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HIGH-LEVEL NUCLEAR WASTE REPOSITORY AT YUCCA MOUNTAIN, NEVADA

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ABSTRACT

Two complementary numerical models for analyzing high-level nuclear waste emplacement at Yucca Mountain have been developed. A vertical cross-sectional (X-Z) model permits a realistic representation of hydrogeologic features, such as alternating tilting layers of welded and non-welded tuffs, fault zones, and surface topography. An alternative radially symmetric (R-Z) model is more limited in its ability to describe the hydrogeology of the site, but is better suited to model heat transfer in the host rock. Our models include a comprehensive description of multiphase fluid and heat flow processes, including strong enhancements of vapor diffusion from pore-level phase change effects. The neighborhood of the repository is found to partially dry out from the waste heat. A condensation halo of large liquid saturation forms around the drying zone, from which liquid flows downward at large rates. System response to infiltration from the surface and to ventilation of mined openings is evaluated. The impact of the various flow processes on the waste isolation capabilities of the site is discussed.

INTRODUCTION

Emplacement of heat-generating high-level nuclear wastes at Yucca Mountain would give rise to complex multiphase fluid and heat flow processes. These include heat transfer by conduction and advection, phase change phenomena (boiling and condensation), flow of liquid water and gas phase under gravity, capillary, and pressure forces, inter-diffusion of vapor and air, and vapor adsorption and vapor pressure lowering effects. These processes would be played out in a complicated geologic setting with alternating layers of porous and fractured-porous materials, and would be significantly impacted by the actual repository operations (e.g. waste emplacement, ventilation), as well as by natural forcings (e.g. infiltration, barometric pressure variations).

It is the purpose of this paper to present conceptual and numerical models for performance assessment of strongly heat-driven flow processes that would be induced by the thermal load of the repository. Our objective is to develop a preliminary understanding and assessment of flow processes and thermo-hydrologic conditions in the host rock. This should assist in evaluating the suitability of the site for nuclear waste isolation, provide guidance for repository design considerations, pinpoint critical uncertainties that need to be addressed in future work, and serve as a basis for further development of performance assessment models.

MODELING APPROACH

An "ideal" performance assessment model would include a comprehensive description of all relevant physical and chemical processes affecting repository and host rock behavior. It would also represent the important hydrogeologic features of the potential repository site in full explicit detail.

Fluid and heat flow fields around a nuclear waste repository at Yucca Mountain would be three-dimensional, due to irregular waste emplacement geometries, and because of geologic irregularities, such as the presence of tilting layers of welded (porous-fractured) and non-welded (porous) tuffs, and irregular surface geometry. Fully three-dimensional simulations of highly non-linear multiphase fluid and heat flow processes are feasible but are extremely demanding computationally. For practical applications it is necessary to make simplifications either in the fluid and heat flow process description, or in the flow system geometry.

The performance assessment models presented here borrow from geothermal and petroleum reservoir simulation methodology to focus on coupled multi-phase fluid and heat flow processes. We attempt a fairly comprehensive description of such processes, but the representation of geologic features and flow system geometry is intentionally left simplistic and schematic. Stripping away nonessential detail aids in understanding and critically evaluating process complexities and uncertainties. It also helps to keep the models simple and flexible enough so that additional detail may be incorporated in the future.

