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NEAR-FIELD THERMAL-HYDROLOGICAL BEHAVIOR FOR ALTERNATIVE REPOSITORY DESIGNS AT YUCCA MOUNTAIN

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ABSTRACT

Three-dimensional calculations that explicitly represent a realistic mixture of waste packages (WPs) are used to analyze decay-heat-driven thermal-hydrological behavior around emplacement drifts in a potential high-level waste facility at Yucca Mountain. Calculations, using the NUFT code, compare two fundamentally different ways that WPs can be arranged in the repository, with a focus on temperature, relative humidity, and liquid-phase flux on WPs. These quantities strongly affect WP integrity and the mobilization and release of radionuclides from WPs. Point-load spacing, which places the WPs roughly equidistant from each other, thermally isolates WPs from each other, causing large variability in temperature, relative humidity, and liquid-phase flux along the drifts. Line-load spacing, which places WPs nearly end to end in widely spaced drifts, results in more locally intensive and uniform heating along the drifts, causing hotter, drier, and more uniform conditions. A larger and more persistent reduction in relative humidity on WPs occurs if the drifts are backfilled with a low-thermal-conductivity granular material with hydrologic properties that minimize moisture wicking.

INTRODUCTION

The U.S. Department of Energy is investigating the feasibility of disposing of radioactive wastes, including spent nuclear fuel (SNF) from electrical utilities and wastes stored at federal facilities, in the unsaturated zone (UZ) at Yucca Mountain, Nevada. To be feasible, the waste isolation system must limit the release and transport of radionuclides to the accessible environment. A key concern is how water contacts a WP, which affects WP integrity and the mobilization and release of radionuclides from WPs. The ambient relative humidity in the UZ is high ($RH \approx 99\%$) and is therefore corrosive for most candidate WP materials. If RH were reduced enough, WP corrosion rates would be minimal [1]. Two primary modes by which water may contact a WP are (1) condensation of water vapor that forms a liquid film on the WP and (2) liquid-phase flow. The critical factor for the first mode is RH on the WP surface. For the second mode, liquid-phase contact may arise in three ways:

Drift seepage: Advective liquid-phase flow of water that enters the drift (and flows through the backfill if present) as a result of ambient percolation or decay-heat-driven condensate flow.

This can include episodic nonequilibrium fracture flow or a steady seep.

Wicking: Diffusive moisture transport driven by matric potential gradients (resulting from capillary and surface forces, and osmotic effects). Because this process occurs both in the gas phase (as vapor diffusion) and the liquid phase (as imbibition), it does not require a continuous liquid phase.

Cold-trap effect: Axial vapor flow and condensation within the drift is driven by axial variations in temperature T and partial pressure of water vapor P_v along the drift. Water vapor is transported from areas of higher to lower T and P_v where it condenses, causing RH to locally increase (up to 100%). Large condensation rates arise in cooler areas if the following conditions are met: (1) RH is high in the adjacent rock, (2) WP heat output varies substantially from WP to WP, and (3) WPs are thermally isolated from one another.

Much of the debate over various thermal loading designs has focused on the areal mass loading (AML, expressed in metric tons of uranium per acre, MTU/acre). Of the many competing factors (e.g., operational constraints, costs, material responses) to consider in evaluating alternative thermal designs, perhaps most important is the role that decay heat plays in determining the thermal-hydrological (T-H) conditions in and around the emplacement drifts and, in particular, RH and liquid-phase flux on WPs. Decay heat influences the distribution of liquid saturation and liquid-phase flux in the near field and altered zone, affecting radionuclide transport. Decay heat also drives coupled thermal-hydrological-geomechanical-geochemical (T-H-M-C) processes that permanently alter flow and transport properties. These effects may continue to affect radionuclide transport well after decay heat has stopped mobilizing gas- and liquid-phase flow.

Waste packages can be arranged in the repository at Yucca Mountain in two fundamentally different ways. The first approach (the point-load design) attempts to evenly distribute the WP decay heat over the repository area by placing the WPs with roughly the same axial and lateral spacing between WPs, as is done in the advanced conceptual design (ACD) [2]. The second approach (the line-load design) lineally concentrates the WP decay heat by placing the WPs nearly end to end along the drifts. For a given AML, this maximizes the spacing between drifts and minimizes the length of emplacement drifts. We analyzed the reference AML of 83.4 MTU/acre [2] with and without engineered backfill emplaced at the time of repository closure (100 yr); however, other AMLs have also been considered [3]. Decay-heat-driven T-H behavior is markedly different for the point-load and line-load designs.

