portion of the aperture versus effective-pressure curves. Therefore, the magnitude and direction of the components of the hydraulic conductivity tensor should be controlled by the distribution of joints of various orientations. Fractures detected from geophysical logs are generally oriented in a north-south direction and are, within 30° of vertical.

- Flow within individual joints probably occurs within channels. The fluid travels preferentially within regions of large apertures with large sections of the fracture surface containing stagnant fluid or no fluid where the faces are in contact.

- The surrounding matrix material conducts no fluid under natural ground water flow conditions but is physically connected to the fracture fluid through the pore network. Fluid is stored in this pore space and is important to radionuclide migration (see below). The matrix porosities of interest are those of the rock within the fractured regions. Fractures are generally found within the moderately to densely welded tuffs, so the range of matrix porosities of these tuffs (0.06 to 0.09 for densely welded and 0.11 to 0.28 for moderately welded) more accurately reflect the fluid storage of interest rather than the generally wider ranges of values found within a specific lithologic member.

Computer Code Selection

The FEHMN code was selected for the transport simulations for many of the same reasons it was chosen for the site-scale flow modeling discussed above. Using the same code for both ground water flow and contaminant transport modeling also eliminates model setup inconsistencies that may otherwise arise (e.g., block centered vs. node centered grids).

Layering and Gridding

Grid Generation and Grid Resolution Studies

Several three-dimensional grids were generated in support of the site-scale flow and transport modeling effort. Both structured and unstructured grids were developed, tested, and used for sensitivity analyses and flow calibration studies. Structured grids, commonly referred to as finite-difference grids, are easy to generate, but their block-like structure makes it difficult to represent complicated geometries with all but the finest grid resolution. Unstructured grids, like the common finite-element meshes, are more complicated and may consist of triangles and tetrahedrals. They can, however, represent complicated hydrostratigraphy and topography accurately at fairly low resolution. It should be noted that not all finite-element models are formulated to accommodate unstructured grids, and recent developments now allow finite differences to solve unstructured grids.

As was discussed in Section VI.2.1.1, the hydrostratigraphy represented in the geologic model consists of multiple layers of contrasting fluid flow and transport properties. The grid-generation methods used in the transport study allow the stratigraphy to be honored in numerical grids of different resolution so that comparison studies can be performed to test for grid quality and to determine the resolution required for flow and transport simulations. All mesh generation and manipulation is done with the GEOMESH/X3D toolkit (GAB95, GAB96, TRE96).

A series of six structured grids of increasing resolution was used to compare the flow through the model domain to assess the point at which increasing resolution no longer influences the results. This process identifies the resolution required for an accurate simulation of the flow field. A similar study for two unstructured grids demonstrated that the coarser grid used for calibrating the flow model was sufficiently resolved for accuracy. This section also reports on the development of a technique for selectively refining the numerical grid for transport calculations. The method uses the solute transport pathway determined on a coarse grid to identify regions of the model where increased grid resolution is required. The mesh-generation software refines the grid in those areas. After two or more successive applications of this process, the grid is finely resolved along the pathways of solute plume movement, and numerical error associated with insufficient grid resolution is minimized. The main application of this technique is for refining the revised site-scale model for transport calculations.

Approach. This subsection addresses the construction of computational grids that reflect complex geologic structure for saturated-zone flow and transport simulations. The importance of grids are summarized by the authors (ZYV97) with the following questions:

- What resolution is required to represent geology?
- What resolution is required to represent flow and transport processes?
- Can a grid be optimized to represent features and flow processes while keeping the size relatively small?
- If a flow model is calibrated on a coarse grid, is it calibrated on a fine grid?

The authors (ZYV97) point out that these grids must accurately represent the geologic structure and be appropriate for numerically accurate simulations of flow and transport. That is, any error associated with numerical grid discretization must be constrained within specified truncation error tolerances. Understanding the quality of the grids and the effects of grid-related error is necessary for assessing the quality of the simulations and generating a defensible model.

The process of developing flow and transport models for the saturated-zone studies are divided by the authors (ZYV97) into three parts:

- Developing accurate conceptual models of the geology and hydrologic material properties
- Building the grid and prescribing boundary and initial conditions
- Applying the computational physics models of flow, heat transport, and chemical transport

They provide further explanation by explaining that geologic interpretation, stratigraphic model development, and material characterization are performed based on numerous field measurements. The stratigraphic model populated with hydrologic material properties then provides the basis for computational grid development. They also point out that the ability of the numerical grid to represent the geologic complexity directly affects accuracy of the numerical model's approximation of the actual physical system's response.

GEOMESH/X3D (GAB95, GAB96, TRE96) is described by the authors (ZYV97) as a mesh-generation toolkit that can use the hydrostratigraphic model as input to create a numerical grid that represents accurately complex structures and stratigraphy such as faults, pinchouts, and layer truncations. As well as representing geologic structure, this software maintains and distributes physical and chemical attributes such as porosity, permeability, or percent zeolite. The process of populating the numerical grid with hydrologic and transport properties is described in Robinson et al., (ROB97). This process of generating and populating numerical grids from geologic framework models is automated, thus making the entire process easy to implement with fewer user-induced errors. At any step in the process, numerical resolution can be added to a particular subregion, new boundary conditions can be prescribed, or new attributes can be incorporated.

The authors (ZYV97) believe that the grid quality control issues involved in this automated process cannot be over-emphasized. They indicate that a system that uses only electronic processing of the hydrogeologic data is desirable for a defensible model during the licensing process because the interfaces can be qualified and metrics of goodness of representation can be established. These metrics would likely include a volume comparison between the project database hydrogeologic units and the model hydrogeologic units.

A primary objective of their study is to analyze how accurately grids of increasing resolution capture this complex structure and simulate flow. At what resolution is the geometry of the material distribution accurately represented with a structured grid in order to model fluid flow through the aquifer? Because higher grid resolution is more computationally expensive, this information can be used to determine what the desired accuracy of the result is and at what resolution of grid that accuracy would be attained.

<u>Saturated-Zone Unstructured Mesh from Stratamodel Geological Model</u>. Software has been developed to automate the steps required to create a finite-element mesh for flow and transport calculations from a geological framework model.

The steps required to create a grid are:

- Convert Stratamodel Stratigraphic Framework Model (SFM) provided by USGS to hexahedral finite-element grid

- Remove zero volume elements from data structure
- Remove elements with vertical height less than one meter
- Convert hexahedral elements to tetrahedral elements
- Add the points defining the potentiometric surface (surface provided by the USGS)
- Add nodes with specified *xyz* location for measured well-head calibration
- Add nodes above and below well-head calibration nodes to enhance grid quality
- Add buffer zones above potentiometric surface and below bottom boundary
- Assign material values to all nodes
- Optimize the grid connectivity to insure positive finite-element coefficients
- Calculate Voronoi control volumes
- Output node coordinates, node connectivity, nodal volumes, and material and boundary lists

All file conversion, gridding, node distribution, property interpolation, quality checking, and output is carried out within a single integrated gridding tool kit. The authors (ZYV97) believe that this approach insures that the steps taken are reproducible and traceable and modifications to any step in the gridding process can be done without a great deal of labor.

<u>Grid Generation and Property Interpolation</u>. Generation of grids and interpolation of properties from the hydrostratigraphic model onto the numerical grids is performed with GEOMESH/X3D. GEOMESH/X3D is also used for comparing results from different grids, each having different resolution or grid structure. Interpolation with GEOMESH/X3D allows for the superposition on mesh A of the attributes (material number, pressure, saturation, concentration, etc.) belonging to mesh B. This utility is useful when refining a mesh or when comparing meshes of different resolution. The meshes should generally be of the same volume but do not have to coincide exactly. They do not need to have the same discretization, resolution, or element type. Either mesh can be structured or unstructured. For interpolation, a node of mesh A is first located within an element of mesh B. The attributes of the nodes defining the element in mesh B are

then linearly interpolated to the node in mesh A. Output of mesh A from GEOMESH then contains the new attribute values associated with each node. If desired, the mesh-A node is also assigned the material number of the mesh-B element. Elements of mesh A can then be assigned material numbers based on the nodal material numbers that were interpolated from mesh B.

The saturated-zone model domain selected for their grid resolution study is defined by Nevada State Coordinates of 533,340 m to 563,340 m in an east-west direction, 4,046,782 m to 4,091,782 m in the north-south direction, and -754 to 1332 m vertically above sea level. Nineteen materials are assumed located within this volume.

Although a calibrated model must have appropriate heads at each inlet and outflow boundary, to test the resolution of the various grids used, the actual pressure differential between the north and south is not important. For simplicity, a pressure difference of 15 MPa is used for all simulations in this grid resolution study. The isothermal site-scale flow model is run to steady state and the flow out of the model is compared for each grid. The problem was designed to study the errors made only in the representation of the hydrostratigraphy. This was achieved by specifying pressures on the north and south faces of the grid. Thus, the solution is a linear variation in pressure with a corresponding constant flux. Tests with homogeneous meshes confirmed this result. The differences in reported fluxes are a result only of representation errors of the hydrogeologic units. The outlet flux was chosen as the parameter to compare because this parameter is likely to be a primary factor in assessing radionuclide transport to the accessible environment. This flow was obtained by summing the outflow at the south boundary of the model. The flow volumes exhibit asymptotic behavior at higher resolution. Because higher grid resolution is more expensive, this type of analysis is used to determine what the desired accuracy is and at what resolution that accuracy would be attained.

The results of the flux changes with grid resolution can be more easily understood in terms of average grid spacing. The range of grid spacings in the vertical direction is from 696 m to 70 m. The results of the grid resolution study suggest that for saturated-zone flow computations, 100-m vertical grid resolution may be sufficient if structured or finite-difference gridding is used. This resolution is a finer grid than is commonly used in saturated-zone simulations of Yucca Mountain. In the subsection below, runs with unstructured-grid representations are presented to determine the resolution necessary for unstructured grids. The authors (ZYV97) anticipate that the restrictions of grid resolution will be somewhat relaxed if the stratigraphy is captured directly in the unstructured numerical grid. However, note also that this grid resolution study was conducted using total outflow water flux. If a criterion based on radionuclide transport was used, the result would most likely imply the need for higher grid resolution due to the nature of simulating transport using the advection-dispersion equation. The authors (ZYV97) believe that selective grid refinement in the region near the repository and close to the water table in the pathways to the accessible environment will be required for radionuclide transport.

Unstructured Grid Studies. As stated in above, it is anticipated that the unstructured grid would produce closer flux agreement between grids of different resolution than the structured study. To investigate this hypothesis, the authors (ZYV97) generated a finer-resolution model by refining the stratigraphic framework model (SFM). This model has approximately 2X resolution in the *x*, *y*, and *z* directions. The volume of each stratigraphic unit is identical to the lower-resolution model. The boundary conditions used are the same as in the structured grid studies-- that is, a 15 MPa difference between the north and south faces with no flow on the top, bottom, east, and west. Again, the flux flowing out of the south face is compared. The results were 3,290 kg/s for the lower-resolution model (9,279 nodes) and 3760 kg/s for the higher-resolution model (49,895 nodes). The flow rates differ by about twelve percent. The authors (ZYV97) believe that the results indicate that the flow calibration with the lower-resolution model is sufficient but some caution is warranted. The authors (ZYV97) also indicate that time constraints precluded additional resolution studies, and conclude that these studies point to a need to systematically study grid refinement and its relation to both flow and transport.

Grid Refinement Around Plumes. To adequately model contaminant transport through porous media, a computational grid will require refinement beyond that required for flow modeling. This requirement is true of the grid used for USGS/LANL site-scale saturated-zone flow simulations of the regional aquifer beneath Yucca Mountain discussed in Section VI.2.1.1 (CZA97). The authors (ZYV97) of the transport modeling study developed an approach for grid refinement that refines only that part of the grid where most contaminant migration occurs, thus minimizing the number of nodes added to the grid to assure an accurate transport solution. The refinement technique uses the results of a transport solution computed on a grid that is expected to be too coarse for an accurate transport solution. The preliminary coarse grid is then refined in the region where most contaminant migration occurs (e.g., within a specified isoconcentration surface). The flow and transport solution is recalculated on the refined grid. This grid may then be refined again within an isoconcentration surface that is generally of lower concentration than used for the initial refinement. Refinement is complete when the breakthrough curves computed at some compliance point no longer vary within a specified tolerance level. This approach is a form of adaptive mesh refinement that uses the problem solution to guide the refinement process. The technique, which uses the GEOMESH/X3D grid-generation system, was first tested on a rectangular grid with a single porous medium. This case is discussed, as it is useful in explaining the refinement methodology. The technique, tested below, was planned to be employed in FY98 to the 250-m sampled SFM currently being developed by the USGS.

For the single porous media test, a criterion is needed to determine when the grid is adequately refined. The authors (ZYV97) chose to look for convergence in the breakthrough curve at a downstream compliance point. The breakthrough monitoring location was chosen as the uppermost, central node of the grid at the downstream boundary. The authors (ibid.) found that the original constant-concentration source used for grid refinement results in different solute mass-flux input rates with the different grids. Therefore, transport solutions were rerun with the various grids using constant tracer flux so that each simulation would receive the same mass, and the breakthrough curves could then be compared. As the grid is refined, breakthrough to the monitoring point advances slightly in time and the steady-state breakthrough concentration generally increases. This result occurs because the plume exhibits less numerical dispersion around its centerline and with depth. There is little difference between the solutions for the grids with 28,511 and 57,450 nodes indicating that the 28,511-node grid is adequately refined. It should be noted that if values of dispersion or time steps are changed the grid may not be sufficiently refined.

The authors (ibid.) indicate that future work will apply the refinement technique discussed above to the USGS/Los Alamos multiple-material saturated-zone model. Refinement will be based on the concentration of a steady plume generated with the calibrated flow field. Nodes added during refinement are assigned material properties based on the original SFM discussed previously. The original nodes remain in the grid and retain their material properties. Refinement of the USGS/Los Alamos model was not pursued in this study. The authors (ibid.) indicate that the coarse 1500-m spacing of the current SFM is inadequately refined to justify refinement for transport simulations. They further note that an updated SFM with 250-m spacing will be incorporated in future work. The authors (ibid.) also believe that this refined SFM has adequate stratigraphic information to work ideally with the concentration adaptive mesh refinement technique.

Initial and Boundary Conditions

The form of the flow boundary conditions employed in obtaining a calibrated model plays a large role in the model results, especially with respect to subsequent transport predictions. A model calibrated to measured head values is a nonunique solution that must be constrained with measured or estimated flux values at boundaries. Simply put, if only head boundary conditions are used, the total flux is directly proportional to the values of permeability in the model; increasing or decreasing each permeability value by a fixed ratio changes the total flux by that same fraction. At the site scale, the flux values into and out of the flow domain cannot be directly tied to major recharge and discharge values because these occur outside the model domain. Because this is the case, there is a need to tie the flux values into and out of model faces to a larger-scale model. The authors (ZVY97) intend to further investigate the interplay between the calibrated regional model and the site-scale model.

The original plan for the site-scale model was to use fluxes or head data from the regional model as boundary conditions for the site-scale model. However, there are several problems in applying fluxes directly. The first is that the site model has sixteen units represented within its boundaries, whereas the regional-scale model represents only three units in this region. This difference presents problems in assigning fluxes to nodes with widely varying permeabilities. The second problem is that the calibrated heads for the regional model deviated the most from well data near the northern boundary of the site-scale model. Thus, fluxes were apt to be most inaccurate in that region. Because of these problems, the fixed head boundary conditions were derived from measured head data. Because of the fixed head conditions, solutions are valid for permeability ratios only. Fluxes must therefore be compared to those predicted by the regional-scale model to insure consistency.

Because of the need for finer resolution (primarily in the z direction), the site-scale model was developed with a smaller horizontal extent than previous site-scale models. The model dimensions are approximately 30 km by 45 km. The compilation of all relevant data was done by the USGS, and these data were then organized into a Stratigraphic Framework Model. The SFM provided the basis for all grid generation. The grid building effort produced 15 grids for testing. The grid used in the calibration was on a 1500 x 1500 m areal spacing that consisted of 5,485 nodes, 29,760 elements, and 40,548 internode connections. The calibration of this model is described in section VI.2.1.1. A good calibration on an initial modeling exercise was obtained, but large flux values pointed to a systematic error in the geometric part of the flow terms. This problem was subsequently corrected, and the flow results revealed more realistic fluxes. The corrected model results were performed on a grid containing 9,279 nodes, 52,461 elements, and 67,324 internode connections. The increase in the number of nodes was due to the inclusion of model "buffer zones" that play no part in the solution but improve the definition of the potentiometric surface. These zones are assigned values of zero for both porosity and permeability and, therefore, do not enter into the fluid flow calculation. Only the layers sandwiched between the upper and lower buffer zones are part of the flow model itself.

The source term boundary is treated as a mass-flux introduction to the saturated zone.