We have developed two complementary two-dimensional models, a vertical section (X-Z) model (Figure 1) patterned after stratigraphic sections developed by Klavetter and Peters,[1] and a cylindrically symmetric (R-Z) model (Figure 2). The X-Z model obviously can provide a more realistic representation of hydrogeologic features such as tilting of lithologic units, presence of fault zones, and irregular surface topography, but it gives a poorer approximation for repository heat transfer. The R-Z model is more limited and schematic in its ability to describe the hydrogeology of the site, but it is better suited to model the "volumetric" nature of heat transfer into the host rock. Furthermore, in the R-Z model one central waste package, assumed emplaced vertically, can be represented explicitly through fine gridding at small radial distances. This makes possible a more accurate prediction of thermo-hydrologic conditions near the waste packages than could be attained with models that apply
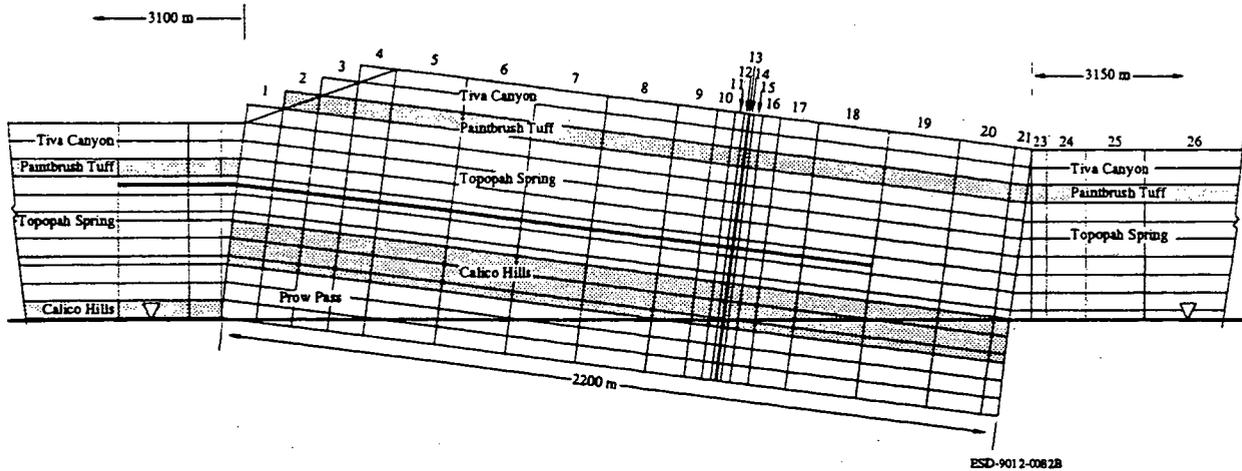
Figure 1. Computational grid for two-dimensional east-west vertical section (X-Z) model of Yucca Mountain.
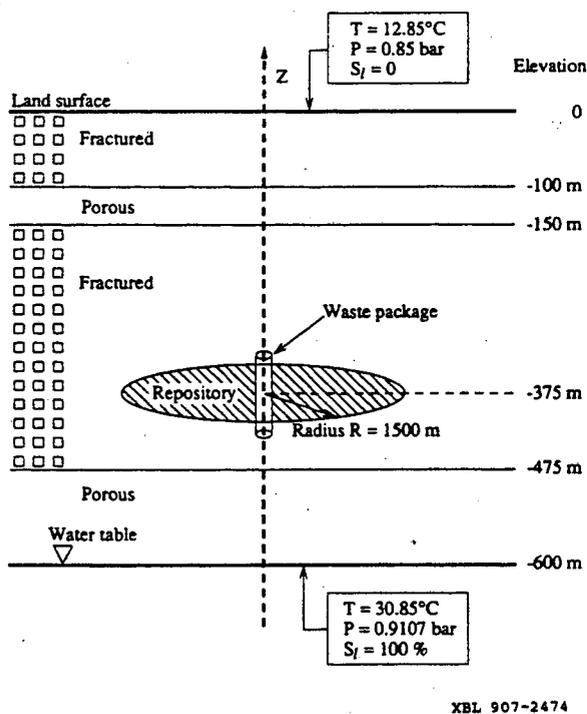

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Figure 2. Two-dimensional radially symmetric (R-Z) model of a high-level nuclear waste repository at Yucca Mountain.

waste heat only in a volumetrically averaged manner. It also permits a detailed definition of "interior" boundary conditions at the surface of the emplacement hole, which is crucial for a realistic representation of the interaction between the waste packages and the mined openings. As will be shown below, this interaction has important ramifications for repository ventilation and

moisture status in the host rock surrounding the repository. Both models are closely tied together through parameter choices and intercomparisons. Their strengths and weaknesses are complementary so that when taken together they can provide increased confidence for predictions.

The computational grid of the R-Z model consists of 21 layers with 30 blocks in radial direction, for a total of 630 grid blocks. Layer thicknesses range from 2.5 m near the waste packages to a maximum of 50 m; radial grid increments range from .061 m near the waste package to 1881 m at the outer perimeter. The X-Z model (Figure 1) consists of a central section of 20 layers with 21 columns of grid blocks, tilted by 7°, and two attached sections without tilt. The western section has 16 layers and 6 columns, the eastern section has 13 layers and 7 columns. Finer gridding is used near the repository level, and in the region of the Ghost Dance fault system (near column 13 of the tilted section). This makes possible an investigation of the effects of the fault on flow;[2] however, in the simulations reported here hydrogeologic parameters in the fault region have been chosen identical to the "background" values away from the fault.