Three-dimensional calculations are required to adequately represent drift-scale T-H behavior. Models based on the NUFT code [4] were developed to carry out such calculations [3]. A major factor to be considered in the selection of a repository design is that WP heat generation varies substantially in the WP inventory. Whereas defense high-level waste (DHLW) generates a negligible amount of heat, spent nuclear fuel (SNF) initially can generate as much as 18 kW per WP. The influence of WP heat output variability on T , RH , and liquid-phase flux experienced by WPs is markedly different for the point-load and line-load designs. A key motivation for the point-load design is to limit peak drift-wall and WP temperatures regardless of the WP sequence along the drifts. A certain degree of thermal management of the waste stream (i.e., controlling WP sequencing) may be required for line-load spacing to sufficiently limit peak temperatures.

NUMERICAL MODELS AND ASSUMPTIONS

Model calculations were conducted with the NUFT code [4], which was developed at Lawrence Livermore National Laboratory to simulate the coupled transport of water, vapor, air, and heat in fractured porous media. We included all major hydrostratigraphic units in the UZ [5] and assumed they are horizontal and of uniform thickness. The initial and boundary conditions are the same as those used in past studies [3,6]. We assumed a bulk permeability k_b of 280 millidarcy, and an initial vertical liquid saturation profile based on a percolation flux of 0.3 mm/yr. However, a wide range of other conditions (including percolation fluxes ranging from 0 to 5 mm/yr) have also been considered [3,6]. The atmospheric RH is assumed to be 100%, so the model allows no loss of moisture by vapor diffusion to the atmosphere. Because actual (desert) RH is much less than 100%, the model underrepresents this loss.

The models include six major WP types (Fig. 1), resulting in a WP inventory that is representative of that assumed for the ACD [2]. The four SNF WP types are: (1) 40-yr-old 12-PWR WPs, (2) 26-yr-old 44-BWR WPs, (3) 26-yr-old 21-PWR WPs, and (4) 10-yr-old 21-PWR WPs. The two types of DHLW are Hanford site and Savannah River site DHLW WPs. The ACD assumes that 27% of the WPs contain DHLW, which is similar to the assumption made in this study that 30% of the WPs contain DHLW. The WP inventory described in Ref. 2 has an average heat output at the time of emplacement of 7.18 and 1.5 kW for the SNF and DHLW WPs, respectively. In our models, the SNF and DHLW averages are 7.84 and 2.4 kW. The SNF and DHLW WPs are assumed to have lengths of 5.68 and 3.68 m, respectively; all WPs are assumed to have a diameter of 1.8 m. The drift diameter is assumed to be 5.5 m, which is similar to the ACD assumption of 5 m [2]. We also considered a 5-m-diameter drift and found little difference in T-H behavior between 5- and 5.5-m-diameter drifts. For thermal radiation in the drift, a WP emissivity of 0.8 is assumed; a WP emissivity of 0.3 has also been considered [3]. For the backfill cases, a granular backfill with hydrological properties similar to sand was assumed; crushed rock from the welded Topopah Spring tuff (TSw2) unit, which is where the potential repository horizon occurs, has also been considered [3]. Backfill thermal conductivities K_{th} of 0.3 and 0.6 W/m°C were considered. The invert is assumed to consist of a granular fill with the same properties as the backfill. For the line-load backfill cases, it is assumed that measures are taken to prevent backfill from filling the small gap separating WPs. For the ACD backfill cases, backfill fills the space separating WPs.

The models are applicable to areas of the repository far enough away from the edge to remain unaffected by edge-cooling effects. This allows the use of periodic no-mass/heat-flow boundaries that correspond to (1) the drift centerline, (2) the pillar centerline, (3) the plane transverse to the middle of the Hanford site DHLW WP, and (4) the plane transverse to the middle of the 10-yr-old 21-PWR WP. The ACD assumes a drift spacing of 22.5 m and places WPs on the basis of a constant lineal mass loading (LML) of 0.46 MTU/m along the drift (Fig. 1). For the line-load design, we assumed a 0.1-m gap between WPs, an LML of 1.11 MTU/m and a drift spacing of 53.8 m (Fig. 1).