Model Parameterization

In section VI.2.1.1, a number of unwanted features in the geologic framework model of the current site-scale model are described, that make it difficult to produce accurate transport results in the vicinity of Yucca Mountain. These features do not significantly impact the calibration of the flow model but make simulations problematic. In parallel to producing this calibrated site-scale model, the USGS has been developing an updated geologic framework model with more up-to-date geologic interpretation near Yucca Mountain. The authors' (ZYV97) plan is to develop grids and calibrated flow solutions on this revised model in FY98 and to use this revised flow model as the platform for performing radionuclide transport calculation.

The main difference between the two framework models is that the discretization of the revised-site SFM is finer (250 m) than the older-site SFM (1500 m). This difference leads to smoother transitions between and more realistic representations of the hydrogeologic units. Additional data from the ISM framework model (ZEL96) were incorporated into the 250-m framework model. This approach gives better resolution to the volcanic units. The representation of the upper volcanic confining unit (UVCU, Unit 14) is of importance due to its predominance in the control of the flow beneath the potential repository site. The UVCU appears primarily in the northern half of the 250-m framework model, with relatively isolated bodies in the southern part of the modeled area. The UVCU does not appear as a large body in the central part of the model, as it does in the 1500-m framework model. It appears that the configuration of the UVCU in the 250-m framework model may produce the steep hydraulic gradients in the north, where it exists, and have a less dominant control on the flow field in the southern and central parts, where it does not exist.

With regard to transport, the authors (ZYV97) note that a revised flow model based on this geologic interpretation will correct the problems in the current version and allow realistic simulations from the potential repository to hypothetical accessible environment locations as far as 25 km from the site.

Model Calibration

The transport model used the flow field of the calibrated sub-site model to predict contaminant transport migration directions and velocities. Since there is no contaminant field data (e.g., existing contaminant concentrations in monitoring wells) on which to perform a transport calibration the authors (ZYV97) did not conduct any further model calibration.

Predictive Simulations

Several models and numerical techniques are used to obtain results for radionuclide transport in the saturated zone. First, a technique based on numerical convolution is developed to link the unsaturated-zone breakthrough curves at the water table to the saturated-zone transport system. In this method, the inputs are the mass flux of radionuclides reaching the water table versus time, along with a generic breakthrough curve in the saturated zone, computed as the response at a downstream location to a constant injection of radionuclides at the footprint of the proposed repository. The numerical implementation of the method was verified by performing a full calculation using the actual time-varying input from an unsaturated-zone calculation as input to the saturated-zone model. The method allows a variety of input flux curves to be computed quickly without recomputing the saturated-zone calculation each time. Assumptions inherent to the convolution technique include steady-state flow and linear transport processes, which, for sorption, implies that the linear-sorption isotherm model must be used. The authors (ZVY97) believe that the linear-K_d sorption model is not overly restrictive because one can select a K_d value that conservatively bounds the sorption behavior predicted by a nonlinear-sorption isotherm model.

Before proceeding to more complex site-specific models, a simplified three-dimensional flow and transport model is presented to examine the importance of several transport parameters that are difficult to investigate fully with the current site-scale models. Dispersivity is established as one of the key uncertain parameters that influence the concentration (and hence dose) at accessible environment compliance points. The transverse dispersivity is actually a more sensitive parameter for dilution because it governs the degree of lateral spreading of the plume.

Matrix diffusion, established as a valid process in the field test of Reimus and Turin (REI97), affects the breakthrough times at a downstream location but, to a first approximation, does not influence the peak concentration unless radioactive decay is significant. Another important factor regarding matrix diffusion is that it allows radionuclides to contact minerals in the rock matrix that potentially sorb radionuclides. Even small amounts of sorption have a large effect on breakthrough times and peak concentrations. Finally, this simplified model was used to illustrate that the saturated-zone transport system has the ability to dilute spikes of high concentration and short duration that come from bypassing of the unsaturated zone through fractures. Thus, the authors (ZYV97) believe that the saturated zone provides an important component in a "defense-in-depth" strategy in which uncertainties leading to poor performance in one part of the repository system are mitigated by the performance of another radionuclide transport barrier.

To simulate radionuclide transport from the footprint of the repository to a 5-km compliance point, the sub-site-scale model was used. This model was chosen as an appropriate substitute to performing these calculations using the site-scale model because of the more accurate representation of the geology near Yucca Mountain. When the site-scale model is revised to use the new hydrostratigraphic data based on a 250 x 250-m geologic grid, all calculations will be performed with the site-scale model itself. The sub-site-scale flow model captures the large hydraulic gradient and flow through the geologic strata of relevance downstream of the repository footprint, including the Prow Pass, Bullfrog, and Tram Tuffs units. Radionuclides travel to the east and south from the footprint to a 5-km compliance point. Releases into the Prow Pass unit travel in a more easterly direction than releases in the other units; releases into the Tram unit at the south end of the footprint travel almost due south. All releases follow the dipping stratigraphy, indicating downward movement of radionuclides. This effect may be important if upcoming field studies reveal more reducing conditions with depth, because sorption coefficients of ^{99}Tc and ^{237}Np are likely to be much higher and solubilities much lower under reducing conditions.

Transport times to a hypothetical 5-km compliance point under conditions in which the effective porosity is the matrix porosity are on the order of a few thousand years; much shorter transport times result from an assumption of less matrix diffusion. However, the extent of matrix diffusion itself only influences the arrival time rather than the concentration at the downstream location. This effect is in contrast to differences in fluid flux that may occur due to future wetter climates, which result in earlier travel times but may also lower concentrations (greater dilution).

Sorption of radionuclides such as ^{237}Np onto zeolitic tuffs in the saturated zone also leads to significant retardation and longer travel times to a 5-km compliance point.

The results of the sub-site-scale model are then used as input to transport calculations to a hypothetical 20-km compliance point in the site-scale model. Simulations assuming both fracture-like and matrix-like effective porosities in the fractured tuff were performed to investigate the importance of this parameter. In both simulations, the alluvium present along the transport pathways were assigned high porosity. In this set of calculations, the nature of transport in the fractured tuffs is less important as the system becomes increasingly dominated by long predicted travel times in the alluvium. Thus, even if the tuffs are presumed to have a low effective porosity, travel times of 10,000 years or more are predicted in the alluvium alone. Furthermore, the results show that even small amounts of sorption in the alluvium shift travel times to values on the order of 50,000 years, and predicted concentrations at the compliance point are lower than in the absence of sorption. Clearly, for more distant compliance points, the flow and transport behavior of the alluvium becomes increasingly the controlling factor in saturated-zone performance.

The influence of repository heat on saturated-zone flow and transport of radionuclides is also studied using the subsite-scale model. Repository waste heat creates a zone of higher-than-ambient temperature that extends vertically into the saturated zone and along the prevailing flow pathway from the repository. However, the predicted impact on transport of ^{99}Tc to a 5-km compliance point is very small. One outstanding issue related to repository heat is the possibility of temporary or durable changes to the permeability and porosity due to temperature-dependent rock-water interactions. If these effects turn out to be minor, then repository waste heat has minimal influence on the migration of radionuclides through the saturated zone.

Integrated transport predictions are presented in which are linked to the unsaturated-zone transport model of Robinson et al. (ROB97) with the subsite-scale model to predict the transport of the key radionuclides ^{99}Tc, ^{237}Np, and the isotopes of plutonium. In Robinson et al. (ROB97), the authors investigated the performance of the unsaturated-zone system for different infiltration rates that could result from changes to the present-day climate. These predictions of radionuclide mass flux at the water table are input to convolution calculations to predict the combined unsaturated/saturated-zone performance at 5 km. For the unsaturated-zone performance predicted in Robinson et al. (ROB97), the integrated response in the saturated zone for ^{237}Np and ^{99}Tc is a direct consequence of dilution of percolating unsaturated-zone fluid with flowing saturated-zone ground water. Therefore, poorer predicted unsaturated-zone performance under wetter future-climate scenarios translates directly to higher predicted concentrations in the saturated zone. Sorption onto zeolites in the saturated zone should provide a considerable delay in arrival times for ^{237}Np. For plutonium, rather than climate change or sorption to the host rock, the key factor influencing concentrations is the propensity of plutonium to sorb to mobile colloids.

Regarding the nature of flow and transport in the fractured tuffs, the authors (ZYV97) experimented with different flow and transport models to investigate different methods of simulating this dual-porosity system. A dual-porosity particle-tracking model for transport was invoked, and the influence of matrix diffusion properties was examined. The results follow those of the matrix-diffusion conceptual model, but several factors argue against its use in large-scale transport model predictions. First, the particle-tracking module does not at present handle the dispersion coefficient tensor formulated as longitudinal and transverse components. Furthermore, although the diffusion model accurately simulates the case of diffusion into an infinite matrix continuum, finite fracture spacings are not part of the model as currently constituted. Therefore, particle tracking cannot be used in site-scale models. A finite-element dual-porosity solution was also investigated. As expected, the dual-porosity flow simulation yielded virtually identical steady-state results to the single-continuum model. Transport results captured the two extremes (fracture-dominated and pervasive matrix diffusion) but failed to produce accurate results for small but non-negligible diffusion into the rock matrix.

VI.2.1.3 TSPA-VA Implementation of Saturated Zone Modeling Analysis

The Saturated Zone Flow and Transport Technical Basis Document for the Total System Performance Assessment - Viability Assessment provides a detailed description of the means by which the saturated zone flow and transport modeling, as presented in sections VI.2.1.1 and VI.2.1.2, has been integrated into the total system performance. The following sections outline the basic components of the saturated zone modeling performed in the TSPA-VA.

Synopsis of TSPA-VA Approach

Past TSPAs focused on the biosphere interface located 5 km from the repository. Alternatively, the TSPA-VA is now focused on calculating radionuclide doses 20 km downgradient from the repository; the DOE indicates that this is due to changes in guidance that were based upon recommendations from the National Research Council (NRC95).

As presented in the previous sections, numerical models were used for the purpose of characterizing and understanding the flow and transport at the regional, site and sub-site scales and to perform TSPA-VA calculations. The conceptual models, upon which the numerical models were developed are based upon all available data and knowledge about the saturated zone. Likewise, the TSPA flow and transport models were developed based upon site knowledge, input from the workshops and expert elicitations, as well as insights provided by the numerical modeling results.

To support TSPA-VA calculations a base-case numerical model was developed for the saturated zone to evaluate the migration of radionuclides from their introduction at the water table below the repository to the release point to the biosphere. In order to estimate the uncertainty associated with the base case scenario, sensitivity analyses were also performed.

A hierarchy of models was used to simulate the movement of ground water and the transport of radionuclides in the saturated zone. Explicit, two- and three-dimensional modeling was not used to simulate radionuclide concentrations because it can generate numerical dispersion, which artificially lowers the concentrations, particularly when matrix diffusion is occurring. The TSPA 3-D saturated zone flow model as described in the preceding sections was used only to determine flowpaths through the saturated zone and potential impacts due to climatic change which are discussed later in this section. The TSPA 1-D saturated zone transport model was developed based on the flow paths from the 3-D flow modeling and used to determine concentration breakthrough curves at a distance of 20 km for unity release of radionuclides from six streamtubes. The saturated zone transport component of the analysis was linked to the transport calculations for the unsaturated zone through which contaminants migrate downward in percolating ground water from the repository to the water table (e.g., the spatial and temporal distributions of simulated mass flux at the water table). The linking was accomplished by using the convolutional integral technique to combine the unit breakthrough curves calculated by the TSPA one dimensional saturated zone transport model with the time-varying radionuclide sources from the unsaturated zone. Changes in the saturated zone flow and transport system in response to climatic variations were incorporated for the three discrete climate states (dry, long-term average, and superpluvial) considered in the other components of the TSPA-VA. Specific discharge and volumetric ground water flow rate in the saturated zone stream tubes were scaled in transport simulations to reflect climate state. The saturated zone transport results were linked to the biosphere analysis by the simulated time history, or system response as a function of time, of radionuclide concentration in ground water produced from a hypothetical well located at the biosphere interface. The biosphere was assumed to be located 20 km from the repository. Radionuclide concentrations in the hypothetical well water were then used in the biosphere component to calculate doses received by the public.

For the base case, uncertainty in the saturated zone system was evaluated through Monte Carlo variation in the input parameters used in the TSPA one dimensional saturated zone transport model. Primarily, the uncertainty in radionuclide transport parameters was evaluated. The one-dimensional saturated zone transport model was used to calculate 101 unit breakthrough curves (100 Monte Carlo simulations and the expected value or base case). The results of the one dimensional saturated zone transport calculation are located in a "family" of unit radionuclide concentration breakthrough curves. For each TSPA-VA Repository Integration Program (RIP) realization, a saturated zone unit breakthrough curve was randomly selected for use in the convolution integral method.

The TSPA-VA sensitivity studies were designed to examine five of the key issues related to the base case saturated zone analysis assumptions. The sensitivity studies were performed to provide information about the importance of these issues with respect to repository performance. The effect of dilution in the saturated zone and vertical transverse dispersivity was investigated to address concerns from the Saturated Zone Expert Elicitation Panel. The impact of including heterogenity and large-scale flow channelization in a three-dimensional flow and transport model was also studied. A two-dimensional dual-porosity transport model was used to calculate radionuclide concentrations to examine the effect of the base case assumptions of a single continuum and using effective porosity as a surrogate for the matrix diffusion process. In addition, alternative conceptual models of colloid-facilitated plutonium (Pu) transport were developed and implemented for sensitivity analysis.

<u>TSPA Flow System Conceptualization</u>

<u>Regional-Scale Saturated Zone Flow Model</u>. The regional-scale 3-D flow model for the TSPA-VA was developed by D'Agnese et al. (DAG97a) to characterize the conditions of the present day ground water flow in the Death Valley region. The numerical code used for the regional

flow model was MODFLOWP (HIL92). MODFLOWP is an adaptation of the U.S. Geological Survey 3-D, finite-difference modular ground water flow model, MODFLOW (MCD88).

The finite-difference mesh used for the USGS regional flow modeling consists of 163 rows, 153 columns, and three layers. The grid cells were oriented north-south and were of uniform size, with side dimensions of 1,500 m. This results in a modeled area that is 244 km long and 229 km wide. The layers represent conditions at 0-500 m, 500-1,250 m, and 1,250-2,750 m below the estimated water table. The first and second layers were designed to simulate local and sub-regional flow paths mostly within the valley-fill alluvium, volcanic rocks and shallow carbonate rocks. The third (lowest) layer simulates deep regional flow paths in the volcanic, carbonate and clastic rocks.

From the perspective of the TSPA-VA, the most important output from the USGS regional scale model was information to determine a ground water flux multiplier for the long-term average and superpluvial climate conditions assumed for the base-case TSPA-VA analysis. The ground water flux multipliers were used to calculate a ground water flux for each of the climate states relative to present day conditions which is required as input to the TSPA one-dimensional saturated zone model discussed later.

With respect to model calibration, the TSPA-VA states:

> *These results* [calibration]*, suggest that additional calibration may significantly improve model accuracy. This analysis suggests that the model is a reasonable representation of the physical system, but evidence of model inaccuracies exists. Inaccuracies in the simulated ground water fluxes in the flow model are generally proportional to uncertainty in the overall ground water budget of the region. The model continues to undergo development for future use by the YMP and the environmental restoration program at the Nevada Test Site.*

<u>Site-Scale Saturated Zone Flow Model</u>. Note: In a number of places the TSPA appears to be inconsistent with the actual reference documents. For example, in Milestone SP25CM3A (ZYV97) that describes the site scale modeling work it is indicated that the modeled area is 30 by 45 km, rather than 20 by 36 km as indicated in the TSPA.

The site-scale flow model developed by Zyvoloski et al., (ZYV97) and used to support the TSPA-VA was developed using FEHM (ZYV83). The 3-D flow model that was developed incorporated an area of about 20 km by 36 km to a depth of 950 m below the water table. The model grid is a uniform orthogonal mesh with 500-m x 500-m x 50-m elements.

The results of the site-scale model calibration appear to be better than that for the regional scale model. The results of the site-scale saturated zone flow model were used in the TSPA to estimate flow path lengths and directions through each of the hydrostratigraphic units downstream from the repository. This was done via a particle-tracking analysis, which only simulates advective flow and does not account for dilution due to dispersion. The calculated flow path lengths were incorporated into the 1-D saturated zone transport simulations discussed below.

The TSPA states, with regard to limitations, in the site-specific flow model:

> *The main concern is related to the problem of large numerical dispersion inherent with the use of a relatively coarse grid (cell size is 500 m x 500m x 50 m) when performing transport calculations. The desire to minimize spurious transverse dispersion for the SZ analyses necessitated the use of 1-D streamtubes for the transport calculations of the SZ analysis, which could be more finely discretized (grids spaced at 5 m intervals).*

One-Dimensional Saturated Zone Transport Model

The TSPA 1-D saturated zone transport model was developed to simulate the radionuclide concentration breakthrough curves that form the basis of the TSPA-VA calculations performed with the RIP computer program. Each radionuclide was transported separately in the analysis. The DOE indicates that they chose the 1-D transport simulation method because *of the desire to eliminate spurious dilution of the radionuclide concentration resulting from numerical dispersion, which can occur in coarsely gridded 3-D solute transport simulations.*

The DOE goes on to state that *Solute transport simulation using a 1-D numerical model precludes dilution from transverse dispersion, by definition. The dilution from transverse dispersion was explicitly specified in this modeling, as a post-processing step. This dilution factor was treated as a stochastic parameter, as described in Section 8.4.2.* Essentially, the DOE dilutes the concentrations of the radionuclides reaching the down gradient well by a factor of 1 to 100, which they obtained from the expert elicitation panel estimates.