Most of the multiphase fluid and heat flow processes expected near heat-generating high-level wastes emplaced in the vadose zone are well understood. Application of comprehensive process models is limited at present by uncertainties of site-specific parameters for the Yucca Mountain site. Our parameter choices for a reference case are discussed in laboratory reports.[3,4] Briefly, the non-welded units (Paintbrush Tuff and Calico Hills) are represented as porous media with permeability of 18 millidarcy. Characteristic curves (capillary pressure and relative permeability) are represented by van Genuchten's model,[5] with parameters as determined by Peters et al.[6] for Paintbrush sample GU4-2, and Calico Hills sample GU3-15. The welded units (Tiva Canyon and Topopah Spring) are modeled as fractured-porous media, using an effective continuum approximation.[7,8] Unfractured matrix permeability is 1.9 microdarcy, with characteristic curves as determined by Peters et al.[6] for Topopah Spring sample G4-6. Fracture network permeability is assumed to be 18

millidarcy. Porosities are taken as 0.18% for the fracture network, and 10% for the composite medium. Previous modeling studies have shown that thermal and hydrologic conditions near waste packages are very sensitive to the relative permeability and capillary pressure behavior of fractures which is poorly known at present.[9] In this paper we have assumed a "sequential saturation" approximation in which liquid is immobile in the fractures as long as the matrix is not fully saturated.[3,4,10]

A difficult aspect of the simulations is the presence of coupled multi-phase fluid and heat flow processes with vastly different response times. Indeed, propagation of gas phase pressure disturbances on the repository scale (1 km) is expected to occur in a matter of months, propagation of thermal disturbances over such distance will require several 10,000 years, and capillary pressure disturbances in the tight Topopah Spring matrix rock will require in excess of 100,000 years (see Table 1). Even slower processes evolve from subtle couplings between formation temperatures, liquid saturations, and saturation-dependent thermal conductivities. Additional numerical complications arise from (1) the extreme permeability contrast of perhaps 4-6 orders of magnitude between fracture networks and unfractured rock matrix, (2) the large range of relevant spatial scales, ranging from centimeters for resolving important changes near the waste packages to hundreds of meters for repository-wide flow processes, and for interactions involving land surface and water table boundary conditions, and (3) the highly non-linear parameter dependencies for variably-saturated media, especially during phase change processes (drying and re-wetting).

Table 1. Characteristic Times for Multiphase Processes (*)

Process	Hydrogeologic Unit	
	Topopah Spring	Calico Hills
Heat conduction	29,900 yrs	51,100 yrs
Liquid flow	234,700 yrs	176 yrs
Gas flow	207 days	127 yrs
Vapor diffusion	1,480 yrs	1,480 yrs
Air diffusion	84,600 yrs	26,900 yrs

*For a propagation distance of x = 1000 m, calculated from $t = x^2/D$, where D is the appropriate diffusivity.[8]

Our modeling approach builds on previous studies of thermal and hydrologic conditions from waste package,[7,8,9] to repository scale.[11] All calculations were performed on an IBM RS/6000 workstation, using Lawrence Berkeley Laboratory's general-purpose multiphase fluid and heat flow simulator TOUGH2.[12] The formation fluids are modeled as two-phase (liquid, gas) two-component (pure water without salinity, air "pseudo-component"). A comment is in order about the treatment of "interface quantities" between grid blocks in the integral finite difference approximation. At lithologic contacts between porous and fractured-porous units we use full upstream weighting for both absolute and relative permeabilities. The more common procedure of using upstream weighting only for relative permeability and employing harmonic weighting for

absolute permeability has been shown to lead to serious errors (spurious flow resistances) in heterogeneous media with large variability in permeability and capillary pressure behavior.[4]

