The Impact of Natural Convection on Near-Field TH Processes in the Fractured Rock at Yucca Mountain

J. T. Birkholzer[1], N. Halecky[1,3], S. W. Webb[2], P. F. Peterson[3], and G.S. Bodvarsson[1]

[1]*Lawrence Berkeley National Laboratory, MS 90-1116, Berkeley, CA 94720*
[2]*Sandia National Laboratories, MS-0718, Albuquerque, NM 87185*
[3]*University of California at Berkeley, Department of Nuclear Engineering, MC 1730, Berkeley, CA 94720*

Abstract – The heat output of the radioactive waste proposed to be emplaced at Yucca Mountain will strongly affect the thermal-hydrological (TH) conditions in and near the geologic repository for thousands of years. Recent computational fluid dynamics (CFD) analysis has demonstrated that the emplacement tunnels (drifts) will act as important conduits for gas flows driven by natural convection. As a result, vapor generated from boiling/evaporation of formation water near elevated-temperature sections of the drifts may effectively be transported to cooler end sections (where no waste is emplaced), would condense there, and subsequently drain into underlying rock units. To study these processes, we have developed a new simulation method that couples existing tools for simulating TH conditions in the fractured formation with modules that approximate natural convection in heated emplacement drifts. The new method is applied to evaluate the future TH conditions at Yucca Mountain in a three-dimensional model domain comprising a representative emplacement drift and the surrounding fractured rock.

I. INTRODUCTION

In the last few decades, extensive scientific investigations have been conducted at Yucca Mountain, Nevada, to explore whether the site is suitable for geologic disposal of high-level radioactive waste [1]. The heat produced by the radioactive waste will significantly change the thermal and hydrological environment at Yucca Mountain, affecting both the host rock and the conditions within the tunnels. Pore-water vaporization and subsequent condensation will lead to a large saturation and flux redistribution in the near-drift fractured rock. As vapor enters the emplacement drifts, the relative humidity will increase. Understanding and predicting these changes—in both the natural system and the drifts—is essential for evaluating the future performance of the repository in terms of canister corrosion and radionuclide containment.

The thermally driven flow processes to be expected in the fractured rock at Yucca Mountain have been investigated in various modeling studies (e.g., [2]–[4]). Gas flow along emplacement drifts has usually been neglected in these models, either because individual drifts were not represented at all or were treated as closed systems without axial flow and transport components. As a result, the models predict that the majority of the vapor produced from boiling/evaporation of formation water remains in the fractured rock. In reality, there may be considerable vapor transport from the fractured formation into the emplacement drifts. The importance of this vapor transfer depends largely on the presence of a transport mechanism that can move vapor away from the vapor-producing sections to the cold end of the drifts. Recent CFD simulations suggest that large-scale axial convection cells would form within emplacement drifts, providing such a transport mechanism [5]–[6].

In this paper, we describe a new simulation method that simultaneously handles mass and heat transport in the fractured formation *and* in the emplacement drifts. The model concepts used for the partially saturated fractured rock are based on existing models as described, for example, in [2]–[4]. In-drift natural convection is approximated as a binary diffusion process, with effective dispersion coefficients estimated from supporting CFD analyses described in [5] and [6]. This approach is similar to a comparative modeling study documented in [7]. The new simulation method is applied to study the future TH conditions at Yucca Mountain in a three-dimensional domain comprising one representative drift and the surrounding fractured rock. Our main objective is to better understand how natural convection in drifts affects the near-drift TH processes, particularly with respect to the saturation changes and flux perturbations in the fractured rock.

II. DISCUSSION OF BASIC TH PROCESSES

At Yucca Mountain, the heat emanating from the waste packages will be effectively transferred to the drift walls, mostly via thermal radiation. At early stages after emplacement, temperatures in the partially saturated formation near the drifts will heat up to above-boiling conditions. As a result, the initially mostly stagnant pore water in the rock matrix will become mobile through boiling (see Figure 1a). Vaporization causes a pressure increase, which will drive the vapor away from the boiling region, both into more distant rock regions (where the vapor will condense and enhance liquid fluxes) as well as back into the drifts (where relative humidity will increase). At later times, when temperatures will decrease below boiling, the rock mass near the drifts will gradually rewet (Figure 1b). For drifts with average temperature conditions, rewetting will occur roughly a few hundred years after boiling has ceased, a time period during which natural convection processes within the drifts are still important.