The six stream tubes for the 1-D transport simulations can be conceptualized as follows: They are a combined width of 3,000 m and range between 10 and 20 m in vertical depth. This depth is important as it will have a significant impact on dilution. The volumetric flow rate of the ground water through each streamtube was determined at the water table from flow simulations using the site-scale flow model developed by Bodvarsson et al. (BOD97) for the unsaturated zone. The cross-sectional area of each streamtube was specified to be proportional to the volumetric ground water flow area. The specific discharge within the streamtubes in the saturated zone was 0.6 m/y for current climatic conditions.

Simulations of the radionuclide transport in the saturated zone for the TSPA-VA calculations were performed using FEHM. The streamtubes were 20 km long, with regular grid spacing in the tubes of 5 m. The radionuclide 1-D transport simulations were performed assuming a steady, unit (1 g/y) radionuclide mass source at the upstream end of the streamtube (i.e., the water table at the base of the unsaturated zone below the water table). Transport of each radionuclide was simulated separately in the 1-D simulations. Transport simulations with the 1-D stream tube approach implicitly assume complete mixing of the radionuclide in the volumetric ground water specific to each streamtube.

The convolution method was used in the TSPA-VA calculations to determine the radionuclide concentration in the saturated zone, 20 km downgradient of the repository as a function of the transient radionuclide mass flux at the water table beneath the repository.

<u>Implementation with the RIP Computer Code</u>

With the exception of the potential for colloidal transport of plutonium, all of the saturated and unsaturated zone flow and transport parameters were sampled independently in RIP. At each time step within the RIP simulation, the current climate state and the radionuclide mass flux at the water table for each of the radionuclides from each of the six source subregions were passed to the convolution integral subroutine. The convolution integral subroutine calculated the concentration of each radionuclide for each of the six streamtubes at the 20 km distance from the repository for that time step, including reduction of concentration from the dilution factor as discussed in the next section. The simulated radionuclide concentrations were passed by the RIP simulator to the biosphere component of the TSPA-VA at this point for dose calculation.

Development of Parameter Distributions and Uncertainty

The DOE indicated that the key uncertain parameters in the analysis were the following: (1) effective porosity in the volcanic units and the alluvium/undifferentiated valley-fill unit; (2) distribution coefficients for sorbing radionuclides; (3) the ratio of the radionuclide mass in aqueous and colloidal forms for colloid-facilitated transport of plutonium; (4) longitudinal dispersivity; (5) the fraction of flowpath through the alluvium; and (6) the dilution factor.

A seventh uncertainty that should have been included is the degree to which fractures and matrix are interacting (i.e., importance of matrix diffusion).

Uncertainty in radionuclide transport through the saturated zone was incorporated in the TSPA-VA by varying key transport parameters for 100 realizations. All input parameters required for the transport model were assumed to be either stochastic with an associated distribution or constant. If the parameter was assumed to be stochastic, its distribution was determined and then sampled using the Latin Hypercube Sampling module of the RIP code to obtain 100 sets of input parameters. Since LHS tends to underestimate the variance on the mean, the DOE should ensure statistical convergence.

The Saturated Zone Expert Elicitation Panel provided input for the input parameters and distributions. For example, the panel estimated that the dilution factor ranged between 1 and 100 with a median value of about 10.

VI.2.1.4 Saturated Zone Information Needs

TSPA-VA Identified Needs

Regional Scale Flow Modeling

The Death Valley regional flow system consists of ground water moving through a 3-D body of consolidated and unconsolidated materials. The 3D hydrogeologic framework model described the characteristics of this saturated volume. The upper boundary of the flow system is the water table. The lower boundary of the flow system is located at a depth where ground water flow is dominantly horizontal and moves with such small velocities that the volumes of water involved do not significantly impact regional flow estimates. The lateral limits of the regional flow system may be either no-flow or potential-flow boundaries. No-flow conditions exist where ground water movement across the boundary is prevented by physical barriers or divergence of ground water flow paths. Flow exists where ground water potentiometric gradients permit flow across a boundary.

For purposes of conceptualization and subsequent numerical simulation, the limits of the flow system for the regional model were selected based on reevaluation of previously defined flow system boundaries, the potentiometric surface developed for the regional modeling study, and the hydrogeologic framework model. Very little hard data exist to support a precise definition of the western extent of the flow system. The western boundary of the flow system is therefore placed to coincide with the eastern edge of the Death Valley saltpan which is interpreted as the terminal sink of the flow system.

The water budget for the Death Valley regional ground water flow system is difficult to compute, because inflow and outflow volumes are poorly defined for many areas. In addition, the large size of this regional system precludes the comprehensive and accurate assessment of all inflows to and outflows from the system. Previous attempts to estimate water budgets for various parts of the flow system did not use consistent boundaries, so the budgets cannot be readily compared. The regional model uses a lumped-budget approach; each component of the ground water budget is defined by a single lumped value even though it may have been calculated originally for separate areas in the basin. This lumped-budget approach permits an encapsulated view of the system, but the authors (ZYV97) point out that errors are inevitable in the estimates. Short of physical measurements modeling is probably the best means of resolving these errors.

Problems with the regional model are indicated by weighted residuals that are not entirely random, indicating some model error. This is related to the occurrence of large positive weighted residuals for hydraulic heads, where simulated hydraulic heads are distinctly lower than the observed values, and large negative weighted residuals for spring flows, where simulated flows are distinctly less than observed flows. The problem is also related to nonnormally distributed less extreme weighted residuals. These results, combined with the previously discussed observation that every model update considered thus far, significantly improved model fit, suggests that additional calibration may significantly improve model accuracy. While the authors (ZYV97) believe that the model is a reasonable representation of the physical system, evidence of important model error exists.

Site-Scale Flow Modeling

Objectives of the modeling. The authors (ZYV97) outlined the objectives of the site-scale model as the following:

1. Provide a large-scale description of the hydrogeologic framework of the site saturated zone flow system based on a sampling of 1500 m by 1500 m mesh;

2. Provide a mechanism to extend model calibration and sensitivity testing of parameters used in the model;

3. Provide the flow field for doing preliminary transport simulations and estimates of ground water travel time through the use of additional transport related capabilities within FEHM; and

4. Provide initial estimates of permeability for 16 hydrogeologic units from the SFM and two additional zones of small permeability and recharge at Fortymile Wash.

Model Limitations

The authors (ZYV97) outlined the model limitations as follows:

1. **Simulations are restricted to fully saturated conditions from the water table and below.** Although the model was built using a framework model that extended to land surface, the unsaturated zone was not included as part of the flow model. The unsaturated zone was omitted because of time constraints and the long execution times for forward simulation runs associated with two-phase flow problems.

2. **The model does not account for variations in temperature within the flow system.** Temperature varies within the ground water flow system and may be a useful constraint in identifying acceptable model representations of both temperature and hydraulic head. The preliminary status of the model limited the extent to which temperature could be evaluated. Furthermore, the temperature of the system was specified at a uniform 44°C which may be too high to represent the average temperature.

3. **It is likely that the flow model is non-unique.** Coordinated adjustments in permeability values (either higher or lower by some multiplier) might lead to similar hydraulic head distribution and calibration. Because fluxes were not specified explicitly at either the upgradient or downgradient ends of the model, the

model is less constrained as it would be with fluxes included in the calibration. However, because some permeability values (of admittedly minimal accuracy) were specified explicitly throughout the parameter estimation, the model was partially constrained which likely caused the parameter estimation process to converge in many instances.

4. **The large hydraulic gradient is poorly understood and greatly affects model calibration, simulated permeability values, and flux.** Additional data and testing are required to adequately characterize this feature. Testing and reconfiguration of monitoring intervals within borehole USW G-2 could be done to provide permeability, flow-survey, temperature, and hydraulic-head data at different depths, particularly for the middle volcanic aquifer. Construction of additional boreholes in the large hydraulic gradient area, such as a corehole into the middle volcanic aquifer adjacent to drillhole WT-6, could provide useful vertical gradient, hydraulic-head, saturation, and permeability data. The authors (ZYV97) believe that the site-scale model was successful in representing the large hydraulic gradient through the incorporation of a vertical barrier to flow, but other representations are possible.

5. **Flux into the site model domain is poorly defined and remains one of the most elusive of model variables.** The quality of the model is in part a measure of the understanding of the distribution and amount of recharge within the model domain. Comparison of fluxes into and out of the model is dependent on available data, which although greatly lacking will not likely be improved substantially through additional field studies. Water levels within the flow system could still be adjusting to recharge supplied during climatically wetter conditions. If such a condition exists, the effect may be too subtle to observe with the available hydraulic data. Adjusting water-level conditions could be evaluated using the regional model to replicate conditions necessary to observe the effect of increased recharge under past wetter climates.

6. **Limited hydraulic-test data exist for constraining permeability values used in the model.** Few hydraulic-test data are available that involve multiple observation wells within the model domain from which huge-scale transmissivity or hydraulic conductivity values can be derived. The exception to this condition is the C-hole-complex hydraulic testing which is optimally located for conditions at Yucca Mountain and provides a test involving a large volume of the middle volcanic aquifer. However, the C-hole testing is in a highly fractured area and might not be representative of the entire area. In general, the model does not distinguish between the permeability of the rock matrix, fractures, or faults. It is possible to add large-scale features such as faults explicitly within the model by regridding, but hydraulic characteristics for faults in the saturated zone are not presently available.

7. **Definition of the hydrogeologic units within the model is limited by the sampling interval used (1,500 m).** By sampling the framework model at a smaller interval (for example, 250 m) better resolution of the hydrogeologic units could be obtained. but resulting in a larger computation mesh. Experience from the site-scale modeling exercise suggests that this approach is warranted and likely would succeed. However, higher resolution sampling alone may be insufficient to explicitly represent faults.

As noted above, comparisons of flux from the regional model showed almost twice the amount discharging from the southern end of the site model, and substantially different amounts for the north and east sides. The major flux differences between the two models occur in the northeast corner where a large part of the recharge from the north is diverted east and discharges in part because of the interaction of the constant-head boundaries and the imposed east-west barrier needed to represent the large-hydraulic gradient.

The authors (ZYV97) observe that on initial inspection, model match to hydraulic-head data and the resulting distribution of residuals have some problems. Although permeability values for all of the hydrogeologic units used in the model lie within reported literature values, reported values for individual units have large ranges. Furthermore, in the case of the middle volcanic aquifer, values of permeability from large-scale hydraulic testing at the C-hole complex were three orders of magnitude larger than those used in the model. This discrepancy may be indicative of model error, or alternately, the possibility of a local, large-permeability zone not represented in the present model. Finally, any model calibrated using hydraulic heads alone is subject to error in simulated flux.

Improvements suggested by the authors (ZYV97) for future model developments include:

- Conduct sensitivity analyses with regard to which model variables have the greatest effect when varied on the sum of squared residuals for hydraulic head. This would provide a guide for additional field studies to reduce uncertainty in the model.

- Refine hydrogeologic framework model to better define the distribution of the hydrogeologic units. In particular, the upper volcanic confining unit is currently over-represented. This discrepancy substantially influences simulated flow and transport simulations.

- Use higher resolution sampling of the hydrogeologic framework model to better delineate unit offsets caused by faulting. This would result in a denser finite-element mesh, resulting in longer execution times, but would provide a more realistic portrayal of the flow system than is available in the model.

- Add major faults explicitly as surfaces within a refined version of the hydrogeologic frame-work model, so that their potential as barriers to flow or as fast pathways to the accessible environment may be evaluated.

- Decouple permeability parameters for the upper and middle volcanic aquifers to the extent practical during model calibration. This separation of the two primary volcanic aquifers at Yucca Mountain within the model would better represent the permeability distribution.

- Recalibrate the existing model with larger values of permeability in the middle volcanic aquifer and the upper volcanic aquifer.

- Incorporate additional data into the formal model calibration. This could include flux data from the regional model for at least one face of the model and borehole-temperature data to better constrain the solution.

- Fluxes should be extracted from a refined, improved version of the USGS regional model of D'Agnese et. al. (in press) in which the topmost layer has been subdivided to better represent the hydrogeologic units at Yucca Mountain and in the Amargosa Desert.

- Include vertical flux through the bottom of the model based on regional model values.

- Use hydrochemical and isotopic data as a check against flow model results.

<u>Sub-Site-Scale Flow Modeling</u>

For the sub-site scale modeling the authors (COH97) reached a number of conclusions regarding the adequacy of the existing data base. These conclusions/recommendations include:

- The properties of the Bullfrog need further characterization since (a) this unit is by far the most important for flow in the saturated zone due to its large fracture permeability, and (b) it underlies the repository at the water table.

- Fault properties need further characterization due to their obvious effects on flow at the sub-site scale.

- Measurements of fracture porosity must be made so that models can better estimate pore velocity.

- Geochemical sampling that considers vertical hydrochemical variations is needed to understand the 3-D nature of flow in the saturated zone.

- Investigation by numerical simulation of the large hydraulic gradient should be undertaken. The authors (COH97) believe that the existing unsaturated and saturated zone models contain enough geologic detail and process modeling capability to make a credible attempt in this direction. Coupling of the two models can be done to facilitate these analyses.

- Because chemical components undergo mixing and dilution due to flow and fracture-matrix interactions, the processes of flow and transport are coupled and should be considered together.

- Additional hydraulic tests and well placement should be designed to focus on fault properties and the Bullfrog unit.

- Extensions of the grid should be made to decrease boundary effects and better model transient pumping tests.

- The grid should be extended spatially to model flow and mixing at greater distances from the repository.

- Advanced visualization techniques should be brought to bear on the problem of elucidating the complex 3-D flows observed in the simulations.

Contaminant Transport Modeling

Conclusions and Recommendations. The authors (COH97) developed the following conclusions and recommendations with respect to the contaminant transport modeling:

- Grid resolution was found to be critical for both flow and transport.

- The transport simulations are very sensitive to matrix diffusion.

- Continue close collaborative effort with the USGS site flow modeling. Continue to update the Stratigraphic Framework Model with the best available data and establish quantitative measures of grid fidelity to the SFM.

- Perform preliminary transport simulations during continued flow calibration efforts. This effort will uncover early possible incompatibilities between the flow and transport conceptual models and will eliminate any problems in sampling frequency that may result in an inaccurate representation of units. This parallel computation may also uncover potential fast paths for radionuclides that can be corroborated or dismissed with supporting thermal or geochemical data. In this way, transport modeling will provide a tool for improving the flow model. By establishing the effect on the radionuclide flux at the compliance boundaries, flow model improvements, such as creating a detailed inlet flux map, may be evaluated with respect to their importance to performance assessment.

- Enlarge the modeling domain of the site-scale model north of the large hydraulic gradient area where the calibration of the regional model is better and the fluxes of the regional model are more defensible. This approach will also allow better redistribution of fluxes from the three-layer regional model to the sixteen-layer site-scale model.

- Use the 250-m sampling of the SFM. This effort will provide sufficient resolution, in the vicinity of Yucca Mountain for transport calculations.

- Use stochastic approach for transport modeling to better characterize uncertainties in the dispersive mixing process occurring at subgrid block scales.

NRC Identified Needs

The NRC is developing a strategy for reviewing the performance of the proposed repository. As currently envisioned, the elements of this strategy necessary to determine acceptability of repository performance are defined by the NRC as key technical issues of the subsystem abstractions. As part of this process, the NRC has developed Acceptance Criteria for the key issues of the DOE TSPA that will ultimately be used to determine the viability of the repository at Yucca Mountain. This NRC evaluation is very relevant in assessing whether the methods and information presented by the DOE have the potential to produce results that are defensible under regulatory reviews.

The two NRC status reports that are most pertinent to ground water flow and contaminant transport are entitled *Issue Resolution Status Report - Key Technical Issue: Unsaturated and Saturated Flow under Isothermal Conditions* and *Issue Resolution Status Report - Key Technical Issue: Radionuclide Transport.*

The following discussion is organized by key technical issues. Under each issue, the NRC's Acceptance Criteria are presented and their assessment as to whether DOE has met the Criteria is provided.