PRE-EMPLACEMENT CONDITIONS

What are the appropriate initial conditions to be used for modeling repository performance at Yucca Mountain? Depending on the history of external perturbations (such as changes in infiltration due to variable climatic conditions), and on internal response times, natural hydrogeologic systems may or may not be close to steady-state conditions. For thick unsaturated zones with tight rock matrix internal system response times may be large, in excess of 100,000 years (Table 1). Moisture conditions at Yucca Mountain are therefore most likely not in a steady state; however, they will be in a stable state in the sense that, in the absence of man-made perturbations, changes in the flow system will occur very slowly. As an approximation to this stable state prior to waste emplacement, we develop a state with steady fluid and heat flows. For the R-Z model the steady initial state is one-dimensional in the sense that all flows are vertical. The steady state is obtained by numerical simulation, applying realistic boundary conditions of ambient pressures for both aqueous and gas phases, and natural geothermal gradients (Figure 2). For the reference case net infiltration is assumed to be zero. Because of the vastly different response times of different processes, a head-on approach trying to run the system to steady state from some arbitrary initial conditions is not very practical. Instead, we go through a parameter-stepping approach, in which we first obtain steady heat conduction for a system with zero permeability. Subsequently gas pressures are equilibrated for conditions of uniform permeability and immobile water. Finally, a steady state for coupled multiphase fluid and heat flow is obtained by introducing proper characteristic curves, heterogeneous permeability, and air-vapor diffusion in the gas phase. The R-Z model is then initialized with this one-dimensional steady state. Development of an initial steady state suitable for studying effects of the repository heat source in the X-Z model follows a similar approach as in the R-Z model, but is somewhat more involved due to added pressure and temperature effects from the tilting of layers.

Gas diffusion in porous media is customarily described by Fick's law, with "free" diffusivities modified by applying a strength factor

$$B = \phi \cdot S_{gas} \cdot \tau \qquad (1)$$

to account for pore space volume and tortuosity effects. For typical porous media, the strength factor B is of order .03 ($\phi = .3$, $S_{gas} = .5$, $\tau = .2$). However, from soil science studies it is well established that vapor diffusivity in porous media is strongly enhanced from pore-level phase change effects mediated by liquid islands; typical values for B are of order 1.[4] Assuming that vapor diffusion enhancement in tuffs is similar to what has been observed in sands, we find that a "normal" geothermal gradient of .03°C/m will cause an upward diffusive vapor flux approximately equivalent to .04 mm/yr of water, in good agreement with Ross' estimate of .03 mm/yr.[13] With zero net infiltration at the land surface, the upward vapor diffusion must be balanced by downflow of liquid condensate at a rate of .04 mm/yr. This liquid flux, although small, is not insignificant relative to the saturated

hydraulic conductivity of the unfractured welded tuffs; indeed, the permeability of 1.9 microdarcy corresponds to a hydraulic conductivity of .6 mm/yr. Thus the downflow of condensate to balance upward vapor diffusion has a strong impact on steady-state saturation distributions in the welded tuffs. Our steady-state saturation profile in the Topopah Spring unit is similar to that obtained by Buscheck and Nitao[14] without consideration of enhanced vapor diffusion for .045 mm/yr net infiltration.

RESPONSE TO WASTE EMPLACEMENT

Subsequent to attainment of steady-state conditions, we have simulated, for a time period of 10^5 years, the system response to emplacement of high-level nuclear waste packages. During these simulations water table and land surface (atmospheric) boundaries are maintained at constant conditions. In the R-Z model we also maintain initial vertical profiles of gas pressures, water saturations, and temperatures at the outer (R = 5,000 m) boundary. The wastes are assumed to be 10 years out-of-reactor, and are emplaced instantaneously at an initial heat load of 57 kW/acre. At an initial power level of 3.051 kW the repository area per waste package is 213.2 m^2. Limited sensitivity studies were carried out to evaluate effects of different rates of water infiltration, and of variations in repository operations during the waste emplacement phase.

After heat generation is first turned on the flow system is undergoing rapid changes in temperature and moisture conditions, and the simulation proceeds with small time steps. As the pace of changes slows, and waste heat generation declines, time steps grow to large values. For the R-Z model the simulation takes 38 time steps for 1 year, 104 time steps for 100 years, and 197 time steps in total to reach 10^5 years.