Vapor entering the emplacement drifts from the fractured porous rock is subject to effective axial mixing transport as a result of natural convection processes. Such mixing can reduce the overall moisture content in heated drift sections because of the presence of the unheated drift ends (turnouts). Principles of thermodynamics suggest that the maximum amount of vapor that can be present in air decreases with declining temperature. Thus, the warm vapor-rich gases moving from heated drift sections toward the drift turnouts—caused by natural convection processes—will be depleted of most of their vapor content through condensation on cooler rock surfaces. (As shown in Figure 1, the condensate will drain away from the repository into underlying rock units.) At the same time, vapor-poor gas will circulate towards the emplacement sections of the drifts, thereby reducing the moisture content and the relative humidity in these areas. This effect, in turn, will generate a concentration gradient between the fractured rock and the in-drift environment, causing diffusive vapor transport from the formation into the drift.

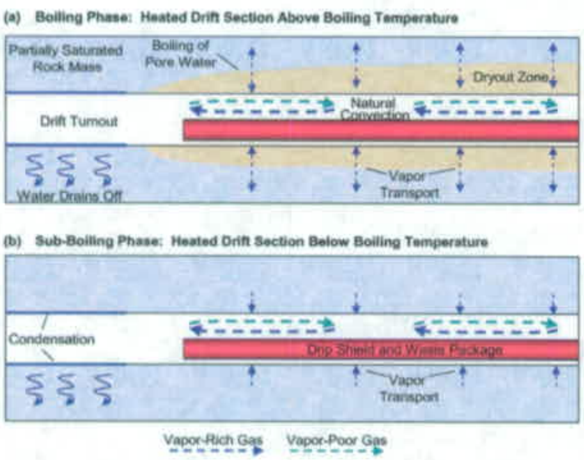

Fig. 1. Schematic of expected TH processes along emplacement drift (modified from [6]).

III. MODELING APPROACH

III.A. Fractured Rock Mass

The modeling framework for simulating the TH conditions in the near-field fractured rock is adopted from existing TH models for Yucca Mountain (e.g., [2]–[4]). The relevant TH processes in the heated rock mass are the convective and diffusive movement of gaseous and liquid phases of components water and air (under pressure, viscous, capillary, and gravity forces); transport of latent and sensible heat; phase transition between liquid and vapor; and vapor pressure lowering. The fractured rock is described using a dual permeability concept, assuming two separate but interacting continua that overlap with each other in space [8]. One continuum describes flow and transport in the fracture network; the other describes flow and transport in the rock matrix. Disequilibrium conditions between fractures and matrix and the related mass and heat transfer can be efficiently modeled with dual permeability formulations, avoiding the need to explicitly account for individual fractures.

III.B. Emplacement Drift

In this work, a detailed representation of in-drift gas flow processes is not essential. Rather, of primary importance is the global large-scale vapor transport in the drift and the impact that in-drift natural convection has on the TH conditions in the near-drift fractured rock. The latter requires a reasonable approximation of axial vapor transport along the drifts, but not a detailed resolution of convective flow patterns. Thus, we assume that in-drift transport of vapor and air can be characterized as an axial diffusion process, using mass dispersion coefficients provided by complementary CFD simulations [5]. Two sets of dispersion values were derived in [5], representing strong versus moderate convective mixing (see Table 1). As pointed out in [5], the two sets provide first-order approximations for the possible range of convective mixing in Yucca Mountain drifts. The values given for both sets are much larger than the standard molecular diffusion coefficient of vapor-air mixtures (2×10^{-5} m^2/s).

Table 1: Mass dispersion coefficients (m^2/s) given in [5]

Cases	300 yrs	1000 yrs	3000 yrs
Case 1: Strong convective mixing	0.1	0.1	0.1
Case 2: Moderate convective mixing	0.008	0.004	0.004

III.C. Heat and Mass Transfer between Rock Mass and Drift

The heat and mass transfer between the gas flow in the drifts and the adjacent fractured rock is calculated from empirical boundary-layer correlations given in the literature. It is well known that such transfer is affected by the presence of a surficial fluid boundary layer, where the motion of particles is retarded compared to the free stream velocity. Extensive experimental and theoretical work has been conducted in the past decades to study and describe these processes (mostly in mechanical engineering applications), and empirical correlations have been developed for heat and mass transfer through the boundary layers for simplified geometries. The correlations used in this study are derived from the case of free convection in the annular space between long horizontal eccentric cylinders, which roughly represents the geometry of an open drift with a drip shield/waste package assembly. See details in [6].