Figure 1. Plan view of the WP layout represented in the models for (a) the ACD point-load design and (b) the line-load design. Both designs result in AML = 83.4 MTU/acre.

The respective designs have linear power loadings (LPL) of 0.5 and 1.2 kW/m. Assuming the WP inventory described in Ref. 2, a 5.335-m length for all SNF WPs (which is a more recent assumption), and a 0.1-m gap between WPs results in an LPL of 1.13 kW/m, similar to the value used in this study.

DISCUSSION OF MODEL RESULTS

A key question is whether liquid-phase flux, arising from ambient percolation flux and decay-heat-mobilized condensate flux, may enter emplacement drifts or, at the very least, prevent dryout (and RH reduction) from occurring in the adjacent rock. For an 83.4-MTU/acre repository, the overall magnitude of the condensate flux depends on AML, not on LML [3]; consequently, the point-load and line-load 83.4-MTU/acre designs mobilize the same overall magnitude of condensate flux. Moreover, liquid-phase flux in the vicinity of an 83.4-MTU/acre repository is dominated by condensate flux for 2000–5000 yr [3]. Superheated conditions and a reduction in RH in the repository rock will occur if the local heat flux q_H is enough to evaporate the local incoming liquid-phase mass flux q_{liq} as expressed by the following relation:

$$q_H > q_{liq} \rho_{liq} h_{fg} \quad (1)$$

where ρ_{liq} is the mass density of water and h_{fg} is the specific latent heat of vaporization. If q_{liq} is too large, q_H is insufficient to generate superheated conditions. Near the drift, q_H is proportional to LML; further out in the rock, it is proportional to AML after the thermal fields have coalesced. Spatial

Figure 2. Temperature and relative humidity in rock at upper drift wall at various WP locations for (a,c) the ACD point-load design and (b,d) the line-load design.

variability in either q_H or q_{liq} can result in local regions where q_{liq} will prevail. Because q_H increases with proximity to the drift, it is more likely for q_{liq} to prevail in the rock away from the drifts (e.g., at the pillar centerline), rather than near the drifts. Near the drifts, q_H will be 2.4 times greater (on average) for the line-load design than for the point-load design. Moreover, the q_H at the pillar centerline will be less for the line-load design than for the point-load design, increasing the likelihood that condensate will shed through the pillar of the line-load design. The point-load design results in spatial variability in both q_H and q_{liq} along the drift. Cooler intervals of the point-load drifts are more likely to be overwhelmed by q_{liq} as a result of condensate being displaced from hotter to cooler regions and because q_H is less there; the net result is higher RH and heat pipes above the cooler intervals of the point-load drift, which increase the local cooling rate and the likelihood of seepage into the drift.

The marked difference in drift-scale T-H behavior between the point-load and line-load designs for no backfill is evident in Fig. 2. The axial WP spacing in the point-load design is large enough to thermally isolate the WPs from each other; peak drift-wall temperatures range from 107 to 158°C, and peak WP temperatures range from 112 to 186°C (Table I). The close axial WP spacing in the line-load design results in efficient WP-to-WP thermal-radiative heat transfer, so that, in spite of their different heating histories, all WPs experience similar (and more beneficial) T and RH conditions. For the no-backfill cases, the coolest and most humid WP in the line-load design always has a lower RH than the hottest and least humid WP in the ACD point-load design (Fig. 3 and Table I). The line-load design results in: (1) more locally intensive (and uniform) rock dryout around the drifts, (2) more effective condensate shedding between the drifts, and (3) less condensate buildup above the drifts.