Assuming that waste emplacement holes are sealed (not ventilated), and that fractures have negligible effective permeability for liquid water at ambient suction conditions, simulated system behavior is as follows. Temperatures near the waste packages rise to a maximum of approximately 180°C at about 10 years after waste emplacement, and then slowly decline to about 120°C at 100 years, 85°C at 1,000 years, and 40°C at 10,000 years (Figure 3). Average rock temperatures at the repository horizon peak at 95°C. Formation waters boil near the waste packages; the vapor is driven away from the heat sources by advection and diffusion, with diffusion dominating when enhancements from pore-level phase change effects are taken into account (see the discussion following Equation 1). Complete dry-out occurs only within a small region of a few meters around the waste packages, while partial drying occurs in a region of approximately 100 m thickness above and below the repository (Figures 4 and 5). Beyond the region of partial drying a halo of increased liquid saturation forms from vapor condensation. The most important effect of the partial drying and condensation is that, near the repository level, very strong capillary pressure gradients are generated. Their effects on liquid phase flow is much stronger than gravity effects, so that liquid flows towards rather than away from the repository. The region of partial dry-out is long-lived; even 10,000 years after waste emplacement only approximately half of the liquid originally in place in a region of 30 m thickness above and below the repository will have been restored to that region.
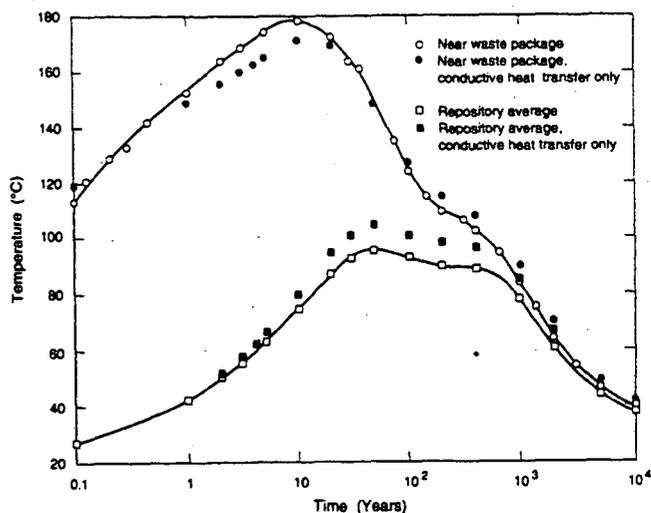

Figure 3. Simulated temperatures in the host rock in the R-Z model.

Our simulations predict sizeable downward flow of condensate towards the repository horizon. Averaged over the repository area, downward liquid flux from the condensation halo is 13.3 mm/yr at 10 years, 7.0 mm/yr at 100 years, and 1.3 mm/yr at 1,000 years. Even larger condensate fluxes are predicted near the waste packages, namely, 44.8 mm/yr at 10 years, and 10.0 mm/yr at 100 years. The vapor migration and condensation is expected to take place primarily in the fractures. The relatively large condensate fluxes predicted from our simulations suggest that the fracture-matrix system may not attain capillary equilibrium, and that downflow of condensate may involve a significant fracture component.

The predicted partial dry-out near the repository level has important consequences for waste isolation: As long as water flows towards rather than away from the repository no contaminant release through aqueous pathways is possible. Partial dry-out would provide a long-lasting capillary "trap" that would prevent dissolved contaminants from reaching the accessible environment. However, the possibility that water may flow along localized fracture paths without reaching larger-scale capillary and thermal equilibrium can not be ruled out at present. Such nonequilibrium water may be able to flow across the repository horizon even when on average strong capillary suction conditions would be present in the neighborhood of the repository.

At the nominal effective gas phase permeability of approximately 20 millidarcy in both welded and non-welded units the temperature field is not much affected by phase change and flow processes. A calculation using heat conduction only (no fluid flow) predicts temperatures to within 5–8°C or better, as compared to a calculation with full allowance for multiphase effects (Figure 3). This suggests that, unless effective permeability of the fracture network in the welded units should turn out to be substantially larger than 20 millidarcy, a "conduction only" calculation would be adequate for evaluating thermal performance of the repository. However, maximum host rock temperatures near the waste packages cannot be predicted with confidence at
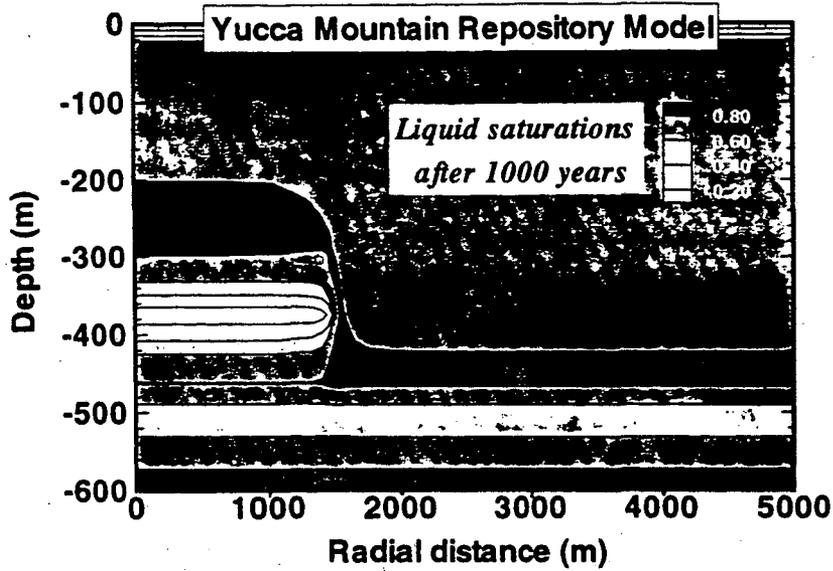
Figure 4. Simulated water saturation distribution after 1,000 years in the R-Z model.