III.D. Modeling with TOUGH2

By approximating natural convection as a binary diffusion process, the in-drift mass- and heat-transport processes can be simulated with standard methodologies applied for Darcy-type flow and transport. For this study, we implemented a new drift simulation module into TOUGH2, a general-purpose simulator for coupled transport of multiphase, multicomponent fluid mixtures in porous and fractured media [9]. In addition to various other applications, TOUGH2 has been widely used for simulating TH processes in the fractured rock at Yucca Mountain (e.g., [3] and [4]). The new version of TOUGH2 is applied to simultaneously solve for mass and heat transport within the drift and in the surrounding fractured rock, with the drift defined by a solution domain that requires certain modifications and parameter specifications. These are described in detail in [10].

Three-dimensional simulation runs were performed for a representative emplacement drift of 600 m length located in one of the southern panels of the repository. In the vertical direction, the model comprises the entire unsaturated zone, having the ground surface as the upper model boundary and the groundwater table as the lower model boundary. In axial drift direction (y-direction), symmetry allows for reducing the model to half of the drift plus sufficient volumes of fractured rock beyond the drift end to provide adequate boundary conditions. Model boundary conditions and material properties are described elsewhere [10], and shall not be repeated here.

IV. MODEL RESULTS

Our model simulations cover the first 5,000 years after emplacement of radioactive waste. Interested in the impact of natural convection, we focus on the postclosure period and run the simulations until the impact of natural convection becomes marginal because of decreasing temperatures. Two main simulation cases are considered using the two sets of effective dispersion coefficients given in Table 1 (Cases 1 and 2). For comparison, we also study a simulation case where axial transport along the drift is neglected (Case 3). This is achieved by removing all open drift elements from the numerical grid, thus making the drift an impermeable boundary to the fractured rock mass. The only remaining in-drift elements are those representing the drip shield/waste package assembly; these elements are connected to the drift wall to allow for radiative heat transfer.

Let us first evaluate the heat-related TH processes in a vertical cross section along the drift. We select Case 1, which features strong convective mixing along the drift, and show model results at 500 years after emplacement, representative of the expected situation towards the end of the boiling period at Yucca Mountain. Figure 2a depicts temperature and liquid saturation contours as well as liquid flux vectors for the fracture continuum and the drift, while Figure 2b plots vapor concentration (derived as the mass fraction of vapor in the gas phase) and liquid saturation contours in the matrix continuum and in the drift. Both the matrix and fracture saturation contours show that a large volume of rock has desaturated in the vicinity of the heated section of the drift, with the region of reduced liquid saturation extending several meters into the formation. The dryout region below the drift is larger than above, where further saturation decrease is limited by the percolation flux arriving at the boiling zone and the gravity-driven reflux of condensate.

Because large amounts of pore water have boiled off, the vapor concentration in the gas phase has increased significantly in the heated rock regions, with maximum values above 0.7 a few meters away from the drift (initial vapor concentration is close to zero). Part of the vapor moves effectively within the highly permeable fractures out into the distant rock mass. As a result, elevated vapor concentrations of 0.3 and more can be seen at distances of 30 m above and below the heated drift. That condensation of vapor occurs in these cooler rock regions can be inferred from the elevated matrix saturations, which reach maximum values well above the initial saturation value of 0.85. This saturation increase is caused by condensation of vapor on the fracture walls and subsequent imbibition into the matrix pores. The fracture continuum does not exhibit a corresponding saturation buildup, because the bulk of the condensate drains off immediately as a result of the large fracture permeability combined with the small fracture capillarity.