NRC's Issue/Subissue Statement

The NRC developed these Issue Resolution Status Reports with the primary objective to assess all aspects of the ambient hydrogeologic regime at Yucca Mountain that have the potential to compromise the performance of the proposed repository. The secondary objective was to develop review procedures and to conduct technical investigations to assess the adequacy of DOE's characterization of key site- and regional-scale hydrogeologic processes and features that may adversely affect performance. The primary issues identified by NRC with respect to the hydrologic regime are the following:

- Hydrologic Effects of Climate Change
- Present-Day Shallow Infiltration
- Deep Percolation (Present and Future)
- Saturated Zone Ambient Flow Conditions and Dilution Processes
- Matrix Diffusion
- Radionuclide Transport Through Porous Rock
- Radionuclide Transport Through Alluvium
- Radionuclide Transport Through Fractured Rock

The following sections discuss each of the above issues by presenting its relevance to PA, as well as NRC's Acceptance Criteria and resolution status with respect to the TSPA-LA.

Issue Resolution Status

Hydrogeologic Effects of Climate Change

Relevance to PA. For the DOE to adequately demonstrate and quantify in its Total System Performance Assessment (TSPA) the effects that climate change might have on repository performance, the NRC believes that it should consider how these effects interplay with the other factors within and between key elements in the engineered and natural subsystems of the repository. Climate change and its hydrologic effects are important factors that need to be abstracted into three of the key elements of the engineered and natural subsystems: (1) spatial and temporal distribution of flow; (2) flow rate in water production zones; and (3) location and lifestyle of critical group (includes consideration of water-table rise).

A description of the technical basis for review methods and acceptance criteria for the subissues of climate change and hydrologic effects of climate change is presented in NRC97a. An important new paper on Devils Hole was published in 1997; however, at this time the NRC has not changed the previously developed acceptance criteria.

The NRC has previously recommended (NRC97a, p. 8) a pragmatic approach to address climate change. Under this approach, global, enhanced, greenhouse warming would be presumed to last no more than several thousand years, and that, about 3,000 years into the future, the climate at Yucca Mountain will resume global cooling predicted by the Milankovitch orbital theory of climate. Pluvial conditions should be expected to dominate at least several thousand years of the next 10,000 years. According to NRC's analysis past climate conditions were cooler and wetter than today, about 60 to 80 percent of the time.

<u>NRC Acceptance Criteria</u>. In the NRC's Technical Review of the TSPA-LA, it will determine whether DOE has reasonably complied with the Acceptance Criteria listed below:

1. Climate projections based primarily on paleoclimate data are acceptable for use in performance assessments of the Yucca Mountain site. During its review, the staff should determine whether the DOE has made a reasonably complete search of paleoclimate data that are available for the Yucca Mountain site and region, and has satisfactorily documented the results. Staff should determine that, at a minimum, the DOE has considered information contained in Winograd et al. (WIN92); Szabo, et al. (SZA94); and other reports that may become available.

2. The DOE's projections of long-term climate change are acceptable if these projected changes are consistent with evidence from the paleoclimate data. Specifically, NRC staff should determine whether the DOE has evaluated long-term climate change based on known patterns of climatic cycles during the Quaternary, especially the last 500 ky. The current analysis indicates that these cycles included roughly 100,000 year cycles of glacial/interglacial climates, with interglacials lasting about 20,000 years.

3. The NRC will not require climate modeling to estimate the range of future climates. If the DOE uses numerical climate models, NRC staff will determine whether such models were calibrated with paleoclimate data before they were

used for projection of future climate, and that their use suitably simulates the historical record.

4. Values for climatic parameters (time(s) of onset of climate change; mean annual precipitation (MAP); mean annual temperature (MAT); etc.) to be used in DOE's safety case should be adequately justified. This includes determination of whether appropriate scientific data were used, reasonably interpreted, and appropriately synthesized into parameters such as MAP, MAT, and long-term climate variability. The current knowledge about these parameters, coupled with past climate change, will require that, as a bounding condition, a return to full pluvial climate (higher precipitation and lower temperatures) be considered for at least a part of the 10,000 year period (current information does not support persistence of present-day climate for a duration of 10,000 years or more). The current interpretations of paleoclimate data indicate an increase in MAP by a factor of 2 to 3 and a lowering of MAT of 5-10°C (9-18°F) during the pluvial climate episodes.

5. If the DOE uses expert elicitation to arrive at values of climate parameters, the NRC will determine whether the guidance in the Branch Technical Position on Expert Elicitation (NRC96) was followed by the DOE.

6. Bounding values of climate-induced effects (for example water-table rise) based primarily on paleoclimate data will be acceptable. The NRC should determine whether the DOE has made a reasonably complete search of paleoclimate data pertinent to water-table rise and other effects (for example, changes in precipitation and geochemistry) of climate change that are available for the Yucca Mountain site and region, and has satisfactorily documented the results. In evaluating the DOE's analyses, NRC staff should determine whether, at a minimum, DOE has fully considered information contained in Paces, et al. (PAC96), Szabo, et al. (SZA94), and other reports that may become available.

7. It will be acceptable for the DOE to use regional and sub-regional models for the saturated zone to predict climate-induced consequences if these models are calibrated with the paleohydrology data. NRC staff should determine whether the DOE's models of the consequences of climate change are consistent with evidence from the extensive paleoclimate data base. Specifically, climate-induced water-table rise is expected to occur in response to elevated precipitation during future pluvial climate episodes, and the staff should determine whether the DOE's estimates of climate-induced, water-table rise are consistent with the paleoclimate data. The current estimate of water-table rise during the late Pleistocene is 120 m (394 ft). The NRC should determine whether the DOE's assumptions about climate-induced, water-table rise over 10,000 years, if different from 120 m (394 ft), are adequately justified.

8. Based on judgment and analysis, NRC staff will determine whether the DOE has adequately incorporated future climate changes and associated effects in its performance assessments. Current information does not support an assumption that present-day climate will persist unchanged for 10,000 years or more. The NRC staff should keep in mind that the consequences of climate change may be coupled to other events and processes and therefore the projections of water-table rise that are used in total system performance may be different from those based solely on climate change.

9. The collection, documentation, and development of data, models, and computer codes have been performed under acceptable QA procedures. If they were not subject to an acceptable QA procedure, they must be appropriately qualified.

<u>Status of Issue Resolution at the NRC Staff Level</u>. In Attachment E of the *Issue Resolution Status Report - Technical Issue: Unsaturated and Saturated Flow* the NRC presents their current concerns related to the potential influence of climate change on ground water flow. The text indicates that the NRC has identified no open items solely related to future climate change and associated hydrologic effects.

Present-Day Shallow Infiltration

<u>Relevance to PA</u>. NRC believes that present-day shallow infiltration is a key hydrologic factor in the isolation of high level wastes within the proposed geologic repository at Yucca Mountain. Present day shallow infiltration should be reasonably understood to provide initial conditions for projecting future hydrologic changes, because the Earth's climate could change significantly during the time that wastes will remain hazardous. Climate controls the range of precipitation that, in part, controls the rates of infiltration, deep percolation, and ground water flux through a geologic repository located in an unsaturated environment. Water flow through a geologic repository and its environs depends on both surface processes (precipitation, evapotranspiration, overland flow, and infiltration) and subsurface processes (deep percolation, moisture recirculation, and lateral flow). Changes in infiltration will likely induce other changes, such as regional fluctuations in the elevation of the water table. Water-table rise would reduce the thickness of the unsaturated zone barrier. Therefore, future changes in climate could alter infiltration from present-day rates and significantly influence the ability of a repository to isolate waste.

The importance of ground water flux as the key parameter for repository performance in an unsaturated zone is well known, and has been further emphasized in DOE's 1995 Total System Performance Assessment (TSPA). On page ES-30 of that report it is stated that:

> *...in the overall TSPA analyses, an over-arching theme comes back again and again as being the driving factor impacting the predicted results. Simply stated, it is the amount of water present in the natural and engineered systems and the magnitude of aqueous flux through these systems that controls the overall predicted performance.... Therefore, information on...[this topic]...remains the key need to enhance the representativeness of future iterations of TSPA.*

Sensitivity studies clearly showed the predominance of percolation flux in estimating cumulative radionuclide releases and peak radiation doses over a 10,000-year period (DOE95).

The DOE's "Waste Containment and Isolation Strategy" (DOE96) likewise states that "performance assessments have shown that seepage into the emplacement drifts is the most important determinant of the ability of the site to contain and isolate waste." This conclusion was reiterated in the DOE's recently published Repository Safety Strategy (DOE98). The importance of infiltration as a hydrologic parameter was also recognized by the NRC in its Iterative Performance Assessment Phase 2. The NRC (NRC95, p. 10-4) states that "Although the flux of liquid water through the repository depends on...infiltration, hydraulic conductivity, and porosity, performance correlates most strongly to infiltration."

In Section 5.1.2 of the DOE's 1998 TSPA-VA, the sensitivity to infiltration is investigated by skewing the probabilities to the higher infiltration rates than used in the base case simulations. The results of this analysis showed relatively small differences in the overall peak individual dose rates largely because other factors such as seepage and waste package corrosion uncertainties.

The NRC believes that, for the DOE to adequately demonstrate and quantify in its TSPA-LA the effects that present-day infiltration might have on repository performance, it should consider how these effects interplay with the other factors within and between key elements in the engineered and natural subsystems of the repository.

NRC97b provides a description of the technical basis for review methods for the issue on present-day shallow infiltration.

NRC Acceptance Criteria. In the NRC's Technical Review of the TSPA-LA it will determine whether the DOE has reasonably complied with the Acceptance Criteria listed below:

(1) The NRC shall determine whether the DOE has estimated shallow infiltration for use in the PA of Yucca Mountain using mathematical models that incorporate site-specific climatic, surface, and subsurface information. The staff will also determine whether the DOE provided sufficient evidence that the mathematical models were reasonably verified with site data. These data would include measured infiltration data and indirect evidence such as geochemical and geothermal data. The DOE may choose to use a vertical one-dimensional (1-D) model to simulate infiltration. However, in that case, the DOE should reasonably show that the fundamental effects of heterogeneities, time-varying boundary conditions, evapotranspiration, depth of soil cover, and surface-water runoff have been considered in ways that do not underestimate infiltration.

(2) The NRC shall determine whether the DOE has: (1) appropriately analyzed infiltration at appropriate time and space scales; and (2) has tested the abstracted model against more detailed models to assure that it produces reasonable results for shallow infiltration under conditions of interest. Recent studies by the NRC (STO96) and the DOE (FLI94, FLI95, FLI96) suggest that shallow infiltration is relatively high in areas where rocks are covered with shallow soils or channels and relatively low in areas where soil cover is deep. In addition, infiltration takes place episodically in time with areas having a shallow soil cover contributing more frequently.

(3) The NRC shall determine whether the DOE has characterized shallow infiltration in the form of either probability distributions or deterministic upper-bound values for PA, and whether the DOE has provided sufficient data and analyses to justify the chosen probability distribution or bounding value. The DOE's expert elicitation on unsaturated zone flow (GEO97) resulted in various estimates of a related parameter, the ground water percolation flux at the depth of the proposed repository. The estimated aggregate mean flux was approximately 10 mm/yr. The panelists estimated the 95th-percentile percolation flux over a range from 10 to 50 mm/yr, with an aggregate estimate of 30 mm/yr. An independent NRC staff assessment of an upper bound for yearly shallow infiltration under present climatic conditions is about 25 mm, which is somewhat less than the aggregate 95^{th} percentile flux estimated by the expert panel.

(4) The DOE's estimates of the probability distribution or upper bound for present-day shallow infiltration need not be refined further if the DOE demonstrates through TSPA and associated sensitivity analyses that such refinements will not significantly alter the estimate of total-system performance.

(5) If used, expert elicitations should have been conducted and documented using the guidance in the Branch Technical Position on Expert Elicitation (NRC96), or other acceptable approaches.

6) The NRC will determine whether the collection, documentation, and development of data, models, and computer codes have been performed under acceptable QA procedures. If they were not subject to an acceptable QA procedure, they have been appropriately qualified.

Status of Issue Resolution at the NRC Staff Level. In Attachment F of the *Issue Resolution Status Report - Key Technical Issues: Unsaturated and Saturated Flow* the NRC presents their current concerns related to Present-Day Shallow Infiltration. The text indicates that the NRC staff has identified no open items solely related to Present-Day Shallow Infiltration.

Deep Percolation (Present and Future)

Relevance to PA. The importance of ground water flux as the key parameter for waste isolation at Yucca Mountain is well known.

Deep percolation is related to two of the key elements of the engineered and natural subsystems: (1) quantity and chemistry of water contacting waste packages and waste forms; and (2) spatial and temporal distribution of flow.

The NRC's technical review of the DOE's treatment of deep percolation is to be based on an evaluation of the completeness and applicability of the data and evaluations presented by the DOE. The NRC expects that the DOE will summarize or document the results of all significant-related studies that have been conducted in the Yucca Mountain vicinity.

NRC Acceptance Criteria and Resolution Status. In the NRC's Technical Review of the TSPA-LA it will determine whether the DOE has reasonably complied with the Acceptance Criteria listed below. The results of the NRC's most recent analyses and issue resolutions are also presented.

(1) It will be acceptable for the DOE to estimate present-day deep percolation by using (1) a reasonable upper bound based on available data; or (2) through a demonstration in TSPA and associated sensitivity analyses that further refinement of the estimate will not significantly alter the estimate of total-system performance. In the latter case, the NRC will conduct an independent analysis to judge the appropriateness of the estimate. In the VA analysis, it will be acceptable to use the aggregate distribution for areally averaged percolation flux estimated

through the expert elicitation (i.e., GEO97). The DOE's current infiltration map (e.g., FLI96) may be used to account for spatial variations in percolation.

According to the NRC, the base-case percolation flux as described by DOE appears acceptable at this time because it is similar to that estimated through expert elicitation (GEO97). If this base-case flux is used by the DOE, this acceptance criterion will be met. The status of this issue is open pending review of the DOE's VA.

(2) The DOE's estimate of future percolation will be acceptable if it provides a reasonable basis for assumed long-term average net infiltration and percolation flux. It will be acceptable to apply spatial- and temporal-average values of deep percolation through the use of an abstracted deep percolation model in PA. In arriving at spatial- and temporal-average values: variability is appropriately considered; model parameters are averaged over appropriate time and space scales; and the abstracted model is tested against more detailed models and field observations to assure that it produces reasonably conservative dose estimates. The current understanding is that a vertical one dimensional model, capable of considering heterogeneities and time-varying boundary conditions at the ground surface, may be sufficient for such calculations above the repository, while a vertically oriented, two dimensional model or three dimensional model may be necessary below the repository.

According to the NRC's analysis, the DOE currently (AND98) assumes that long-term average precipitation at Yucca Mountain will be twice as high as present conditions and long-term average percolation will be six times greater. The assumption about long-term average precipitation at Yucca Mountain is reasonably consistent with that recommended in Attachment E (NRC97a). It is not yet clear whether a six-fold increase in long-term average percolation is reasonable. The staff will make that determination after review of DOE submittals.

The NRC staff considers that the LBNL 3-D site-scale model may be too coarse to provide more than a general indication of subsurface processes at Yucca Mountain, but note that significant model refinement may be computationally infeasible. Despite these reservations, the NRC staff endorse the LBNL philosophy of using all available sources of information to calibrate the site-scale model, and agree that, for many purposes, homogeneous effective properties for each layer obtained through inverse modeling may be adequate.

The NRC staff supports the use of the DKM (i.e., dual permeability) approach for site-scale flow modeling as long as the DOE demonstrates that the results bound the effect of episodic infiltration and percolation pulses.

The NRC staff considers that approaches used by the DOE to estimate parameters for flow and transport simulations generally use sound methods, particularly in the most recent work. The NRC staff notes, however, that subgrid heterogeneity is not explicitly and transparently addressed in the approaches, and caution that failure to consider subgrid heterogeneity may lead to qualitatively incorrect results. Small scale modeling of heterogeneous zones is one approach that may be used to support use of uniform properties in hydrostratigraphic units of the site-scale UZ flow model.

The staff have reasons to believe that recharge and percolation in the Yucca Mountain region may increase in the next few decades due to replacement of native shrubs by invading brome grasses. The effect will likely be to replace the zero distributed recharge occurring in the alluvial basins with, perhaps, 1 to 10 mm/yr under current conditions. Recharge in upland areas like Yucca Mountain may also increase. The effect may be significantly greater during pluvial periods. This point is based on infiltration simulations, and on observations of increased streamflows where invasions of Bromus species have occurred in Nevada.

The status of this issue is open pending review of the DOE's VA.

(3) It will be acceptable for the DOE to conservatively assume that the fraction of deep percolation that intercepts disposal drifts also drips onto waste packages. Technical bases should be provided for deep percolation that is considered to bypass emplacement drifts. These technical bases should use field observations, experimental data from the ESF, calculations based on mass balance, tracer studies, and data from natural analog sites. Likely changes in percolation rates and patterns due to climate change should also be considered. Also, the abstracted model used in PA should be tested against more detailed models and field observations to assure that it produces reasonably conservative dose estimates. It is known that the amount of deep percolation into the waste emplacement drifts is sensitive to fast flow in fracture zones. Such flow paths need to be considered in the DOE's calculations

According to the NRC's analysis, the DOE is developing an approach for estimating seepage into drifts. The current DOE approach for drift-scale modeling for isothermal flow is apparently to represent the fracture system as an equivalent continuum with or without incorporating the matrix continuum (NIT97). However, it is not clear that the fracture system can be represented as a continuum at the scale of an emplacement drift based on the average fracture spacings in the repository horizons and the grid size in the numerical model. The NRC believes that alternative approaches will be needed to support estimates of seepage.