RZ Liquid Saturation Profiles (R=705.16 m)   XZ Liquid Saturation Profiles (X = 1100 m column)
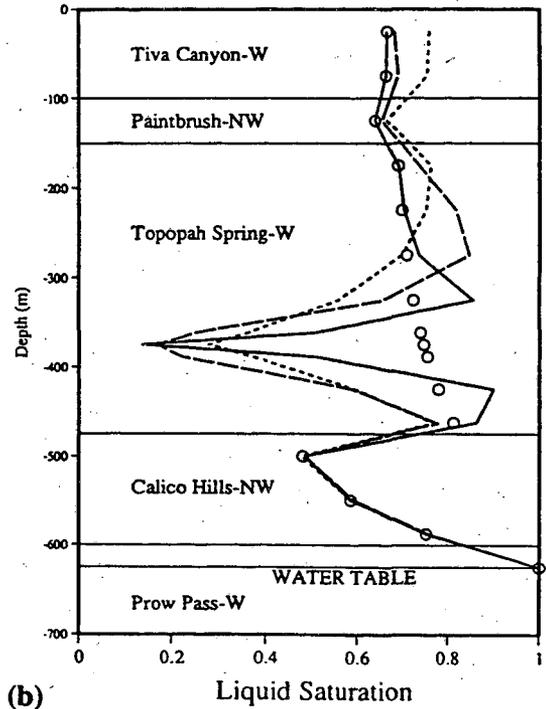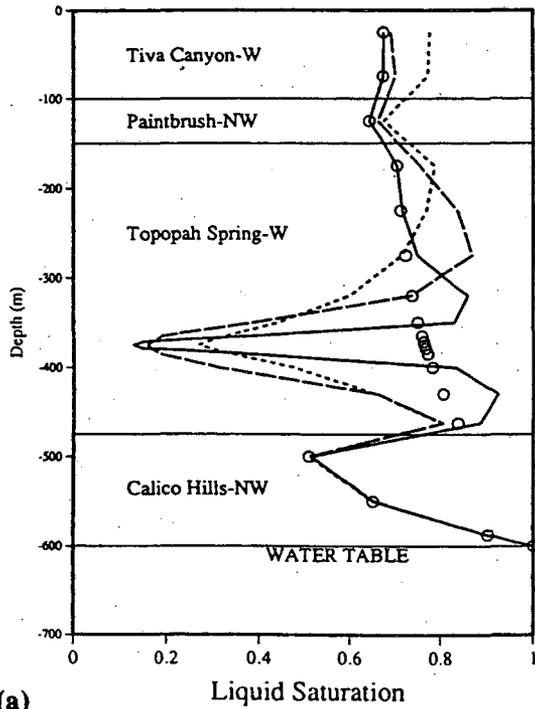

(a)

(b)

Figure 5. Simulated water saturation profiles. (a) R-Z model at R = 705.16 m radius, (b) X-Z model at column 8 (see Figure 1).

the present time, due to poorly known behavior of rough-walled rock fractures in partially saturated conditions. If at ambient suction conditions in the Topopah Spring unit water would have significant mobility in the fractures persistent heat pipe conditions would develop that would prevent temperatures from rising much beyond 100°C[8]. Heater experiments performed by Zimmerman and coworkers in G-tunnel, Nevada Test Site,[15,16] suggest that development of persistent heat pipe conditions, while not a ubiquitous phenomenon, is a distinct possibility.[8] Indeed, several thermocouples in these experiments registered temperatures near 94°C for extended time periods. This happens to be the boiling temperature at ambient pressures in G-tunnel, indicating persistent two-phase conditions.