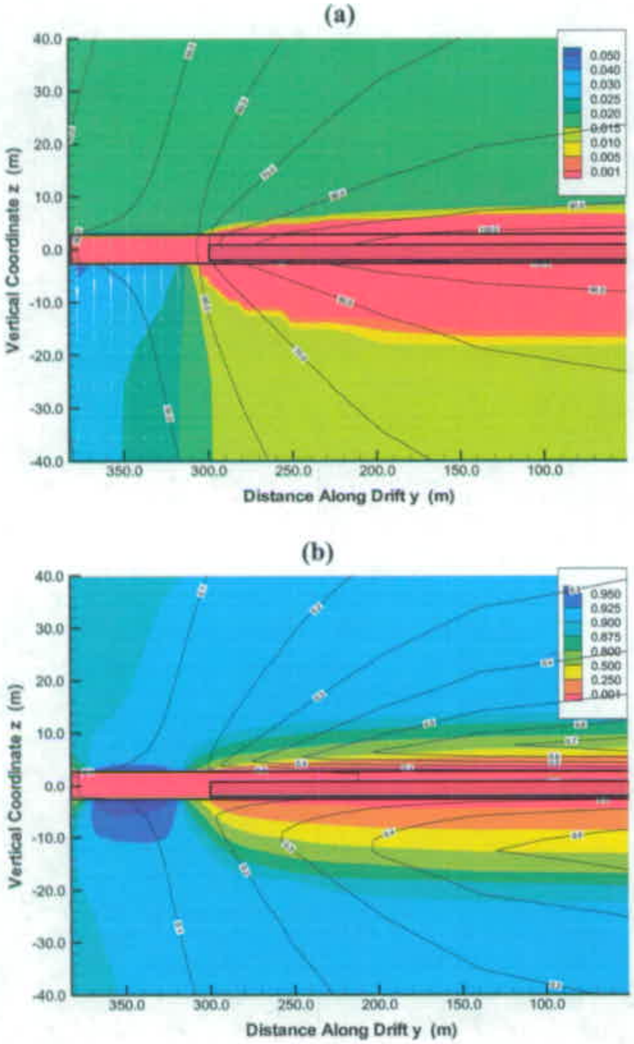

Fig. 2. Simulated TH conditions for Case 1 in vertical cross section along drift after 500 years. (a) Colored contours show fracture saturation; contour lines show temperature in the rock mass and in the drift. (b) Colored contours show matrix saturation; contour lines show vapor concentration in the matrix and in the drift. The distance along the drift is measured with y = 0 in the center of the heated section of the drift. The heated section of the drift ends at y = 300 m, followed by a 90 m long unheated end section.

Notice the pronounced saturation buildup near the unheated end section of the drift in both Figures 2a and 2b, indicating that a significant amount of the vapor produced in the rock mass enters the drift, migrates in axial direction (as a result of circulating gas flows from natural convection), and eventually condenses on the cooler drift wall surfaces (Figure 2a). Most of the condensate drains towards the drift bottom through the invert and downward into the fracture continuum. As a result, fracture saturation increases strongly below the drift, and significant gravity-driven liquid fluxes occur, driving water away into the underlying formations. A small fraction of the condensate imbibes from the drift walls into the matrix pores as a result of capillary forces. The impact of imbibition can be seen in the elevated matrix saturations both above and below the drift end (Figure 2b). Despite the saturation increase, the liquid fluxes in the matrix are much smaller than those in the fracture continuum. In fact, when plotted on the same length scale, the flux vectors in the matrix are too small to be visible.

While vapor-rich gas is driven from the heated drift section towards the unheated drift turnout, vapor-poor gas moves back, thereby reducing the in-drift vapor concentration near the heat-producing waste packages. This effect, present along the entire length of the emplacement section, causes a steep vapor concentration gradient between the fractured rock mass and the drift. For example, Figure 2b shows that the maximum vapor concentration in the drift is between 0.2 and 0.3, which compares to a maximum value of more than 0.7 in the rock. As a result of this concentration difference, vapor migrates from the heated rock mass into the drift not just by pressure-driven convective flow, but also by diffusion.

More detail on the in-drift moisture conditions—and the effect of different degrees of natural convection—is given in Figure 3, showing relative humidity profiles along the drift centerline for Cases 1 and 2, respectively. Relative humidity of less than 100% in the drift indicates that evaporative conditions exist; i.e., pore water present in the adjacent fractured rock would be subject to evaporation. Relative humidity equal to 100%, on the other hand, implies that there is no evaporation, and that any vapor mass exceeding the corresponding vapor concentration would condense.