Although direct measurement of percolation flux at spatial and temporal scales relevant to modeling at Yucca Mountain is difficult to accomplish, the NRC staff believes that efforts should continue to identify pathways and measure percolation in the field at Yucca Mountain. A number of field tests designed to investigate percolation and seepage rates are planned or currently in progress, notably the alcove and niche infiltration tests and testing planned for the east-west drift in the TSw (WAN98). The direct measurement of percolation flux is encouraged, and the DOE should consider, to the extent practicable, that the proposed east-west drift be allowed to equilibrate with ambient conditions by closing down the tunnel for a period of time. The east-west drift has a significant lateral extent for observing seepage and dripping into the tunnel under ambient conditions, and will cross beneath what are expected to be areas of relatively high infiltration.

Besides providing independent estimates of deep percolation rates, the NRC staff will review whether or not the data used in the methods described in the following sections were extensively incorporated, either directly or as constraints, into the calibration process for the LBNL site-scale numerical model of the flow field (BOD97).

The NRC believes that another possible way that the DOE can demonstrate a reasonable approach is to assume that the fraction of percolating water that contacts waste packages is at least as great as the amount that intercepts disposal drifts. This means that most deep percolation will bypass waste packages because the disposal drifts occupy a relatively small areal percentage of the repository. This approach is probably reasonable and conservative given the tendency of underground openings to divert UZ flow laterally. It may not be reasonable to assume that all packages will receive equal amounts of dripping. Many may receive little or no dripping, while others could experience greater than average dripping over long time periods, especially during pluvial climate episodes.

The issue remains open pending review of DOE’s VA and key supporting documents.

(4) It will be acceptable for the DOE to conservatively assume that all deep percolation below the repository level bypasses the bulk of the units of the CHn formation, either by lateral movement above the units or through vertical flow through fractures and faults. Technical bases should be developed for any deep percolation considered to flow vertically through the matrix of the nonwelded zone. Such technical bases should consider spatial and temporal variability and the scales at which model parameters have been-averaged. Also, the abstracted model has been tested against more detailed models and field observations to assure that it produces reasonably conservative dose estimates.

According to the NRC's current understanding, flow will occur predominantly vertically as matrix flow through the nonwelded vitric zones, including those that are slightly altered. Water will tend to perch upon highly zeolitized horizons and move laterally until vertical structures are encountered. Flow through fractures and fault systems will also occur. The NRC staff believes that the heterogeneity of the hydraulic properties and the characteristics of the fractures cross-cutting the units of the CHn are both poorly known. The field-scale UZ transport test at Busted Butte will significantly improve the conceptual model of flow through the CHn, but it will also contribute significant data for characterizing hydraulic properties, thus reducing uncertainty in flow rates below the repository. The DOE is continuing to work on flow below the repository, with one objective being to estimate how much bypass flux is reasonable.

The status of this issue remains open pending review of DOE's VA and reports on results from the Busted Butte hydrologic test facility.

(5) If used, DOE's expert elicitations should have been conducted and documented using the guidance in the Branch Technical Position on Expert Elicitation (NRC96), or other acceptable approaches.

The NRC has concluded that the expert elicitation on DOE's unsaturated flow model (i.e., GEO97) was conducted and documented in an acceptable way. Consequently this issue is closed and the staff have no further questions at this time.

(6) The NRC will determine whether the collection, documentation, and development of data, models, and computer codes have been performed under acceptable QA procedures. If they were not subject to an acceptable QA procedure, they have been appropriately qualified.

The NRC has not yet analyzed this issue and determined the path to resolution.

Summary of Deep Percolation Topics That NRC Believes Warrant Further Analysis. Significant variability of flow and transport pathways and travel times is expected to occur at Yucca Mountain due to the natural heterogeneity, stratification, alteration, fracturing, and other characteristics of the site. The extent to which such heterogeneities of the flow system should be incorporated into the DOE site-scale UZ flow model depends on their importance for estimating seepage into the repository and flow below the repository. Conceptualizations of flow in the UZ at Yucca Mountain have ranged from single-continuum models, to equivalent continuum models, to dual- and multiple- continuum models, to discrete-fracture models, as the importance of particular components of the flow system was examined. Given the matrix permeability values (FLI96) and assuming a unit hydraulic gradient, ground water flowing only in the matrix would move sufficiently slowly that it would take many tens of thousands of years for shallow infiltration to go through the repository horizon and arrive at the SZ. In contrast, both geochemical evidence and transient-flow modeling have suggested that a significant amount of ground water flux occurs in the fracture system, and that these fluxes can travel at much faster rates than in the matrix. Fluxes in the fracture systems may move sufficiently fast that some component of shallow infiltration reaches the water table in tens to hundreds of years. Differing conceptualizations of the link between the matrix and fracture systems and flow processes in the fractures cause important differences between alternative conceptual models. The differences in the conceptualizations can have a strong impact on PA modeling and, as such, are the focus of the discussion in this section.

The development of both the repository-scale and drift-scale conceptual models at Yucca Mountain may be partitioned into:

(1) Percolation processes above the repository, which affect the spatial and temporal distribution of water moving through the repository horizon

(2) Percolation processes at the drift scale, which affect the release of radionuclides from the repository

(3) Percolation processes below the repository, which affect the transport of radionuclides from the repository to the SZ

Saturated Zone Ambient Flow Conditions and Dilution Processes

Relevance to PA. This issue is important to repository performance because it constitutes an important potential pathway for radionuclide transport from the repository to the environment and receptor locations. Saturated zone characteristics will influence how future societies may use ground water resources in the Yucca Mountain region. The SZ also contributes to repository performance through: (1) magnitude and direction of ground water flow; (2) geochemical retardation; and (3) dilution of radionuclides. The time of arrival and the concentration of radionuclides at the receptor locations are based on the average ground water fluxes and velocities and the geochemical conditions encountered along the flow paths. Longer residence times will provide opportunity for radioactive decay, and the ground water pathways will affect transport due to retardation and adsorption.

The concentration of radionuclides at the receptor locations is also affected by the dilution processes during transport (dispersion and ground water intrabasin mixing) and pumping. The importance of dilution of radionuclides in the ground water is a central issue for dose reduction in the PA. The DOE TSPA-VA identifies dilution in the saturated zone below the repository as one of the five major system attributes most important for PA.

The Repository Safety Strategy (DOE98) notes that "Significant flow must occur in the saturated zone in order for the radionuclide-bearing flux that percolates to the water table to be diluted. The magnitude of mixing and dispersion also must be established because certain conditions have been noted to lead to persistence of contaminant plumes...However, even persistent contaminant plumes may themselves be subject to significant dilution when mixed with other water in a producing well."

Ambient flow conditions in the saturated zone are related to three of the key elements of the engineered and natural subsystems: (1) flow rates in water-production zones; (2) dilution of radionuclides in ground water (dispersion and well pumping); and (3) location and lifestyle of the critical group.

NRC Acceptance Criteria and Resolution Status. In the NRC's Technical Review of the TSPA-LA it will determine whether DOE has reasonably complied with the Acceptance Criteria listed below. The results of NRC's most recent analysis of the issue are also presented.

(1) The staff shall determine whether the DOE considered conceptual flow and data uncertainties. Uncertainties due to sparse data in some areas or low confidence in the data interpretations (e.g., LUC96; also CZA97) should have been considered by analyzing reasonable conceptual flow alternatives supported by site data, or by demonstrating through sensitivity studies that the uncertainties have little impact on repository performance.

According to the NRC's analysis, the reference Luckey, et al. (LUC96) does an excellent job of describing various conceptual models of site-scale hydrology as they were known at that time. The staff will exercise professional judgment in determining whether DOE has reasonably treated the conceptual and data uncertainties in performance assessments or has shown that they will not adversely impact performance.

This issue is open.

(2) The staff shall determine whether, based on site data, the DOE has reasonably delineated approximate flow paths from beneath the repository to potential receptor locations. Flow paths should consider: (i) aquifers (volcanic, alluvium, and carbonate) and continuity of flow regimes; (ii) flow domains (matrix and fracture); (iii) flow directions; (iv) flow velocities (approximate Darcy fluxes and average linear velocities); and (v) vertical hydraulic gradients, including the potential flow direction between the Paleozoic carbonate aquifer and the volcanic aquifers. Hydraulic and tracer testing along paths to potential receptor locations should be conducted on a scale large enough to include a statistically representative elementary volume in alluvium and in the fracture network in tuffs: A sufficient number of tests should be conducted to reasonably reduce the uncertainty in hydraulic and transport properties of the units downgradient from the proposed repository, including approximate delineation of the southerly zone where the water table transitions from tuffs to alluvium. These values, along with existing data such as that from the C-wells complex (e.g., GEL97), should be used in ground water flux calculations and mathematical models.

According to the NRC's analysis, the lack of hydrologic data for alluvium is a data gap in the DOE's site characterization of saturated zone hydrology. Emphasis should be placed on reasonable determinations of heads, transmissivity, hydraulic conductivity, effective porosity, and dispersion coefficients. The hydraulic and geochemical characteristics of the likely flowpath that exists south of well JF-3 have not been evaluated. It is unknown at which locations the water table transitions from fractured tuff to overlying alluvium. The saturated thicknesses, hydraulic properties, and geochemical properties of alluvium have not been determined for the region that lies between well JF-3 and the Amargosa Desert. The DOE's cooperative well drilling program with Nye County, Nevada could accomplish this if the wells are sited and tested to characterize the hydrology along likely flow paths in a timely manner.

The staff believe that the three-phase SZ testing strategy described in Reimus, et al. (REI97) could, if implemented, significantly improve understanding of the hydrogeologic system. New wells may be needed, but possible locations for such testing using existing wells would include (1) J-12, JF-3, and J-13; (2) H-4, SD-12, and WT-2; or (3) SD-6 and H-5. Other combinations are also possible, and other wells could be expected to respond to long-term pumping tests. Because fractures and faults have preferred orientations, and can act as preferred flow pathways, quantitative studies require that more than one representative elementary volume of rock be sampled.

Based on the available potentiometric head data, flow from the proposed repository is likely to be in a southeasterly direction (i.e., along the natural hydraulic gradient) toward Fortymile Wash. This is the general direction of flow that was interpreted by panelists in a recent expert elicitation on the site saturated zone (GEO98), and is also the flow pattern that is best supported by hydraulic head data. Southeasterly flow is the direction used in the NRC/CNWRA performance assessment model where saturated zone flow and transport are simulated in a series of stream tubes. Radionuclides reaching the saturated zone from the repository along this southeasterly flow path would migrate along fracture-dominated pathways in the tuff aquifers in the general direction of well J-12, and thence, southward in saturated alluvium toward the Amargosa Desert. The southeasterly flow path assumes that the fractured tuff aquifer is an equivalent porous medium at the site scale under isotropic conditions. Treating the aquifer as an equivalent medium at a large scale is supported by the pervasiveness in the tuffs of faults and fractures oriented in many directions, and by results of long-term testing at the C-wells. The NRC staff plans to continue its analysis of the previous and ongoing C-wells testing.

As noted above, ground water flow in the tuff aquifer is dominated by structural features. This causes anisotropic conditions where structures may act as high- and/or low-permeability zones, and this is most evident at small spatial scales. At larger scales the hydrologic properties of interconnected fault and fracture networks are expected to dominate flow conditions. Because of uncertainties about large-scale anisotropy, current DOE simulations assume that ~10-percent of transport pathways never come into contact with saturated alluvium. Data from aquifer pumping tests in the C-well complex are now being analyzed to determine whether large-scale anisotropic effects are evident. There are presently no data concerning the isotropy of saturated alluvium.

The staff's current model is subject to revision as new site data are collected and analyzed. Due to sparse data in some areas and uncertainties in the interpretation, the staff continues to analyze whether there are other viable SZ conceptual flow models which can be supported by available data. For example, the staff is examining whether there is evidence of site-scale aquifer anisotropy that could shift SZ flow patterns significantly away from the direction of the observed southeasterly natural hydraulic gradient.

A promising new approach exists that may greatly improve the isotopic dating of ground waters with the ^{14}C technique, leading to better estimates of average ground water residence times. Residence time is related to average regional ground water velocity. Thomas (THO96) describes the separation of dissolved organic carbon from ground water using reverse osmosis and ultrafiltration methods. The staff believes that this method should be applied to samples collected at Yucca Mountain to provide an independent estimate of the apparent ground water velocities in the system and the average time of travel from principal recharge zones to Yucca Mountain. This technique has been applied to ground water in the vicinity of Devils Hole, and indicates that ground water residence times in the carbonate aquifer feeding Devils Hole are about 2000-3000 years (WIN97), significantly less than earlier estimates.

Information about flow conditions in the Paleozoic carbonate aquifer beneath Yucca Mountain is based on only one well, USW p#1. Heads in this well are about 22 m higher in the Paleozoic carbonate aquifer and lower volcanic confining units than in the Crater Flat tuffs (lower volcanic aquifer), indicating a strong upward gradient. Likewise, heads in the lower volcanic confining units in wells H-l and H-3 are also higher than in the Crater Flat Tuffs, providing evidence that significant upward hydraulic potentials probably exist over most of the site east of Solitario Canyon. This condition is favorable for waste isolation because an upward gradient, if maintained in the future, would protect the deep Paleozoic carbonate aquifers from contamination. The DOE's cooperative drilling program with Nye County, NV, should provide timely additional data regarding the vertical gradients between the Paleozoic carbonate aquifers and overlying tuffs or alluvium. It should also be noted that large differences in ground water chemistry between the carbonate aquifer system and the Crater Flat tuffs suggest that upward fluxes are relatively small compared to those introduced by lateral flow within the tuffs.

The issue remains open pending review of the DOE submittals (e.g., VA, data for alluvium and tuffs) and staff analysis of effects of large-scale anisotropy. The staff will determine what adjustments, if any, to general flow paths are warranted.

(3) The staff should determine whether the DOE has provided a hydrologic assessment to describe likely causes of the "moderate hydraulic gradient" and the "large hydraulic gradient."

According to the NRC's analysis, at, or west of, Yucca Mountain is a zone of relatively low permeability that tends to restrict flow from west to east. Based on current understanding, the SCF and associated splays are the most likely cause of the 45-m head change known as the "moderate hydraulic gradient." There is evidence that ground water crosses the fault, but actual fluxes are not known. The tendency to restrict flow probably decreases toward the north as fault displacement decreases. The fault displacement reaches a minimum at a hinge point, about one km southwest of well G-2. When completed, well SD-6 located at the crest of Yucca Mountain should be used to conduct pumping tests beneath the western repository block near the Solitario Canyon fault, and to obtain estimates of transmissive properties beneath that part of Yucca Mountain. Hydraulic testing at SD-6 should provide new insights about the nature of the so-called "moderate hydraulic gradient."

Well WT-24 is currently being drilled to improve the DOE's understanding of the so-called large-hydraulic gradient. The NRC believes that a sufficient understanding can be obtained through the drilling and testing of WT-24. Preliminary data show that a perched zone is present near the top of the Calico Hills in this well, and that the regional potentiometric surface is also more than 100 m higher than in wells immediately to the south.
This issue remains open pending submittal and staff review of the DOE reports on the drilling and testing of wells WT-24 and SD-6. Preliminary water-level elevations have been reported (WT-24: 839.5 m; SD-6: 731.5). The data remain preliminary because the wells are still being constructed, and staff await formal reports from the DOE on testing and data collection at these wells.

(4) The staff shall determine whether the DOE has provided maps of approximate potentiometric contours for an area that, at a minimum, includes wells J-l 1 on the east, VH-1, VH-2, and the GEXA Well on the west, UE-29a #2 to the north, and domestic and irrigation wells south of Amargosa Valley (Lathrop Wells). Maps of regional and site-scale recharge and discharge should be provided, along with

site-scale hydrostratigraphic cross sections constructed along the paths to the accessible environment, and flow-net analysis of the site-scale SZ.

The NRC has not completed its analysis of this issue which remains open.

(5) The staff shall determine whether the DOE has characterized key hydrologic parameters in the form of either probability distributions or deterministic bounding values. These parameters include transmissivity, hydraulic gradient, porosity (effective, matrix, and fracture), and effective aquifer thickness. The DOE's parameters should be reasonably consistent with site data.

Based on the NRC's analysis, the DOE is apparently using probability distributions to represent key hydrologic parameters in TSPA, an approach that is acceptable to the staff. Staff will review DOE submittals to determine whether the parameters used are reasonably consistent with site data.

The issue remains open pending the NRC's review of DOE's VA.