The last two rows of Table I list the time required to rewet to RH = 65 and 90%. These RH thresholds are important because corrosion studies of the candidate WP materials indicate that the critical RH for significant atmospheric corrosion is 65% if a hygroscopic salt is present on the WP, or

No backfill		
Repository design	ACD point load	Line load
$T_{\text{peak}} (t < 100 \text{ yr})$	112–186 °C	184–214 °C
$RH (t = 100 \text{ yr})$	26–71%	14–19%
$RH (t = 2000 \text{ yr})$	85–94%	71–74%
$RH (t = 10,000 \text{ yr})$	93–99.9%	94–98%
$t(RH = 65\%)$	25–660 yr	1540–1710 yr
$t(RH = 90\%)$	1540–2390 yr	4260–4790 yr

Table I. Temperature and relative humidity RH ranges on WPs for $AML = 83.4 \text{ MTU/acre}$. The last two rows give the time to rewet the RH thresholds for the most humid and least humid WP, respectively.

Backfill ($K_{\text{th}} = 0.6 \text{ W/m } ^\circ\text{C}$)		
Repository design	ACD point load	Line load
$T_{\text{peak}} (t > 100 \text{ yr})$	119–344 °C	245–268 °C
$RH (t = 120 \text{ yr})$	1–55%	2–3%
$RH (t = 2000 \text{ yr})$	43–96%	48–52%
$RH (t = 10,000 \text{ yr})$	62–99.7%	72–80%
$t(RH = 65\%)$	170–12,250 yr	3550–4770 yr
$t(RH = 90\%)$	1340–58,960 yr	26,200–41,030 yr

Backfill ($K_{\text{th}} = 0.3 \text{ W/m } ^\circ\text{C}$)	
ACD point load	Line load
132–537 °C	344–362 °C
0.5–38%	1–1%
24–95%	34–38%
41–99.6%	57–64%
200–27,820 yr	10,600–15,960 yr
1440–104,880 yr	53,330–71,610 yr

90% if the WP surface is free of salt [7]. Whether liquid water can enter the drift and reach (and evaporate on) a WP, leaving a salt buildup, is of critical importance to WP integrity. For the no-backfill cases, the line-load design significantly extends the time required to reach these RH thresholds (relative to the point-load design). When a low- K_{th} backfill (that limits wicking) is used, the time to reach these RH thresholds is further increased for all WPs in the line-load design, while for the point-load design, it is only increased for the SNF WPs (Fig. 4); consequently, DHLW WPs do not experience the benefit of RH reduction in the point-load design. Low- K_{th} (e.g., $0.6 \text{ W/m}^\circ\text{C}$) backfill accentuates thermal isolation in the point-load design, causing large variability in peak WP temperatures (119–344°C), while for the line-load design, peak WP temperatures only range from 245 to 268°C. For the backfill cases, the line-load design substantially decreases the maximum peak WP temperatures (relative to the point-load design).

The additional RH reduction for the backfill cases arises from the large temperature difference (ΔT_{drift}) between the WP and drift wall [6]. This effect (called the “drift- ΔRH effect”) occurs in addition to RH reduction resulting from rock dryout. Assuming uniform P_v in the drift, RH on the WP is given by

$$RH_{\text{wp}} = RH_{\text{dw}} \frac{P_{\text{sat}}(T_{\text{dw}})}{P_{\text{sat}}(T_{\text{wp}})}, \quad (2)$$

where RH_{dw} is RH at the drift wall, T_{dw} and T_{wp} are the drift-wall and WP temperatures. For decreasing backfill K_{th} , ΔT_{drift} increases, resulting in a larger and more persistent reduction in RH . The influence of thermal design on WP integrity is pronounced. For example, the time to reach $RH = 65\%$ is only 25–660 yr for the ACD no-backfill case, while it is 10,600–15,960 yr for the line-load backfill case with $K_{\text{th}} = 0.3 \text{ W/m}^\circ\text{C}$ (Table I). The time to reach $RH = 90\%$ is only 1540–2390 yr for the ACD no-backfill case, while it is 53,330–71,610 yr for the line-load backfill case.

Figure 3. Temperature and relative humidity on upper WP surface for no backfill. Curves are plotted for (a,c) the ACD point-load design and (b,d) the line-load design.