All relative humidity profiles in Figure 3 exhibit strong differences between the heated and unheated drift sections. In the heated section, relative humidity is below 100% at all times, in both Cases 1 and 2. This means that no condensation can occur in the vicinity of the waste packages, and that evaporative conditions exist over the entire simulation period. (We caution, however, that local heat output variation between individual waste packages, which might lead to localized condensation, has not been considered in this analysis.) In the unheated sections, on the other hand, relative humidity is at 100%, which explains the strong condensation patterns observed in Figures 2. In general, the relative humidity values along the heated section are much smaller for Case 1 compared to Case 2, a result of the more intense convective mixing between vapor-poor and vapor-rich drift sections. In Case 2, the relative humidity profiles at 1,000 and 5,000 years show a local minimum at the end of the heated section, with relative humidity locally reduced. This suggests that convective mixing is not strong enough (i.e., that the turbulent circulation patterns are not large enough) to impact the entire emplacement drift; only those sections that are close to the unheated drift turnout are affected during these late time periods.

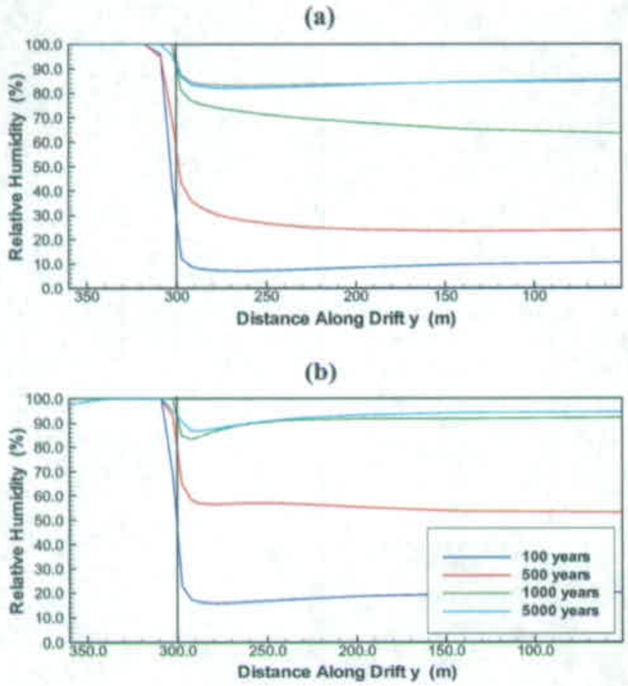

Fig. 3. Relative humidity along drift just above drift center for (a) Case 1 and (b) Case 2.

Let us now analyze in more detail how the observed in-drift conditions affect the moisture exchange between the fractured rock mass and the drift. Figure 4 shows the evolution of the vapor mass transfer integrated over the heated drift section for Cases 1 and 2, respectively. To allow for a direct comparison, the integrated vapor fluxes are given as relative values, divided by the total liquid flux arriving over the footprint of the heated drift section from ambient percolation. The figure exemplifies the importance of the drift as a conduit for vapor transport out of the near-drift fractured rock, particularly in Case 1, where in-drift relative humidity values are small. At early heating stages, the amount of vapor transferred into the drift in Case 1 is almost 10 times higher than the water arrival from natural percolation, suggesting that the vapor source is mostly resident pore water. With time, the magnitude of vapor transfer reduces significantly, but not to negligible values. At 5,000 years, for example, more than 20% of the long-term percolation flux arriving at the drift is still being transferred into the drift by means of vapor transport. In Case 2, featuring moderate convective mixing, vapor transfer is clearly less effective, with relative values of about 5 at early times, which reduce to negligible amounts after about 2,000 years.

Figure 4 also distinguishes between convective and diffusive transport of vapor between the formation and the drift. Convective transport results from the pressure increase in the fractured rock as pore water boils, while diffusive transport is caused by the vapor concentration gradient. In Case 1, diffusion is the dominant transport mechanism, since the strong mixing along the drift ensures small vapor concentrations and thus a large concentration gradient. In Case 2, vapor diffusion is less important, while the magnitude of convective transfer is comparable to Case 1. Thus, the differences between Case 1 and Case 2 are mostly a result of the more or less effective diffusive exchange. Note that in both cases, convective transport is only effective for the first 2,000 years after emplacement.