(6) The staff shall determine whether the DOE has used mathematical ground water model(s) that incorporate site-specific climatic and subsurface information. Sufficient evidence must be presented to show that the models were reasonably calibrated and that the physical system is reasonably represented. The fitted aquifer parameters should compare reasonably well with observed site data. Implicitly- or explicitly-simulated fracturing and faulting should be consistent with the data in the 3-D geologic model. Abstractions should be based on initial and boundary conditions consistent with site-scale modeling (e.g., CZA97) and the regional models of the Death Valley ground water flow system (e.g., DAG97a,b). Abstractions of the ground water models for use in PA simulations should use appropriate spatial- and temporal-averaging techniques.

The NRC has not yet examined this issue in depth and it remains open pending review of DOE's VA.

(7) It will be acceptable for the DOE to conservatively assume no wellbore dilution at a receptor location. If wellbore dilution is used, a demonstration should be provided that reasonable assumptions have been made about well design, aquifer characteristics, plume geometry, withdrawal rates, and capture zone analysis for the receptor location.

The NRC has determined that currently the DOE is taking no explicit credit for wellbore dilution. This is acceptable to the staff, but is inconsistent with a DOE-sponsored expert elicitation

(GEO98) which concluded that significant dilution can be expected through well pumping. If the DOE takes credit for wellbore dilution in future submittals, the staff will evaluate the information to determine if the acceptance criterion has been met.

This issue is resolved and the staff have no further questions at this time.

> (8) It will be acceptable for the DOE to conservatively assume no dilution due to dispersion, or no ground water mixing below the repository footprint, and no mixing of the Yucca Mountain water with water from the north in Fortymile Wash. If intra-basin mixing of ground water is used, a demonstration should be provided that reasonable assumptions have been made about spatial and temporal variations of aquifer properties and ground water volumetric fluxes. If dilution is simulated as dispersion in a numerical transport model, scale-dependent dispersivities, constrained by the analysis in Gelhar, et al. (GEL96), should be used.

The NRC notes that in the recent peer review of DOE's TSPA, panelists observed that the saturated zone model used in the TSPA-VA is likely to result in a non-conservative estimate of dilution due to mixing along the flow path. The model assumes that radionuclides reaching the water table and transported in the ground water would be subjected to widespread and uniform mixing in all of the stream tubes within the flow tube model. If only a small percentage of the waste packages fail, and if the failures are confined to a small area of the repository, which is probably one of the more likely scenarios, the radionuclides will more likely be confined to specific stream tubes and not uniformly mix or spread over all of the stream tubes in the flow tube model. Therefore, the presumed widespread and uniform mixing in the flow tube model is not conservative because it would result in more dilution due to mixing in the flow tube than would actually take place.

For 20-km flowpaths, the DOE appears to be using dilution factors that range from 1-100, with a median value of 12. These estimates were derived from the conclusions of three members of a five-member expert panel (GEO98), and consider dispersion effects. The other two panel members did not estimate the dilution range. The estimates do not include the additional effects of dilution within wellbores or intrabasin mixing. The range and median appear to be conservative because they are reasonably low. The staff will assess the DOE's treatment of dilution in the VA.

(9) The staff shall determine whether the DOE has incorporated key conclusions regarding potential geothermal and seismic effects on the ambient SZ flow system (e.g., NRC92, NWT98).

The NRC's analysis and proposed resolution of this issue remains open pending review of the DOE's VA.

(10) It will be acceptable for the DOE to use estimates and recommendations provided by expert elicitations (e.g., GEO98) as long as the expert elicitation is conducted and documented using the guidance in the Branch Technical Position on Expert Elicitation (NRC96) or other acceptable approaches.

The NRC has concluded that the expert elicitation on saturated zone flow and transport (i.e., GEO98) was conducted and documented in an acceptable way. Consequently, this issue is resolved and the staff have no further questions at this time.

(11) The staff shall determine whether the collection, documentation, and development of data, models, and computer codes have been performed under acceptable QA procedures. If they were not subject to an acceptable QA procedure, they have been appropriately qualified.

The NRC's analysis and proposed resolution of this issue are yet to be determined.

Matrix Diffusion in Saturated and Unsaturated Zones

Relevance to PA. Matrix diffusion is related to two of the key elements of the natural subsystems: (1) distribution of mass flux between fracture and matrix; and (2) retardation in water-production zones and alluvium. At Yucca Mountain, the process of matrix diffusion may impact repository performance because ground water flow, away from the repository, occurs primarily in fractures that account for only a small fraction of total formation porosity. In such hydrologic systems, matrix diffusion can attenuate migration of radionuclides in two ways: (1) it can spread them physically from the flowing fractures into stagnant matrix pore water; and (2) rock matrix can provide a vast increase in mineral surface available for geochemical surface reactions (e.g., sorption) as compared to fracture surfaces alone. The extent to which matrix diffusion can affect repository performance is controlled by the rate of solute diffusion from fractures into rock matrix relative to the time scale for flow through the fracture system to the receptor point. When diffusion is very slow relative to the transport time, the impact is negligible in terms of solute arrival time, but there is a slight long-term attenuation of peak solute concentration. If diffusion is fast relative to transport time, the impact is a significant delay in solute arrival at the receptor point. At intermediate diffusion rates, the impact is a modest delay in initial solute arrival time with significant attenuation of solute concentration.

The Repository Safety Strategy (DOE98) noted that concentrations of radionuclides in ground water can be reduced by matrix diffusion and sorption. If matrix diffusion is limited, there can still be sorption on fracture walls, but the depletion effect will be much smaller.

NRC Acceptance Criteria and Resolution Status. In the NRC's Technical Review of the TSPA-LA it will determine whether the DOE has reasonably complied with the Acceptance Criteria listed below. The results of the NRC's most recent analysis of the issue are also presented.

(1) It will be acceptable for the DOE to conservatively assume no credit for matrix diffusion in the UZ. If credit is taken, then matrix diffusion predictions are consistent with evidence for limited matrix diffusion in the UZ including: (i) geochemical data (e.g., YAN96) that provide evidence of geochemical disequilibrium between matrix and fracture waters in the UZ at Yucca Mountain; and (ii) ^{36}Cl evidence for rapid transport pathways to the repository horizon (e.g., FAB96).

According to the NRC, the UZ radionuclide transport sub-model that is currently used in the DOE TSPA model is described by Robinson, et al. (ROB97). From the model description it is evident that effective diffusion coefficients are selected *a priori* and not correlated within the model to fracture or matrix saturation. Although it is possible to simply reduce the value of the selected diffusion coefficient to be consistent with reduced matrix and fracture saturation, there is no analysis provided to show that selected diffusion coefficients are appropriate for the conditions modeled. Additionally, no analyses of the resultant geochemical differences between matrix and fracture water are provided. Thus it is not possible at this time to assess whether the DOE method of abstracting matrix diffusion into UZ radionuclide transport is suitable for predictions of repository performance.

Available information for Yucca Mountain indicates that fracture-matrix interface area is limited to the wetted surface area within fractures. Similarly, effective diffusion coefficients in the UZ are saturation-dependent and should be proportional to the effective saturated cross-sectional area through which solutes can diffuse. Furthermore, TSPA model predictions should be consistent with UZ geochemical data (e.g., YAN96), which suggest that waters within rock matrix at Yucca Mountain have different geochemical signatures than fracture waters; predictions should also be consistent with ^{36}Cl evidence (e.g., FAB96) for rapid transport pathways to the repository horizon.

The DOE should clearly document the technical basis for assumptions used to estimate the transfer term for fracture-matrix exchange in the dual permeability model for UZ transport. The staff has concerns that the residence time transfer function for the dual continuum model is overestimated, because assuming an immobile reservoir neglects the transfer function accounting for particles moving from the matrix to the fracture.

The issue remains open.

(2) It is acceptable for the DOE to conservatively assume that no matrix diffusion will occur in the SZ (i.e., that all solutes will remain in fractures) during transport through saturated fractured rock aquifers. DOE's inclusion of matrix diffusion in SZ transport models for Yucca Mountain should be reasonably supported by both field and laboratory observations. Acceptable field and lab observations include tracer tests that are conducted over different distance scales and flow rates with multiple tracers of different diffusive properties. Transport models should reasonably match the results of the field tracer tests. Rock matrix and solute properties used to justify the inclusion of matrix diffusion in TSPA models fall within a range that can be supported by laboratory data.

The staff believes there is much greater potential for radionuclide retardation in saturated alluvial deposits than in fractured tuffs. From the proposed repository to potential receptors at a distance of 20 km, flowpaths will probably include significant amounts of saturated alluvium. Matrix diffusion in the Tertiary tuffs would then be of minor significance.

The DOE's current assumptions about matrix diffusion are supported to some extent by field and laboratory results to date. However, the amount of matrix diffusion claimed by the DOE from these results has been disputed by the staff and others. A clearer demonstration of the matrix diffusion phenomenon can be made by (1) using tracers with more variation in physical properties and by testing over different length scales and flow rates; and (2) by demonstrating the degree to which matrix diffusion can actually occur within fractured welded and moderately welded tuffs that are known to act as significant flow zones at Yucca Mountain. Zones that contribute to flow in wells have been identified through borehole logging and hydrologic testing. Samples from those zones should be subjected to visual testing techniques of the type described by researchers like Tidwell, et al. (TID97).

The DOE is assuming that matrix diffusion in the saturated zone occurs over a range of porosity described by a log-triangular distribution that ranges from 0.0001 to 0.2, with a mean of 0.02 (2%). The DOE is simplifying the treatment of matrix diffusion by assuming that the range and mean are equivalent to that assumed for effective (advective) porosity and appear to be reasonably conservative with respect to field and lab tests of matrix diffusion and porosity. However, the DOE's basis for selecting of a log-triangular distribution needs to be clarified, and will be examined in the staff's review of the VA.

In the DOE's evaluation of C-wells tracer tests, the staff is concerned that use of the 50% relative solute concentration arrival times to derive the range of effective porosities has an inherent non-conservatism that could be avoided by basing the effective porosity approach on relatively early solute arrival times (e.g., about 10% relative solute concentration). Finally, it appears that, although the matrix diffusion behavior is different for each solute, the DOE is using the same effective porosity for all solutes. If the DOE intends to neglect this variation in solute behavior, the NRC recommends using the effective porosity derived from the least diffusive solute likely to influence performance.

This issue remains open pending review of DOE's VA.

(3) If used, DOE's expert elicitations should be conducted and documented using the guidance in the Branch Technical Position on Expert Elicitation (NRC96), or other acceptable approaches.

The NRC's analysis and resolution of this issue are yet to be determined.

(4) Staff shall determine whether the collection, documentation, and development of data, models, and computer codes have been performed under acceptable QA procedures. If they were not subject to an acceptable QA procedure, they have been appropriately qualified.

The NRC's analysis and resolution of this issue are yet to be determined.

Radionuclide Transport through Porous Rock

Relevance to PA. When radionuclides pass through porous rock, the interactions between the dissolved radionuclides and the rock surfaces (e.g., sorption) result in retardation of the velocity of the radionuclides relative to the velocity of ground water. The large surface areas of the porous media tend to enhance sorption and consequently retardation. Furthermore, for those radionuclides whose sorption reactions may be kinetically inhibited, the slower average linear velocities of ground water flow in porous media promote the solid-liquid interaction. If the radionuclides exist instead as particulates or as colloids, they may be filtered out as ground water flows through the constricted pores of the matrix. Sorption of radionuclides on solids and filtration of radiocolloids and particulates in the matrix reduces the radionuclide concentration in the liquid. However, the low permeabilities of the matrix of some hydrostratigraphic units at Yucca Mountain may make some rock inaccessible to radionuclide-contaminated water on the timeframe of repository performance.

NRC Acceptance Criteria. The approach that recent performance assessment efforts have used to simulate radionuclide transport in porous rock involves first establishing a ground water flow field. This flow field is generated as a result of hydrologic modeling of the Yucca Mountain system using site-specific parameters, and can be one-, two-, or three-dimensional, depending on the purpose of the modeling effort and the available data. The flow field representing the spatial distribution of ground water velocities is then adjusted by dividing the velocity vectors by the retardation factor, R_f, for each radionuclide, to yield the radionuclide velocity fields. Current approaches model the ground water flow field as a dual continuum representing both fracture and matrix flow at every point in the system.

The following Acceptance Criteria apply to evaluating the DOE estimates and consideration of radionuclide transport through porous rock:

(1) For the estimation of radionuclide transport through porous rock, the DOE has

  a. Determined, through performance assessment calculations, whether radionuclide attenuation processes such as sorption, precipitation, radioactive decay, and colloidal filtration are important to performance

  b. (i) Assumed K_d is zero and radionuclides travel at the rate of ground water flow, if it has been found that radionuclide attenuation is unimportant to performance (in which case, Acceptance Criteria 2 and 3 do not have to be met), or (ii) demonstrated that Criterion 2 or 3 has been met, if radionuclide attenuation in porous rock is important to performance

(2) For the valid application of the K_d approach, using the equation $R_f = 1 + \rho K_d/n$, the DOE has

a. Demonstrated that the flow path acts as an isotropic homogeneous porous medium

b. Demonstrated that appropriate values for the parameters, K_d, n and ρ have been adequately considered (e.g., experimentally determined or measured)

c. Demonstrated that the following assumptions (i.e., linear isotherm, fast reversible sorption reaction, and constant bulk chemistry) are valid

(3) For the valid application of process models such as surface complexation, ion exchange, precipitation/dissolution, and processes involving colloidal material, the DOE has

a. Demonstrated that the flow path acts as an isotropic homogeneous porous medium

b. Demonstrated that values for the parameters used in process models are appropriate

c. (i) Demonstrated that the three implicit assumptions (see 2.c.) are valid, if process models are intended to yield a constant K_d for use in the retardation equation; or (ii) determined transport in a fully coupled dynamic system (e.g., PHREEQC, MULTIFLO, HYDROGEOCHEM, etc.)

(4) Where data are not reasonably or practicably obtained, expert judgement has been used and expert elicitation procedures have been adequately documented. If used, expert elicitations were conducted and documented in accordance with the guidance in NUREG-1563 (NRC96) or other acceptable approaches.

(5) Data and models have been collected, developed, and documented under acceptable Quality Assurance (QA) procedures or if data were not collected under an established QA program, they have been qualified under appropriate QA procedures.

Status of Issue Resolution at the NRC Staff Level. Most of the Yucca Mountain geochemical work in the past twenty years has been directed toward determining the retardation of radionuclides in porous rock. Significant progress has been made to address this issue that is important to waste isolation and repository performance. However, in that time, there have been major changes in the conceptualization of the geologic setting of the repository that impact the relative importance of this issue and the consideration of the point of compliance up to 20 kilometers away from the repository. The greater average infiltration results in a greater proportion of the flux bypassing the sorptive porous rock by flow in fractures. A 20 km point of compliance would result in the need to consider the alluvium along with porous and fractured rock. These major changes reduce the relative importance of radionuclide transport in porous rock on performance assessment.

The NRC considers that the subissue has been met for certain radionuclides but not for others. Some of the radionuclides for which the issue has not been resolved on the staff level may be important to performance.

The NRC finds that the approach adopted by LANL to determine minimum K_d values is logical and defensible. By performing batch sorption tests using site-specific materials, followed by confirmatory tests to establish the validity of the assumptions needed for the constant K_d approach, and then selecting the minimum K_d from all the tests, an acceptable value can be obtained.

In summary, the NRC chose three radionuclides as examples to highlight successes and areas needing further work. They are neptunium, plutonium, and uranium. The minimum K_d approach has worked well for neptunium. The staff recognizes that multiple tests have been performed to establish reasonable K_d values for this radionuclide. Consequently, this issue is being resolved for neptunium. On the other hand, although both batch sorption tests and flow-through column tests have been performed to determine a minimum K_d for plutonium, significant inconsistencies occurred. The NRC staff recognizes plutonium as problematic and encourages further work to establish defensible K_d values. For uranium, geochemical modeling suggests that a uranyl silicate phase, soddyite, could precipitate from solution, given the initial ground water composition. Eliminating the possibility that processes other than sorption (e.g., precipitation) may be contributing to the removal of a radionuclide from solution is necessary for establishing a valid K_d. On the other hand, the thermodynamic modeling could be in error based on parameter uncertainties. To date, it does not appear that flow-through column tests were perfomed with uranium. Consequently, the NRC does not believe that this issue has been resolved.

Radionuclide Transport Through Alluvium

<u>Relevance to PA</u>. Current conceptual models of the alluvium incorporated in performance assessments reflect limited information concerning the physical and chemical conditions of alluvium. For example, in the NRC's TPA 3.1 (NRC98), the alluvium is assumed to be crushed tuff similar to the material used in batch sorption experiments. The DOE model abstraction assumes flow as in a sand column driven by the hydraulic gradient. Furthermore, in the TSPA-VA the DOE assumes there are no preferential pathways in the alluvium. This assumption has

not yet been tested. However, the occurrence of cut and fill structures formed in the alluvium by braided streams as evident in the walls of Forty Mile Canyon may suggest that preferred pathways exist in the alluvium with the potential to reduce mixing and dilution.

