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CALCULATION OF POST-CLOSURE NATURAL CONVECTION HEAT AND MASS TRANSFER IN YUCCA MOUNTAIN DRIFTS

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ABSTRACT

Natural convection heat and mass transfer under post-closure conditions has been calculated for Yucca Mountain drifts using the computational fluid dynamics (CFD) code FLUENT. Calculations have been performed for 300, 1000, 3000, and 10,000 years after repository closure. Effective dispersion coefficients that can be used to calculate mass transfer in the drift have been evaluated as a function of time and boundary temperature tilt.

INTRODUCTION

Yucca Mountain in Nevada has been designated as the site of a high-level nuclear waste repository for the United States. Calculation of in-drift conditions during pre- and post-closure conditions is important in assessing the performance of the repository. During pre-closure, air is forced through the drifts by fans. Subsequently, in the post-closure period, forced convection cooling is discontinued. Heat and mass transfer in the drifts during the post-closure period is addressed in this paper.

In the post-closure period, natural convection and radiation are the main heat transfer mechanisms within the drift. Decay heat from the waste packages is transferred to the surrounding environment and then to the surrounding rock. The post-closure geometry is shown in Figure 1. The waste package sits on a metal pallet and is covered by a thin metallic drip shield. An invert exists at the bottom of the drift that consists of crushed tuff particles. Natural convection and radiation occur between the waste package and the drip shield as well as that portion of the invert under the drip shield. Additional natural convection and radiation occurs between the drip shield and the drift wall and the invert outside of the drip shield. Heat is conducted through the invert mainly by conduction.

The natural convection flow patterns and heat and mass transfer within the drift are modeled by the FLUENT computational fluid dynamics (CFD) code version 6.0.12 (Fluent, 2002). FLUENT solves conservation equations for mass, momentum, and energy for fluids based on the finite

Fig. 1. Yucca Mountain Post-Closure Geometry

volume methodology in open spaces such as in Yucca Mountain drifts. Earlier modeling of in-drift heat transfer relied on a porous media equivalent thermal conductivity approach. Comparison of the two approaches is discussed by Hadgu et al. (2004). Heat is introduced into the model through volumetric heat generation rate inside of the waste packages. Heat is removed from the model as a result of a constant temperature boundary condition imposed as discussed later. Steady-state conditions are assumed.

The methodology for modeling natural convection in the drifts has been developed by comparing FLUENT calculations with experimental data for geometrically-similar horizontal concentric cylinders (Webb et al., 2003a, b) and for scaled Yucca Mountain tests. These data-model comparisons are discussed in more detail later.

The methodology employed includes meshing all the way to the wall and not relying on wall functions. Meshing all the way to the wall requires that the first mesh point have a y^+

value of about 1.0, which leads to significant meshing requirements. y^+ is a dimensionless distance from the wall equal to the actual distance times the wall-friction velocity divided by the viscosity, or yv^*/ν . Meshing all the way to the wall is necessary because the alternative of using wall functions is not appropriate. Wall functions are based on forced convection data and assume that the velocity profile is monotonic. In contrast, the velocity profile in natural convection has a velocity peak near the wall, so wall functions are not appropriate. The use of wall functions is also not appropriate when low-Reynolds number effects are pervasive within the flow domain or in the presence of strong body forces.

The RNG k - ϵ two-equation turbulence model was selected for this analysis. The primary reasons for using the RNG k - ϵ turbulence model are that it allows for variation in the turbulent Prandtl number as a function of flow conditions, it provides a means for including low-Reynolds number effects in the effective viscosity formulation, and it includes an extra term, R_ϵ , in the ϵ -equation to better model separated flows.

As mentioned above, internal natural convection using FLUENT and the above methodology has been validated by comparison to experimental data. The approach has been validated against literature data from Kuehn and Goldstein (1976, 1978) and others for the case of horizontal concentric cylinders in laminar and turbulent flow (Webb et al., 2003b). The FLUENT predictions agree very well with the available overall heat transfer experimental data for gap-width Rayleigh numbers up to 5×10^9 . Three different turbulence models (Spalart-Allmaras, RNG k - ϵ , SST k - ω) showed small differences ($\sim 10\%$) for the highest Rayleigh number, well within the experimental uncertainty. Local heat transfer data from Kuehn and Goldstein (1978) are available at a Rayleigh number of 2.51×10^6 . However, as discussed by Webb et al. (2003b), these data are not adequate to distinguish between the various turbulence models.

The validation of the RNG turbulence model above is limited to the total heat transfer rate and surface temperatures. Experimental data for the horizontal annulus configuration are not available to validate the local heat transfer or the fluid velocities. In order to evaluate the appropriateness of the RNG turbulence model for natural convection, comparison to data for a differentially heated square enclosure has been performed as given by James and Webb (2004). Their results show that all of the two-equation turbulence models examined (standard k - ϵ , RNG k - ϵ , SST k - ω) perform similarly to each other, and that none of the models performs particularly well in the prediction of detailed time-averaged mean quantities including velocity and temperature profiles. Therefore, while the RNG turbulence model is as good as the other engineering turbulence models investigated, there is a significant amount of uncertainty in the results.