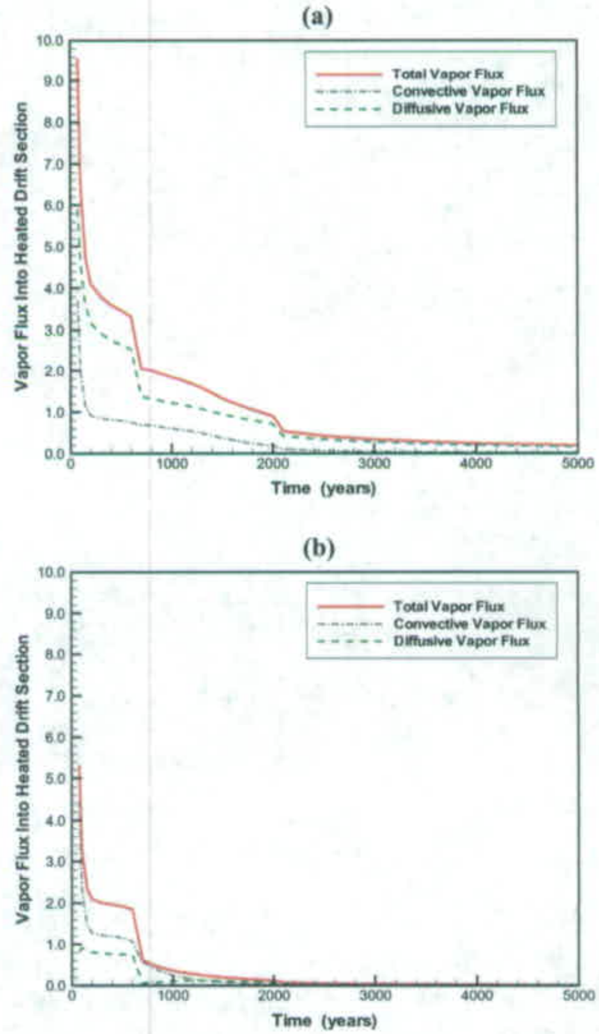

Fig. 4. Evolution of vapor flux from formation to drift integrated over heated drift section for (a) Case 1 and (b) Case 2. Vapor flux is normalized by dividing with ambient percolation flux integrated over the cross-sectional area of the heated drift section.

We now focus our attention on the TH conditions in the near-drift fractured rock. As a starting point, it is useful to plot the evolution of matrix liquid saturation along the drift for selected times (Figure 5). In addition to Cases 1 and 2, we plot results for Case 3, where axial transport along the drift is neglected. Comparison between the cases demonstrates the importance of natural convection. In Case 3, with no vapor transfer between the formation and the drift, the rock mass near the drift resaturates much earlier after the initial dryout than in the other two cases, and arrives at much higher long-term saturation levels along the emplacement section.