For sealed emplacement holes, the impact of heat pipe conditions would be limited to the vicinity (a few meters) of the waste emplacement hole, and would not affect temperature and moisture conditions on a larger scale. For open-hole ventilated conditions, however, heat pipe development could have significant effects, promoting removal of heat and moisture from the system. Waste package-scale simulations have indicated that, when liquid is assumed mobile in the fractures, as much as 2/3 of total heat generated could be removed through ventilated open emplacement holes, and substantial moisture removal could take place to distances of 100 m or more above and below the repository horizon.[8]

A comparison between liquid saturation profiles in the R-Z and X-Z models shows good agreement at all times (Figure 5). This indicates that the X-Z model can provide an adequate approximation to waste heat effects on a larger scale (large compared to waste package dimensions), and that the model is suitable for studying the interaction between the waste heat and actual hydrogeologic features at the site. Of particular interest in this regard are capillary barrier phenomena at sloping contacts between different lithologic units,[17] and the role of fault zones with respect to liquid and gas phase flows.[2]

Gas phase flow effects are more complicated than would be expected from simple thermal buoyancy. Figure 6 shows gas fluxes calculated in the X-Z model at 1,000 years after waste emplacement. It is seen that gas convection is directed away from the repository, with flow being upward above the repository, downward beneath the repository. As noted previously,[11] this effect is due to an interplay between vapor-air diffusion and Darcy flow: Gas phase near the repository is primarily vapor, while away from the repository it is primarily air. Therefore, air diffuses towards the repository, increasing air partial pressure and total gas phase pressure there, and causing the gas phase outflow. The R-Z model shows the same effect.

SENSITIVITY STUDIES

Limited sensitivity studies have been carried out to examine effects of liquid infiltration from the ground surface. Two cases were simulated, with infiltration rates of 1 and 10 mm/yr, respectively, commencing at 1,000 years after waste emplacement. Impacts of the 1 mm/yr infiltration are very minor, even though this rate exceeds the matrix saturated conductivity in the Tiva Canyon and Topopah Spring units. Running the simulation to 10,000 years, fracture flow is found to never extend beyond 50 m depth. Liquid downflow at greater depths occurs entirely through the rock matrix under the combined action of gravity and capillary forces. The condition of liquid flow converging towards the repository that was observed in the "no infiltration" simulations persists even with 1 mm/yr infiltration for the entire 10,000 year period. When a persistent infiltration of 10 mm/yr is switched on at 1,000 years, however, liquid flow patterns are altered. Convergent liquid flow towards the repository horizon persists to 2,000 years, but gives way to downflow all the way to the water table at approximately 3,000 years. However, examining the immediate vicinity of the explicitly represented central waste package, it is observed that convergent liquid flow towards the emplacement hole is maintained to approximately 4,000 years. Subsequently, liquid downflow in the rock matrix extends all the way to the emplacement hole.
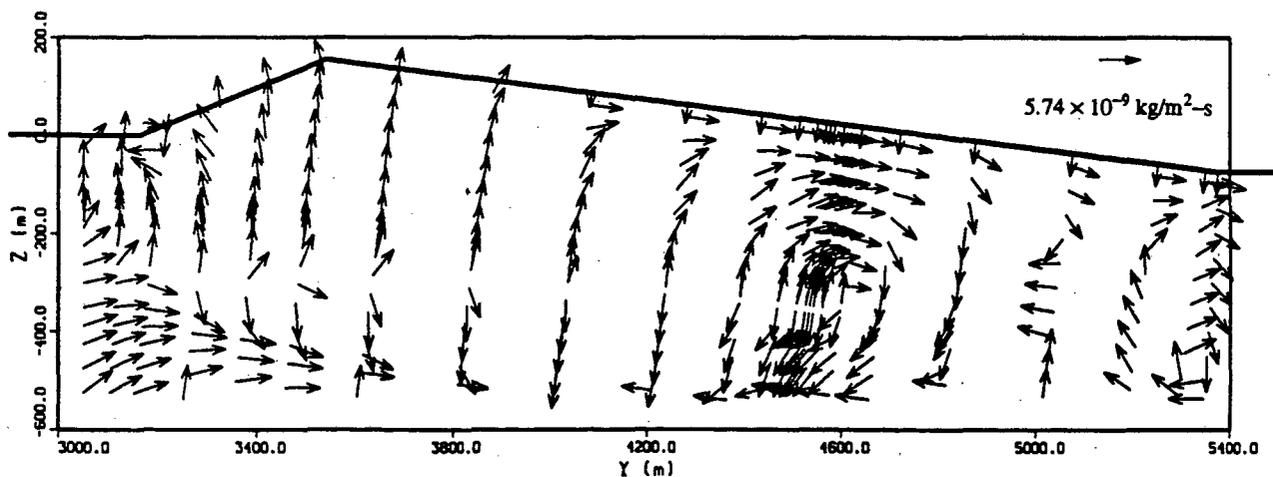