The available experimental data used in the data-model comparisons discussed in the previous paragraphs are at small length scales (gap width ~ 3 cm) compared to the Yucca Mountain geometry (gap width ~ 1.9 m). Therefore, much larger scale tests were conducted. These length scales are at 25% and 44% of full-scale Yucca Mountain drifts. Temperature data-model comparisons show very good agreement between FLUENT and the experimental temperature data as discussed in detail by Dalvit-Dunn et al., (2004).

Velocity data-model comparisons were reasonable with significant uncertainty in the experimental data.

Thermal radiation is very important in the present application, accounting for about 75-80% of the total heat transfer between the waste package and the drift walls. Thermal radiation heat transfer modeled by the discrete ordinates (DO) approach. The DO model solves the radiative transfer equation for a finite number of discrete solid angles. The DO model allows one to solve surface-to-surface radiation and fluid participation radiation. This model is restricted to either gray or non-gray thermal radiation using a banded gray model. The radiative transfer equation accounts for scattering, gas emission, and absorption. The surfaces are treated as gray, diffuse surfaces.

In addition to the heat transfer calculations and fluid velocities, the FLUENT model has also been used to calculate mass dispersion coefficients within the drift due to natural convection flow patterns. These dispersion coefficients are needed for mass transfer within a drift including the transport of water vapor and trace chemicals.

NOMENCLATURE

A	cross sectional area (m ²)
C	concentration
D	effective dispersion coefficient (m ² /s)
L	length (m)
Q	mass flow rate (kg/s)
ρ	fluid density (kg/m ³)

NUMERICAL MODEL

The physical subsystem to be modeled is the region inside of the emplacement drifts as shown earlier in Figure 1. Heat is generated inside of the waste canisters due to the decay of the radioactive materials, which decreases with time. The waste packages are to be emplaced on metal pallets with a small axial gap between packages. The waste packages vary in length and diameter depending on the type of waste in the container. The pallets sit on top of a crushed tuff invert. A thin metallic drip shield covers the waste packages. The emplacement drifts are drilled at regularly spaced intervals into the host rock. The host rock, invert, waste packages, and drip shield are all physically represented in the natural convection models.

After emplacement of the waste, the drift will be ventilated for a period of up to 50 years, which will remove a large fraction of the waste heat as well as some moisture from the drift. The amount of time that a drift is ventilated will vary depending on when the drift is loaded and when the repository is finally closed. At closure, the drip shield is installed to cover the waste packages. The natural convection model is run at specific times after closure of the repository. The linkage of the natural convection models to the environment is through the boundary conditions of the model. The rock temperature five meters into the host rock from the drift wall is used as a radially constant temperature boundary condition for the natural convection models because the effects of in-drift geometry are small at that distance into the rock (BSC, 2001). The rock temperature at this location is calculated from line-source analytical solutions. Initial conditions for the natural convection models are not needed because the constant

temperature boundary condition and the waste package heat generation rate serves to introduce temporal variation into the models.

The movement of heat and mass within the drift are the important processes that are modeled. Conduction, convection, and radiation are all important thermal processes that are contained within the model. Conduction is modeled in all solid materials and turbulent thermal convection and radiation is modeled in the gas phase. In order to develop a dispersion coefficient, some air particles are marked and the flux of that air is calculated between a constant concentration source at one end of the drift segment and a constant concentration sink at the other end of the drift.

NOTE: Not to scale and all waste packages not shown.

Figure 2. Schematic Diagram of Geometry of the Three-Dimensional Natural Convection Model

The domain for the drift CFD models is a half-cylinder 7.75 m radius including the rock. The radius of the drift is 2.75 m (5.5 m diameter) plus a shell of host rock five meters thick on the outer surface of the cylinder. An illustration of the geometry of the model is found in Figure 2. To reduce computational costs, symmetry is assumed down the centerline of the drift.

The waste package sequence is shown in Figure 3. The sequence consists of 6 full packages and 2 half packages at the end, and the sequence is 33.5 m long. The sequence is reflected about itself to give the package sequence in the repository drifts. Two waste package sequences are used in the CFD model. Therefore, the domain is 71 meters long and contains 13 full waste packages and two half-packages.