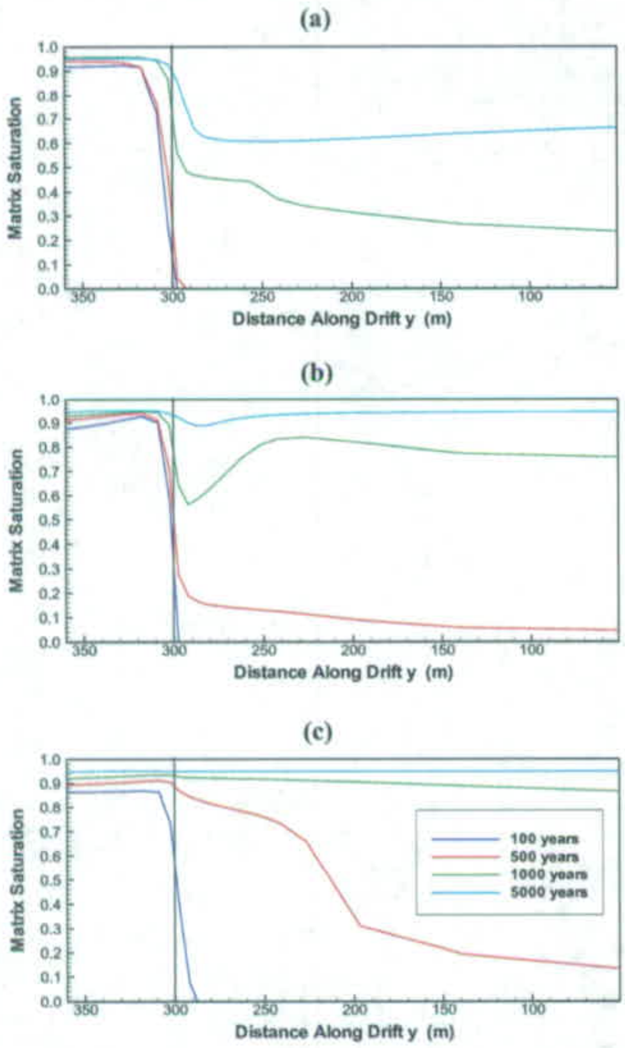

Fig. 5. Matrix saturation along drift just above drift crown for (a) Case 1, (b) Case 2, and (c) Case 3

In Case 1, on the other hand, the matrix pores along the emplacement section are still desaturated at 500 years, while Case 3 already exhibits strong saturation buildup. Further, in Case 1 the maximum saturation at 5,000 years is less than 0.7, indicating that evaporation remains effective, while Cases 2 and 3 end up with maximum saturations of 0.94 and 0.97, respectively. Notice the local minimum in the saturation profiles of Case 2 at 1,000 and 5,000 years, which corresponds to a similar minimum in the relative humidity profiles in Figure 3. Convective mixing reduces the moisture content in the rock matrix, but only over a limited drift length close to the end of the heated section.

The volumetric evolution of rock dryout as a function of time is presented in Figure 6. Rock dryout estimates have been derived by adding the volume of all mesh elements along the heated drift section that have a matrix saturation less than 0.425 (i.e., half of the initial matrix saturation). In Case 1, the total dryout volume calculated from this procedure is as high as 37,000 m^3, which translates into an average circular extent of about 6.5 m dry rock from the drift walls. (Note that the volumetric values are given for a half-drift model with 300 m emplacement length. Values need to be quadrupled for an entire full drift emplacement section with 600 m length.) The maximum value in Case 2 is almost as large as in Case 1 at early heating stages, but the dry rock volume decreases much faster with time. Significantly less drying can be seen in Case 3, where the maximum volume is on the order of 25,000 m^3, about 65% of Case 1.

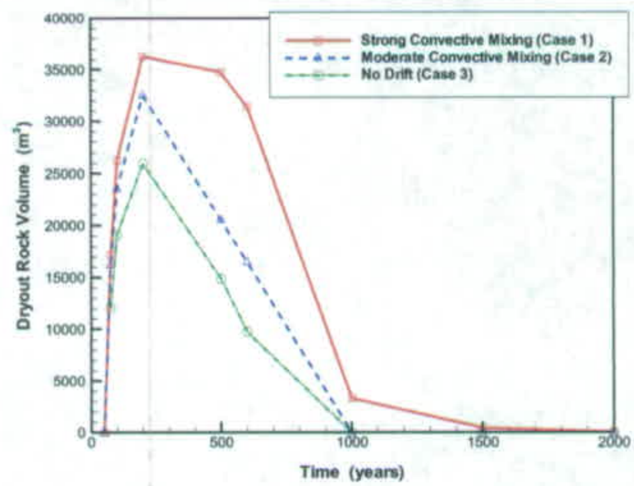

Fig. 6. Evolution of dryout volume of rock mass along heated drift section

It is of interest to determine how these changes in water content affect the heat-induced perturbation of liquid fluxes in the fractured rock. Figure 7 shows the downward liquid fluxes at different times along a horizontal profile chosen close to the center of the heated drift section. The profile is perpendicular to the drift axis; it starts at the sidewall of the drift and extends laterally several meters into the fractured rock. All fluxes are given relative to the ambient natural percolation flux at the considered time; i.e.; fluxes larger than one denote a flux enhancement.

At early heating stages (i.e., 100 and 500 years), vaporization of pore water and subsequent condensation lead to a considerable flux elevation just outside of the dryout zone where the condensate drains off. Note the strong differences between the different simulation cases, with Case 1 showing much less flux enhancement than the other cases because more vapor moves out of the fractured rock into the drift. Flux enhancement during boiling is a concern for repository performance, because it may increase the potential for preferential flow events penetrating the dryout region and possibly dripping into the heated drift [11].