The possibility of hydrothermal alteration of the vitric nonwelded Paintbrush tuff (PTn) unit that overlies the repository is an important issue. If it occurs, it could significantly reduce the ability of the PTn to imbibe (and thereby attenuate) fast fracture flow. These changes may also increase the percolation flux at the repository. The 83.4-MTU/acre point-load and line-load designs drive markedly different changes in T and liquid saturation S_{liq} in the PTn, which are the result of how effectively condensate sheds between the drifts. More efficient condensate shedding between the line-load drifts results in less condensate buildup above the repository than the point-load design. The vertical extent of the upper heat-pipe zone depends on the amount of condensate available (above the repository) to reflux. For the point-load design, the maximum vertical extent of the upper heat-pipe zone is 100 m closer to the ground surface than in the line-load design (Fig. 5a). Figure 5b shows how the larger condensate buildup above the ACD repository inundates the matrix (raising S_{liq} to 99%) in the PTn and causes the peak temperature rise in the PTn to be 30°C higher than in the line-load design. The condensate buildup above the ACD repository causes S_{liq} in the PTn to be greater than ambient for thousands of years. The S_{liq} increase, together with the temperature rise, may be enough to cause hydrothermal alteration that reduces the ability of the PTn to imbibe fast fracture flow. The upper extent of the condensate zone overlying the line-load repository remains well below the PTn; consequently, S_{liq} in the PTn never exceeds ambient. Greater condensate buildup above the ACD point-load repository also causes the peak temperature rise near the ground surface to be almost twice that for the line-load design.

CONCLUSIONS

A three-dimensional model representing a realistic mixture of WPs was used to compare T-H behavior for two different approaches to arranging the WPs in a potential repository at Yucca Mountain. The point-load approach used in the ACD places WPs equidistant from each other to

Figure 4. Temperature and relative humidity on upper WP surface for backfill emplaced at 100 yr with $K_{th} = 0.6 \text{ W/m}^2\text{C}$. Curves are plotted for (a,c) the ACD point-load design and (b,d) the line-load design.

spread the WP decay heat, thereby limiting peak drift-wall and WP temperatures. The line-load approach lineally concentrates the WP decay heat by placing WPs nearly end to end in widely spaced drifts. A key consideration in evaluating alternative WP layouts is the markedly different T-H behavior that occurs in and around drifts, including: (1) how condensate returns to the repository, (2) how much heat is available near the drifts to vaporize incoming liquid water, and (3) the spatial variability in heat flux and condensate flux along the drifts. The line-load design causes the pillar to be a more preferential pathway for condensate drainage than the point-load design. Moreover, the line-load design has 2.4 times the local heat flux near the drifts (on average) to vaporize incoming liquid water than the point-load design. Consequently, it is more difficult for condensate to drain into line-load drifts than point-load drifts; the coolest and most humid WP in the line-load design is always less humid than the hottest and least humid WP in the point-load design. The point-load design thermally isolates WPs from each other, causing large variability in T , RH , and condensate flux along the drifts. The close axial WP spacing in the line-load design allows efficient WP-to-WP heat transfer that homogenizes the heat flux distribution along the drift. When a low- K_{th} backfill is used, this heat-flux homogenization greatly limits peak WP temperatures compared to the point-load design. A larger and more persistent reduction in RH on WPs occurs when the drifts are backfilled with a low- K_{th} granular material that limits wicking.

The line-load design provides the following advantages (compared to the ACD): (1) reduction (up to 60%) in the required length (and number) of emplacement drifts with a corresponding cost reduction, (2) large reduction in backfill volume, (3) narrower range of T and RH for which natural and engineered materials must be tested, (4) less spatially variable drift-scale T-H behavior to be accounted for in performance analyses, (5) all WPs (including DHLW) experience the benefit of RH reduction, (6) decreased probability of condensate flow entering the drifts, (7) decreased tendency for decay-heat-driven temperature and liquid saturation increase (and any resulting hydrothermal alteration) in the PTn unit,

Figure 5. Vertical temperature profile (a) at 1000 yr along a line intersecting the Hanford site DHLW WP for the ACD point-load design and the line-load design. Also plotted (b) are liquid saturation and temperature histories in the PTn unit 295 m above the repository horizon.

and (8) a reduction in peak temperature rise near the ground surface. The cost associated with any WP sequencing that may be necessary to implement the line-load design is worthwhile given the important benefits of this approach.

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