NRC Acceptance Criteria. The DOE considers radionuclide transport a key performance attribute of the natural barrier system in the proposed repository. Retardation of radionuclides through alluvium constitutes a key element of the DOE performance assessment. The NRC requires that the DOE must adequately estimate the transport characteristics of the Yucca Mountain site and appropriately consider radionuclide transport in their assessments of repository performance. The NRC's review process is designed to determine which transport processes have been addressed/assumed by DOE. The review will first identify, whether or not the selected retardation processes are appropriate to the Yucca Mountain system, and second, whether or not they are addressed adequately for those radionuclides of concern.

The following Acceptance Criteria, which are the same as those for radionuclide transport through porous rock, apply to evaluating the DOE estimates and consideration of radionuclide transport through the alluvium:

For the estimation of radionuclide transport through alluvium, the DOE has

b. Determined, through performance assessment calculations, whether radionuclide attenuation processes such as sorption, precipitation, radioactive decay, and colloidal filtration are important to performance
c. (i) Assumed K_d is zero and radionuclides travel at the rate of ground water flow, if it has been found that radionuclide attenuation is unimportant to performance, in which case, Acceptance Criteria 2 and 3 do not have to be met; or, (ii) demonstrated that Criterion 2 or 3 has been met, if radionuclide attenuation in alluvium is important to performance

For the valid application of the K_d approach, using the equation $R_f = 1 + \rho K_d/n$, DOE has

a. Demonstrated that the flow path acts as an isotropic homogeneous porous medium

b. Demonstrated that appropriate values for the parameters, K_d, n and ρ have been adequately considered (e.g., experimentally determined or measured)

c. Demonstrated that the three implicit assumptions (i.e., linear isotherm, fast reversible sorption reaction, and constant bulk chemistry) are valid

For the valid application of process models such as surface complexation, ion exchange, precipitation/dissolution, and processes involving colloidal material, the DOE has

a. Demonstrated that the flow path acts as an isotropic homogeneous porous medium

b. Demonstrated that appropriate values are used in processes models

c. Demonstrated that the three implicit assumptions (as in 2.c.) are valid, if process models are intended to yield a constant K_d for use in the retardation equation; otherwise, determined transport in a fully coupled dynamic system (e.g., PHREEQC, MULTIFLO, HYDROGEOCHEM, etc.)

Where data are not reasonably or practicably obtained, expert judgement has been used and expert elicitation procedures have been adequately documented. If used, expert elicitations were conducted and documented in accordance with the guidance in NUREG-1563 (NRC96) or other acceptable approaches.

Data and models have been collected, developed, and documented under acceptable QA procedures, or if data were not collected under an established QA program, they have been qualified under appropriate QA procedures.

Status of Issue Resolution at the NRC Staff Level. The status of this issue is tied closely to that of the previous issue. However, additional uncertainty is a result of the very limited information collected to date on the mineralogy, ground water, chemistry, and physical flow systems of the alluvium. Past efforts have focused on characterizing the geologic media within 5 kilometers of the repository because of the provisions of the then applicable 40 CFR Part 191. With the resultant increase in the length of the flowpath to the biosphere to 20 kilometers, now being understood as consistent with draft 10 CFR Part 63, a significant portion of relatively uncharacterized geologic media has been added to the system.

Although, like the DOE, the NRC has assumed in earlier modeling that the alluvium acts as a homogeneous porous medium, the NRC also recognizes that little or no information is available to support that assumption. Furthermore, it is recognized by the NRC that treating the alluvium as a homogeneous porous medium may be nonconservative.

The NRC expects that the series of boreholes to be drilled by Nye County in the alluvium will provide significant information concerning its geologic, and hydrologic characteristics. It is expected that the mineralogy will reflect that used in batch sorption experiments for determining sorption coefficients for radionuclides in tuff. If that is so, the NRC believes that the laboratory work needed to address previous issue (i.e., retardation in porous rock) will also address the retardation issues in the alluvium.

The NRC notes that the DOE will need to defend their conceptualization of the alluvium. If the alluvium is a composite of cut and fill structures resulting from the accretion of braided streams, preferred pathways limiting water-rock interaction may result. If on the other hand, the alluvium is homogeneous, the application of experimentally determined K_ds to calculate retardation factors would be appropriate. The NRC indicates that resolution of this issue will await the geologic and hydrologic information to be collected.

Radionuclide Transport through Fractured Rock

Relevance to PA. Recent site characterization activities involving the radioisotopes ^{36}Cl and ^{3}H provide evidence suggesting fast pathways of ground water flow through the unsaturated zone (FAB96). These fast pathways are proposed to occur as a result of flow down faults and fractures. Also, responses from adjacent wells in large-scale hydrologic pump tests (C-Wells) suggest that preferential pathways may exist in the saturated zone at Yucca Mountain (GEL97). If preferential pathways exist from the repository to the critical group, performance may be adversely affected, because portions of the geologic barrier would be bypassed.

In predicting flow and transport through the unsaturated zone, the TSPA-VA takes no credit for retardation of radionuclides in fractures. The rationale for assigning no retardation in the fractures is based on the hypothesis that there is limited capacity for sorption along fractures, and average linear velocities in fractured rock are high, limiting time for interaction between the dissolved radionuclides and the sorbing minerals lining the fracture walls. However, the presence of specific fracture-lining minerals may provide significant opportunity for sorption of specific radionuclides. For example, the manganese oxyhydroxides may strongly sorb plutonium, uranium, and americium; calcite may strongly sorb or coprecipitate neptunium (TRI96).

Since the TSPA-VA does not explicitly incorporate fractures in predicting flow and transport through the saturated zone the potential sorption effects of the fractures and matrix are, in essence, lumped into a single value. The DOE addresses the associated uncertainty by assigning a range, mean and distribution to the sorption values (i.e., K_ds) for each of the hydrologic units.

NRC Acceptance Criteria. The DOE considers radionuclide transport a key performance attribute of the natural barrier system in the proposed repository. Retardation of radionuclides in fractures in the unsaturated zone and in the saturated zone constitutes a key NRC consideration for evaluating the DOE's performance assessment. The NRC notes that the DOE must adequately estimate the transport characteristics of the Yucca Mountain site and appropriately consider radionuclide transport in its assessments of repository performance. The NRC's review process is designed to determine which transport processes have been addressed/assumed by the DOE. The NRC will first identify whether or not the selected retardation processes are appropriate to the Yucca Mountain system, and secondly, whether or not they are addressed adequately for those radionuclides of concern.

The NRC expected to develop Acceptance Criteria for evaluating the DOE estimates and consideration of radionuclide transport through fractured rock in FY99.

Status of Issue Resolution at the NRC Staff Level. The NRC has yet to develop the Acceptance Criteria for this issue. The DOE has performed some experiments using fractured rock. Whereas the retardation factor in fractures is assumed to be 1 (i.e., no sorption) in performance assessments, due to the uncertainty with regard to radionuclide transport in fractured rock, preliminary experiments suggest that some retardation occurs. For example, neptunium experiments have been performed and show reduced recovery and a delay in the breakthrough relative to tritium and technetium.

Criticality in the Far Field

Relevance to PA. The Total System Performance Assessment-Viability Assessment Methods and Assumptions Report (TRW97) states nuclear criticality scenarios will be evaluated. There are some scenarios that could lead to criticality that may affect performance. For example, Bates, et al, (BAT92) found that plutonium released from glass waste form exists predominantly as colloids. If colloidal plutonium could be efficiently filtered in nonwelded bedded units below fractured strata of the repository horizon, it could accumulate sufficient mass for criticality. Consideration of neutron sorbers or poisons, either contributed from the natural system or from the repository may be important. Differences in the mobility may lead to chromatographic separations of fissile material and poisons. A criticality occurring over a long time could produce increasing amounts of fission products and neptunium. Some of the radionuclides generated in a criticality event could be relatively mobile and, thus, could adversely affect performance. Furthermore, criticality could: (1) generate additional colloids, capable of transporting radionuclides unretarded; (2) affect the ground water flow field; or (3) result in gaseous release of volatile radionuclides.

NRC Acceptance Criteria: To be determined.

Status of Issue Resolution of the NRC Staff Level: To be determined.

NWTRB Identified Needs

In their 1999 Report to Congress the Nuclear Waste Technical Review Board makes a number of observations regarding the potential viability of the proposed repository. The following discussion pertains to issues related to ground water flow and contaminant transport in the saturated zone. As a general consideration, the Board indicates that after reviewing the TSPA-VA it has not identified any features or processes that would automatically disqualify the site.

The Board also notes that the TSPA-VA relies heavily in some cases on formal elicitation of expert opinion. The Board maintains that this was necessary and extremely useful, given the lack of field and laboratory data in certain areas and the equivocal nature of some of the data in other areas. However, the Board expresses a concern that expert opinion should not be used as a substitute for data that can be obtained directly from the site, laboratory and other investigations.

The Board also concludes that a significant amount of additional scientific and engineering work will be needed to increase confidence in a site-suitability determination and license application.

The Board's expressed specific concerns with respect to the data needs of the near field (e.g., waste package) environment. However, with respect to ground water flow and contaminant transport in the saturated zone the Board issued a general statement indicating that long-term studies of the natural barriers also will be needed, primarily to verify projections of water movement within the unsaturated and saturated zones near the repository.

The Board also expressed agreement with a DOE-commissioned peer review panel that two types of additional data are needed to improve the credibility of the total system performance assessment part of the TSPA-VA: (1) fundamental data that are essential to the development and implementation of the models; and (2) data sets designed to challenge conceptual models and test the coupled models used in the TSPA-VA.

Peer Review Panel Identified Needs

The Total System Performance Assessment Peer Review Panel raised a number of concerns related to ground water flow and radionuclide transport in the saturated zone. A discussion of their findings are presented below.

In their introductory remarks to this section the Panel states:

> *The current treatment of saturated zone (SZ) flow and transport at Yucca Mountain is far from satisfactory. In part, this may reflect a higher level of interest and activity in UZ processes during the earlier stages of the project. This, in turn, may have resulted in less progress in SZ activities. Admittedly, the SZ encompasses a much larger volume of the mountain than the UZ. Although it does not involve the complexities of the UZ, it represents a much larger problem for site characterization, flow, and transport.*

The Panel identified three main areas where they believe important weaknesses are present in the current treatment:

- The lack of data for some important parameters
- The incomplete nature or site characterization
- Continuing questions regarding the adequacy of the numerical models

The Panel indicates that the first two areas of weaknesses have forced the DOE to rely primarily on estimates of the expert panel that participated in the Saturated Zone Flow and Transport Elicitation Project (GEO98) for guidance on selecting values for key parameters, including dilution and retardation. As a result of comments and recommendations provided by these experts, "Saturated Zone Flow and Transport Preliminary Draft Chapter 2.9 of TSPA-VA" (CRW98), published on February 13, 1998, has been replaced by a revised interpretation of the SZ flow and transport process. However, it is the opinion of the Panel that inherent problems remain. The Panel believes that additional work on this critical subject is needed. The Panel offers the following specific comments.

Lack of Field Data

The Panel indicates that the lack of field data presents a major difficulty. There is a broad area along the projected SZ flow path from Fortymile Wash to the Armagosa Valley, 10 km or more in length, in which no boreholes have been drilled (a number of the Panel's concerns may be alleviated by Nye County's well drilling/testing program as presented in the following section). The Panel maintains that, for this region, there is a resulting absence of data on key subjects such as: subsurface geology, water table configuration, hydraulic parameters, etc. In other words, the Panel is concerned that the characterization of the SZ flow path over about one half of its 20 km length is currently not complete. In addition, the Panel notes that there is an apparent difficulty in estimating vertical flow in the SZ, the location of the lower boundary, and the lack of account for anisotropy and heterogeneity. Furthermore, the Panel references a more detailed discussion of the serious uncertainties resulting from this lack of data presented in a report submitted to the U.S. Nuclear Waste Technical Review Board (GEL98).

The Panel also explains that the difficulty in evaluating the effects of retardation on radionuclide transport, which is needed in determining dose rate, is another inherent problem. There are two critical aspects to this problem: (1) the division of flow between the matrix and fractures in the SZ zone; and (2) the magnitude of the K_d values to be used.

According to the Saturated Zone Expert Elicitation Panel, ground water flow over the 20-km path from the repository site occurs mostly in the volcanic units and alluvium, and flow occurs in only 10% to 20% of the fractures. As indicated above, field data are needed to verify this picture of the SZ zone. Because K_d values in the matrix (especially for Np) can be 10 to 100 times higher than K_d values in the fractures, it is necessary to know what percentage of the radionuclides are in the matrix of the volcanics. Finally, Gelhar (GEL98), a member of the Peer Review Panel, has also indicated that K_d values cannot be used without knowing how representative they are of field conditions.

Incomplete Characterization of the Site

The Panel believes that characterization of the site remains incomplete. In the TSPA-VA, SZ site characterization affects primarily the description of the flow streamtubes, though the estimation of the permeability field and the water fluxes (in both SZ and UZ). The current approach for estimating the permeability field is based on the calibration of pressure heads. The Panel also points out that, in addition to the problem of lack of data over a substantial region of the SZ as mentioned above, it is known (as acknowledged by the DOE in Chapter 8 of the Technical Basis Document) that pressure data inversion does not guarantee uniqueness in parameter estimates. Thus, potential fast paths in the SZ (such as permeability channels) may be underestimated. The Panel maintains that the implications of such a possibility on the transport of radionuclides are significant and cannot be dismissed.

In the same context, the Panel also raises an issue of numerical resolution in the modeling of regional flow, where only 3 vertical layers (spanning 2,750 m) are used to represent the large-scale hydrology and a typical grid has a linear (horizontal) size of the order of 1,500 m. With such limited resolution, the Panel believes that the intra-grid heterogeneity is seriously misrepresented. Their same concern also applies to the site-scale model, which involves a grid resolution of 200 m. The Panel indicates that, given the large range in permeabilities, which spans 7 orders of magnitude, this limited resolution raises the issue of the relevance of numerical predictions regarding the postulated flow fields.

The assumed water fluxes in the SZ and UZ, their variation with different climates and the recharge from the ground surface downgradient from the repository will also affect the description of the streamtubes. The Panel asserts that the uncertainties pertaining to the characterization of the site, the postulated flux multipliers for the future climates (four for the Long-Term Average and six for the Super Pluvial) are also uncertain. Streamtubes are assumed not to vary with time, regardless of the changes in climate, which is assumed to affect only the volume flux through them. The Panel indicates that this assumption is not consistent with the change in the ratio of the water flux though the UZ and the SZ zones, as shown in Table 3.21, Volume 3, of the TSPA-VA. The Panel further points out that instead of being constant, as required by the assumption of a constant streamtube, this ratio is shown to increase more than twofold as the climate changes from present day to super pluvial conditions.

In the current analysis, it is assumed that recharge along Fortymile Wash enters the ground water to the east of the plume, but it does not enter on top of the contaminated water. Recharge on top of the projected flow path would alter the streamlines significantly, resulting in a substantial layer of clean water above the contaminated water. In his report to the NWTRB, Gelhar (GEL98) suggests that such a layer could be 100 to 150 meters thick. The Panel believes that this potentially conservative feature would call into doubt the basic biosphere model in which a farm family is assumed to pump contaminated water from the plume.

<u>Streamtube Approach</u>

In response to the criticism raised by the Expert Elicitation Panel on the SZ Flow and Transport (GEO98), the DOE drastically revised the model of contaminant transport in the SZ in favor of a new formulation based on flow streamtubes. While the Peer Review Panel believes that the streamtube approach is better than the previous coarse-grid numerical models (200m x 200m, x 20m), it also believes that several issues need to be resolved.

The modeling of dispersion and dilution is treated quite empirically, using overall estimates of dilution, provided by the Saturated Zone Flow and Transport Expert Panel. Since the DOE has similarly provided overall dilution factors instead of a more detailed analysis, the net result is that the interaction of plumes containing different radionuclide concentrations is also treated inadequately, in a generally ad hoc manner. The Panel believes that a numerical approach based on a streamtube formalism, well-resolved near the plume and with a correct representation of dispersion and retardation, is feasible (provided that a good description of the heterogeneity from field data is available). Development of such an approach would permit sensitivity studies to be conducted or the effects various factors, including geostatistics, and would circumvent the necessity to rely solely on estimates from an expert panel and/or empirical corrections. At the same time, the Peer Review Panel raises a concern as to why the modeling of the transport problem is treated differently in the UZ (using a particle-tracking method) and in the SZ (using streamtubes with a dilution factor). The Panel maintains that a unified treatment should be feasible and should be adopted.