Later, when boiling has ceased and the fractured rock near the drift resaturates, the maximum vertical fluxes occur close at the drift wall. These fluxes are enhanced because water—arriving at the drift crown from natural percolation—is diverted sideways and around the drift as a result of the capillary barrier at the drift wall. At 1,000 years, the flux enhancement is smallest in Case 1, since water present near the drifts is subject to evaporation. At 5,000 years, the impact of evaporation at 5,000 years is less pronounced in all cases.

III. CONCLUSIONS

We have conducted a numerical study to evaluate how the vapor transport caused by natural convection in waste emplacement drifts will affect the TH conditions in the surrounding fractured rock during the postclosure period at Yucca Mountain. A new simulation method was developed that couples existing model approaches for predicting heat and mass transport in the rock mass with modules that approximate in-drift convection as a binary diffusion process. The work described in this paper was conducted in parallel with TH modeling for performance assessment of Yucca Mountain, to evaluate alternative approaches and their impact on the TH conditions. Three simulation cases were analyzed. The first two cases represent different degrees of convective mixing in drifts. The third case ignores the presence of the drifts as a conduit for vapor transport.

Our simulation results demonstrate the importance of in-drift natural convection. Compared to the simulation case without the drift, convective mixing convection causes

(1) More rock dryout during the boiling period,
(2) Later resaturation of the near-drift rock mass and a smaller long-term saturation value,
(3) Less moisture redistribution within the fractured rock from boiling and condensation, and
(4) Less heat-induced flux perturbation.

These natural convection effects are expected to improve the performance of the repository, since smaller relative humidity values form a more desirable waste package environment. Also, seepage of formation water into the drifts will be reduced under such conditions [12].

The two simulation cases representing strong versus moderate convective mixing exhibit clear differences. The first case shows a much more pronounced reduction of the moisture content in the drift and the rock mass over a longer duration.

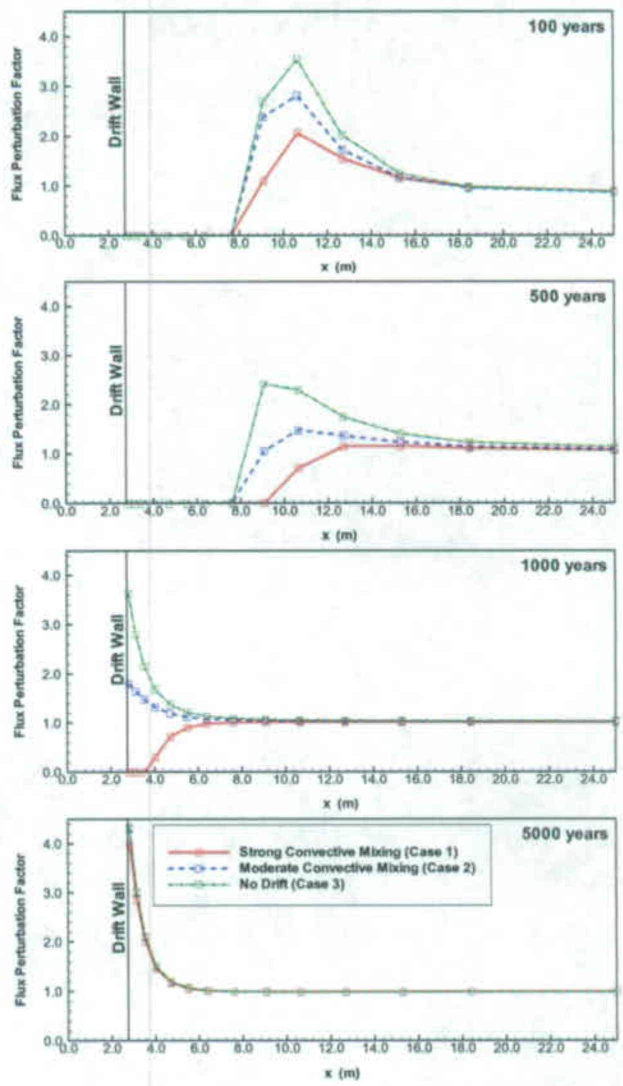

Fig. 7. Vertical liquid fluxes in horizontal profile from drift wall into fractured rock in a drift section close to the center of the drift. Fracture and matrix fluxes have been summed up and divided by ambient percolation flux at the considered time.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of Science and Technology and International, of the U.S. Department of Energy. Review and comments of Y. Tsang and D. Hawkes from Berkeley Lab are greatly appreciated.

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