Figure 6. Simulated gas phase fluxes after 1,000 years in the X-Z model.

A brief study of open-hole emplacement was made, to evaluate the impact of repository ventilation during the operational phase on thermohydrologic conditions in the host rock. Ventilation effects were represented in a schematic way by applying a boundary condition of reduced relative humidity of 90%[18] and constant gas phase pressure at the inner boundary of the central waste package in the R-Z model. Only sensible and latent heat transfer but no conductive heat exchange were permitted at this boundary. The rates of water, air, and heat flow into the explicitly modeled emplacement hole were also applied, properly scaled for areal density of waste packages, to the distributed repository grid blocks.

Compared with sealed emplacement, temperatures near the repository level after 50 years of ventilated operation were approximately 6°C lower, and water saturations were approximately 6% lower. These modest effects are consistent with recent estimates by Danko and Mousset–Jones.[19] Moisture removal from the formation is mostly by vapor diffusion, and occurs at a rate of approximately 10^{-4} kg/s per waste package, with insignificant variations during the 50-year period. Heat removal rate is approximately 300 W per waste package. Total water removed per waste package is approximately 184 m^3 in 50 years. To put this number in perspective: At a formation porosity of 10% and an initial water saturation of 75%, this removal would have completely dried a region extending 5.8 m above and below the repository level. These results pertain to a situation where liquid is assumed immobile in the fractures; much larger effects would be predicted if liquid mobility in the fractures were finite.

DISCUSSION AND CONCLUSIONS

Our studies show that detailed numerical simulations of strongly heat-driven multiphase flow processes over time scales of 100,000 years are feasible in models that represent site-specific hydrogeologic conditions at Yucca Mountain in considerable detail. Thermal effects are found to alter not only the magnitude but in fact the direction of liquid and gas phase flows, so that an understanding of these effects is essential for a realistic assessment of repository performance.

The most important impact of the repository heat load is the development of a zone of partial dry-out around the repository, which is surrounded by a condensation halo of increased water saturation. The region of partial dry-out is predicted to be long-lived and is not easily obliterated even when net infiltration of 1–10 mm/yr is applied. This region may form a capillary "trap," drawing liquid water towards the repository (more or less balanced by outflow of vapor), and thereby adding to the capacity of the site to safely contain hazardous radionuclides. A superficial inspection of simulated flow behavior would appear to suggest that the capillary trap will be totally effective, completely preventing any liquid from migrating away from the repository region as long as capillary pressures are sufficiently negative there. However, it appears unlikely that such an absolute prohibition against liquid flow away from the repository would hold in reality. Most of the vapor condensation above the repository is expected to take place in fractures. Simulated condensation rates for the 57 kW/acre thermal loading considered here are so large that the condensate may not reach capillary equilibrium between fractures and matrix and may in part flow

downward along fast fracture paths. Liquid flow along fast paths across the repository region appears therefore possible even though on average capillary pressures would be more negative there.

It has been suggested recently that waste containment benefits associated with formation dry-out could be enhanced by means of high areal power density.[14] However, it should be noted that increased thermal loading will not only, on average, enhance formation dry-out, but will also increase rates of boiling and condensation, and thereby promote non-equilibrium flow of condensate along fractures. This could in fact have an adverse impact on the containment of hazardous radionuclides, suggesting that the issue of thermal loading should be dealt with cautiously. Clearly, further experimental and theoretical study is needed to develop a better understanding of liquid flow in partially saturated fractures in low-permeability rocks.

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