On the positive side, the Panel notes the excellent analysis, described in the Technical Basis Document, that relates the dilution factor to transverse dispersivity. The Panel asserts that the proposed convolution approach is quite useful for abstraction, assuming that processes, such as adsorption and retardation, remain in the linear regime, and the flow field is at steady state. The

Panel also notes the advances in the analysis of radionuclide sorption on colloids presented in Chapter 8 of the Technical Basis Document, although these are not included in the current TSPA-VA. The Panel believes that one of the most significant advances is that the process is now correctly treated as being dynamic, rather than irreversible.

The Peer Review Panel raise a point regarding the fracture-matrix interaction. In the TSPA-VA model, flow is assumed to occur only through the fractures; the water in the matrix being stagnant. Instead of explicitly modeling mass diffusion from the fracture to the matrix, the approach taken is to introduce an effective, time-independent porosity for the entire system, in which low porosity values reflect limited diffusion, and high values reflect a more enhanced diffusion. A problem with this representation is that the degree of fracture-matrix interaction is fixed a priori, rather than being a time-dependent process as it is, in reality. Given that retardation is associated with the matrix, this assumption will affect the transport predictions.

The Panel also brings forth an issue regarding the averaging the source concentrations over six areas, which here lie at the interface between the UZ and the SZ. As in UZ transport, this assumption introduces an artificial spreading which will lead to non-conservative estimates, particularly at early times (e.g., within the first 10,000 years) when leakage of radionuclides from waste packages is associated with isolated failures. For such failures, the Panel suggested in its third interim report (WHI98) that it is unrealistic to assume that radionuclides will produce a uniform concentration in the ground water beneath the repository across a flow path that is hundreds to thousands of meters wide. Even if multiple releases were to occur, the waste packages that fail could be close to one another within the repository. Such a situation could occur due to a locally aggressive corrosion environment or the fact that adjoining waste packages share a common fabrication problem.

In response to the Panel’s criticism, the DOE conducted a sensitivity analysis of the effect of the source size on the dilution factor at the 20-km point. In this analysis, the degree of the non-conservatism introduced by the approximation made in the TSPA-VA can be assessed. It was found that, as a result of this approximation, the TSPA-VA underestimates the dose rates for the base case parameter values by a factor of 3. A correction was not introduced in the TSPA-VA, however. The Panel agrees with the general results of Arnold’s analysis, and recommends that the current TSPA-VA treatment be modified to correct the existing deficiency. In particular, the Panel believes that the method described in the sensitivity analysis by Arnold and Kuzio

(ARN98) should be applied to the assessment of the exposures that would result from human intrusion and from the juvenile failure of a waste package.

Soil Adsorption of Radionuclides

The TSPA-VA analysis of the performance during the first 10,000 years after repository closure indicates that the estimated doses are due primarily to ^{99}Tc and ^{129}I. The doses at later times from ^{237}Np and ^{239}Pu are projected to be larger. This is due to the fact that the transport of these two actinides though the UZ and SZ will be delayed for extended periods by chemical sorption and, therefore, they will not reach the accessible environment in significant concentrations until a considerably later point in time. No retardation credit is taken for ^{99}Tc and ^{129}I (or for three other radionuclides), based on the lack of observed sorption in batch measurements of K_d values in the laboratory. This decision is described in the TSPA-VA as being conservative. However, the Panel points out that field measurements near the Savannah River Plant and in the vicinity of the Chernobyl nuclear power plant, following the accident at that facility, indicate that radioactive iodine deposited on the ground has been retained in the upper soil layer to about the same extent as plutonium and cesium, (STR96; STR97). The Panel has not conducted a literature review on this issue, but believes that it is likely that measurements taken of areas near the Chernobyl site, for example, would also provide relevant data on the retention or lack of retention of technetium in soil. Regarding the retardation of iodine, the Panel notes that additional data sets are likely to be available from environmental measurements taken at the Hanford site, where radioactive iodine was released during spent fuel reprocessing. Although it appears that some fraction of the deposited radionuclides may be transported to ground water (e.g., as with cesium at the Hanford tank farm), field data suggest that radionuclide does not move unretarded through the soil. It is the Panel's view that the DOE, in preparing the TSPA-VA, unduly emphasized the results of laboratory K_d measurements, and did not appropriately consider the results of field measurements of radionuclide concentrations in the soil following releases that occurred as a result of nuclear power plant accidents and past nuclear facility operations. The Panel further notes that the DOE has now recognized this problem and it is being addressed.

State of Nevada/T-Reg, Inc. Identified Needs

The State of Nevada and their consultant T-Reg believe that structural controls on the flow system have not been adequately addressed in the TSPA-VA. To support their position, they have identified a number of items in the TSPA-VA which they believe are incompatible, not well represented, or nonrepresentative of their structurally controlled conceptual flow field. Most of the nonrepresentativeness occurs in the saturated zone, or in the areal distribution of recharge to the water table, via the unsaturated zone. Each of these items is discussed separately.

<u>Saturated Zone</u>

(1) The TSPA conceptual flow model allows particles of water to move orthogonal to the hydraulic gradient. Anisotropic effects due to structure are not considered. This causes the flow path for releases from the repository to move initially eastward and then southeastward to Forty Mile Wash, then curve back to the southwest to the Amargosa Farms area at a 20 km radius. Utilizing anisotropic transmissivities, flow paths are created which are directly south, then southeast and southwest, considerably shortening the flowpath to the receptors.

(2) Flow path properties used in the "six flow tubes" are not representative of the southerly flow path. This is because the TSPA flow path would take the releases into alluvium at a shorter distance than a more southerly flow path. Thus, out of the 20-km compliance distance, less distance is assigned tuff properties and more is assigned alluvial properties. (The TSPA flow path is actually longer than 20 km.) The alluvial properties are generally more favorable for retarding and dispersing the repository releases than the tuff properties and, in fact, now constitute the most important barrier in the saturated zone. A shorter flow path to the receptors would also be taken in the State's conceptualization.

(3) Alluvial properties assigned may not be representative of valley- fill sediments. According to drilling results of Nye County, presented at the Devils Hole Workshop, the valley fill sediments south of Yucca Mountain are not primarily alluvium. Rather they consist of coarse gravels, tufa, basalts, tuffs and lake bed sediments. The State asserts that sorption, retardation, dispersion and effective porosity assumptions used to describe transport through "alluvium" must be justified.

(4) The State believes that fracture zone effective porosities or hydraulic apertures also need to be reconsidered or verified. Porosities ranging up to 10% or more are used currently. The TSPA sampled a distribution of porosities ranging from 10^{-5} to approximately 20% but the mean value centered near 2-3%. The State points out that normally effective porosities for fractured aquifers range on the order of 0.01 to 0.001. These changes would work to increase the flow velocities inversely, making them higher than most base case scenarios.

(5) Eastward expansion of the water table receptor area appears inconsistent with channelized flow through Ghost Dance fault zone. This eastward expansion could add up to about 25% more area over which to average repository releases from the

unsaturated zone. The State believes that this is inconsistent with results of Bodvarson, shown in the TSPA, where his center of mass calculations show eastward movement cut off by the presence of the Ghost Dance fault (If waste is placed east of the Ghost Dance, then some areas of eastward expansion could be envisioned, but only at these positions, not uniformly across the length of the repository.)

(6) The eastward flow path is not consistent with chemistry data of the USGS, presented at the Devils Hole Work Shop, April 1999, or earlier work. These data do not indicate an eastward flow part, but rather a southerly one for numerous isotopes.

(7) The eastward flow path may not be consistent with temperature data. Temperature calculations must be a part of this flow path analyses. Both data sets (temperature and pressure) must be matched before any flow paths can be believed.

(8) The State also questions the NRC well bore dilution numbers and the DOE dilutions based on the idea of rigid blocks separated by transmissive faults. Nye County drilling results indicate three boundaries in one of their pump tests. These boundaries were not distant and depict a situation where by smaller volumes of water would be available for dilution. Their drilling results also show that pumping rates are highly non-uniform ranging from a few gallons a minute to several hundred gallons per minute. To use huge well bore dilution volumes (10^8 gallons per day) at this point is not justified. The DOE flow path dilution numbers are much smaller than the NRC's but still not based on channelized flow and therefore must be justified.

Infiltration

(1) The State points out that the map of infiltration based on Flint is partially inconsistent with their conceptual model of infiltration. While slope, depth of alluvium, evapotranspiration and elevation are definitely important, so may be some other factors. Flint assumes that where thick alluvium is present idle recharge occurs. The State believes that this may not hold true on the steep western slope of Yucca Mountain. The TSPA-VA infiltration model shows a dry area to the west of the crest of Yucca Mountain rather than a wetter one which the State's conceptualization would predict.

(2) The State asserts that it is possible for runoff to go under the alluvium and into fractures, thus being blanketed from potential evaporation. Given that the PTn unit is not present to divert any infiltration in some areas to the west of the repository, then infiltration is possible directly or nearly so into the Topopah

Springs unit, up gradient of the repository. As stated previously, in the State's conceptual model, the western side would be expected to be wetter than the eastern side.

(3) The State also notes that recent correspondence from Steve Brocum, DOE to the NRC, Sandra Wastler, Monthly Progress Report, dated 03-26-99 indicates that water potentials are higher in the East-West Cross Drift (ECRD) and indicate that the rock is wetter and the moisture is more uniformly distributed than expected. The State points out that the structure here is probably important and explains further that tensional north-south trending smaller structures across the mountain block may be channeling the movement of infiltrating water. By cutting across them in an east-west direction, the ECRD has intercepted more pathways than when they bored north-south in the main drift section, parallel to these features.

(4) Flint et al. (FLI96) and the TSPA-VA infiltration model indicate that the net infiltration is lower in the washes. The State generally concurs, except that they believe higher infiltration occurs in the upper reaches of most washes, not along the lower reaches.

(5) The State believes that infiltration at the water table surface may also not be representative, nor consistent with their model. The TSPA-VA infiltration map shows lower infiltration along the Ghost Dance fault area where the State would assume higher infiltration based on the temperature distribution.

(6) The State also notes that Zell Peterman, USGS has shown what appears to be a plume of younger water along the northwest side of the mountain block. The State would expect that this plume would be infiltrating or recharging in that area. The water table map in the TSPA-VA shows it to be relatively dry.

(7) Breakthrough curves simulating the dry (present day) climate conditions (Figure 3-10 of the TSPA-VA) indicate less than 5% cumulative breakthrough for an unretarded tracer at the water table in less than 800 years with 95% breakthrough between 800-12,000 years. The State believes that it is reasonable that if in the north-south trending drifts, ^{36}Cl is seen within 50 years, that when sampled, the ECRD may also yield ^{36}Cl and perhaps more than in the north-south drift. The State asserts that these low percentages of ground water breakthrough are not justified.

(8) Drift scale seepage assumes a 99.5% reduction of net infiltration. While the State would expect some diversion they would also expect that the infiltration rate of water into the drifts would be on the order of that calculated for G Tunnel, i.e., about 3% of the annual average rainfall. This would allow for 4.5mm/vr into the

tunnel. Instead, VA values are orders of magnitude lower. The State notes that these low values need to be supported.

(9) Seepage Fraction, or number of canisters hit by drips is surprisingly low. The State claims that given their concept of fracture controlled drips and data from the DOE that the ECRD is wetter than expected, no confidence can be assigned to this number. The State further notes that testing in Alcove 1, though shallow with high infiltration applied, is indicative of a potential for more wide spread dripping given that 45% of the roof area catchments had contacted drips.

(10) Drips onto packages are assumed stationary during their flow history. The State believes that this may also not be the case for many reasons (hydraulic, geochemical or tectonic), and further suggests that moving them about over time would tend to wet a larger number of packages.

(11) Sorption and matrix diffusion are assumed to always operate together on sorbing species. The State questions whether this a valid assumption, and notes that it allows for more retardation than may be justified if considering them separately.

(12) Volumetric flux via the drift invert assumes 10% porosity, 99.8% saturation, sorption and diffusion. The State contends that if the invert fails over time, or fractures develop due to tectonic activity, then flow would be focused and radionuclides less retarded. The State further notes that no provision for invert failure or degradation has been made in the TSPA-VA.

<u>State's Conclusions</u>

Based on the concerns identified above, the State made the following three conclusions:

(1) If the basic flow pathways and their characteristics are not correctly interpreted or represented, when they possess qualities which can be measured or tested in the field, then little confidence can be placed on analyses, interpretations or designs which have not been or cannot be tested or verified.

(2) The flow fields need to be calibrated against temperature or other independent variables in order to support flow paths selected.

(3) Future TSPAs will have to modified their flow model to be representative of a structurally controlled flow field.

VI.2.1.5 Nye County Drilling and Characterization Program

As part of its Nuclear Waste Repository Project Office Yucca Mountain Oversight Program, Nye County is conducting an Early Warning Drilling Program (EWDP). The purpose of the EWDP is to establish a ground water monitoring system to protect the residents of Nye County in Amargosa and Pahrump Valleys against potential radionuclide contamination of the ground water system as a result of radionuclide releases from a repository at Yucca Mountain.

The program is also intended to provide geologic and hydrologic characterization data to supplement the DOE program. The EWDP boreholes are located in a highly complex geohydrological regime, about 20 km south of the proposed repository location, which has received very little characterization. Near-surface geologic features are valley-fill alluvium which is potentially very heterogeneous and overlays volcanic rocks such as are beneath Yucca Mountain. Data are to be obtained to characterize the geologic features, ground water flow patterns, and ground water recharge.

Eight drillholes were completed during Phase I of the program in 1999. Four of the drillholes were relatively shallow (a few hundred feet), and the other four went to depths on the order of 2,000 feet. Lithologic logs were recorded, and can be seen on the Nye County website, www.nyecounty.com. The website also provides a map showing the locations of the drillholes, most of which were close to, and along the length of, U.S. Highway 95 south of Yucca Mountain.

The program also includes airborne aeromagnetic surveys which are obtaining data are being used to characterize buried geologic features, to provide details on possible fault conduits in the valley-fill deposits, and to help guide selection of the Phase II drillholes, eight of which are planned. An alluvial tracer complex, which would be an interagency effort involving Nye County, DOE, and Yucca Mountain Project contractors to DOE is also planned.

The current status of the program, and descriptions of the EWDP drillholes and reports on program activities and findings, are available at the Nye County website cited above.

VI.2.1.6 Relationship Between the Hydrologic Regime and the 10,000-Year Compliance Period

As shown by preceding discussion, the geohydrologic regime in the Yucca Mountain region is highly heterogeneous, and the models of ground water flow and radionuclide transport reflect this heterogeneity. Flow occurs principally in fractures in volcanic tuffs, and the valley-fill alluvium south of the proposed repository site has been found to exhibit braiding and other structural features such that there may be principal flow channels in this medium as well as in the volcanic tuffs.

Ground water flow paths and rates, and radionuclide contaminant transport by the ground water, therefore depend on the specific small-scale features of the geohydrologic regime. These characteristics may be significantly affected by seismicity, tectonic movement, climate change, and other natural phenomena expected to occur over the next million years.

How the small-scale features will change in response to these phenomena is uncertain. The validity of very long term projections of repository system performance and radiation doses that are based on current geohydrologic conditions and models of these conditions is therefore highly uncertain, and too uncertain to be the basis for evaluation of compliance with radiation protection standards.

As noted by the National Academy of Sciences Committee that developed the technical basis for the EPA's Yucca Mountain standards, (NAS95), the potential for future occurrence of natural phenomena such as earthquakes may be boundable based on current data and evidence of past phenomena. However, bounding the potential incidence of natural phenomena does not and can not capture the changes in small-scale features that are directly important to repository performance and radiation doses that might be incurred at a specific location.

Factors involved in long-term uncertainty for repository performance are discussed in detail in Section 7.3.11 of the BID. The discussion shows that radiation doses for a compliance evaluation period corresponding to the time of peak dose hundreds of thousands of years in the future cannot be reliably evaluated. The dose evaluations would be subject to the uncertainties associated with the small-scale consequences of diverse, episodic phenomena characterized by bounding estimates.

In contrast, a compliance period of 10,000 years captures a reasonable extrapolation of current natural features and phenomena, such as climate, that affect repository system performance. It also captures the effect of the thermal pulse on repository-scale natural and engineered features, and allows reasonable assessment of the occurrence and consequences of improbable but possible repository-scale phenomena such as intrusion of volcanic magma and, for the Site Recommendation repository engineered design, common-mode failure of a drip shield and the underlying waste package. The 10,000-year compliance period would be expected to exclude low-frequency, high-consequence natural phenomena such as high-intensity seismic activity, which dominate the uncertainty associated with long-term dose predictions.

The 10,000-year compliance period is not, however, so short that it excludes phenomena such as temperature changes and low-rate, low-frequency seepage that affect repository system performance and can be reasonably modeled and accounted for. Principles of reasonable expectation can be applied with confidence as a result of a data base of current conditions and an understanding of the phenomena and features that affect performance over the 10,000-year period.

In summary, the site-specific features of the Yucca Mountain region, which include a highly heterogeneous geohydrologic regime and expectation of long-term phenomena that can and will affect the geohydrologic regime in uncertain ways, reinforce use of the 10,000-year compliance period established for the generic 40 CFR Part 191 standards.

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