Figure 3. Waste Package Sequence

The waste packages have different diameters and lengths as listed in Table 1. There is a 6.1 m gap between the waste packages. The waste package lengths and gaps between packages are honored in the CFD model. Due to computational restrictions on the number of elements, the variability in waste package diameters was not included in this model. Instead, all of the waste packages had a diameter of 1.644 meters, which corresponds to the diameter of the PWR package, which is the most common waste package in the repository. Some other details of the geometry are ignored in the model. The geometry of the drift has been simplified in that the package pallet is not modeled so that the waste package is suspended above the invert. The structural supports on the surface of the drip shield are also not defined in the model. The invert and host rock are modeled as conduction only solids and not porous media. Condensation and evaporation in the drift are also not modeled.

Table 1. Waste Package Information at 300 Years

Waste Package Type	Power (W/P) ^a	Length (m)	Actual Diameter (m)
1/2 21-PWR	8.90E+2	2.5825	1.644
5-HLW-Long	4.64E+0	5.217	2.110
21-PWR	1.41E+3	5.165	1.644
44-BWR	8.00E+2	5.165	1.674
44-BWR-Adj	8.58E+2	5.165	1.674
5-HLW-Short	3.18E+1	3.590	2.110
21-PWR	1.38E+3	5.165	1.644
44-BWR	8.00E+2	5.165	1.674
21-PWR	1.38E+3	5.165	1.644
5-HLW-Short	3.18E+1	3.590	2.110
44-BWR-Adj	8.58E+2	5.165	1.674
44-BWR	8.00E+2	5.165	1.674
21-PWR	1.41E+3	5.165	1.644
5-HLW-Long	4.64E+0	5.217	2.110
1/2 21-PWR	8.90E+2	2.5825	1.644

^aBNC (2003)

Fig. 4. Waste Package Decay Heat Values

The heat generation rate in the packages varies significantly as shown in Figure 4. The PWR packages have the largest decay heat value followed closely by the BWR packages. The HLW waste has a substantially smaller decay heat power than the other two package types.

The temperature at the 5-m thick rock boundary can be calculated by line source solutions assuming conduction heat transfer in the rock. The radial variation in the rock temperature at this location is minor and can be assumed to be constant. There may, however, be significant temperature variation along the drift due to the three-dimensional nature of the repository. Based on line source solutions for the repository, this temperature variation can be up to 4°C over the length of the modeled drift (71 m). This temperature "tilt" has a significant effect on the results.

In the present case, the 5-m thick rock boundary temperature is somewhat arbitrary because condensation and evaporation is neglected. Therefore, in order to make the calculations simpler, an average 5-m thick rock boundary temperature of 77°C (350 K) has been assumed for all times with and without temperature tilt.

Due to the presence of the drip shield, there are two separate fluid regions – inside the drip shield and outside the drip shield. The drip shield is modeled as a zero-thickness boundary that has no thermal resistance. This approximation is appropriate because the drip shield is thin (2 cm thick) and is made out of titanium (thermal conductivity = 21 W/m-K).

The ends of the model are specified as wall boundaries in order to calculate mass dispersion coefficients as detailed in the next paragraph. While this boundary condition is not ideal, it is not expected to influence the results on the interior of the model compared to a more realistic symmetry boundary. To create a mass gradient needed to calculate a dispersion coefficient, a second air component, air2, was incorporated into the model. This second air component was assigned the same properties as air.

Centerline symmetry is a significant assumption. Assuming symmetry implies that the natural convection plumes are steady. If transient plume behavior is to be modeled, a full geometrical model (no centerline symmetry) would be needed to calculate the plume oscillations. Transient plume behavior may be very important in the mass transfer and mixing characteristics in the drift and is currently being investigated.

The DO settings used in the thermal radiation model are theta divisions, phi divisions, theta pixels, and phi pixels (Fluent, 2002). The settings for the present simulations are 3,3,3,3 for the DO model. These values are on the low side but are necessary due to memory limitations. The gray radiation model is applied as a constant emissivity over all wavelengths. For the three-dimensional simulations, the default air absorptivity of 0.01 m⁻¹ is used for all simulations.

Calculations were performed for the no tilt and tilt cases at 300 years, 1000 years, 3000 years, and 10,000 years to investigate the temporal variation of dispersion in the drift. The results are given in the following section.

Even with the centerline symmetry, the y' requirements on the meshing discussed earlier results in a large model. The FLUENT model is about 4,000,000 cells, or control volumes. In addition, the large memory requirements of the radiation model limit the DO settings to less than optimal. These models were run on a 4 CPU cluster (4 Pentium-4 processors) with 8 GB of RAM using the Linux 7.3 operating system. Typical CPU times for adequate convergence is 4-7 days.

RESULTS

Temperature, velocity, and mass transfer/dispersion results are summarized in this section.

a. Temperature

Figure 5 shows the centerline temperatures in the drift for the no tilt case at 300 years for a single waste package sequence. The temperatures include the interior of the waste packages, which are simply modeled as solid carbon steel for simplicity. The interior temperatures are not of particular interest in this figure – rather, the waste package surface temperatures are more important.

Fig. 5 Centerline Temperatures for 300 Years with No Temperature Tilt

As expected, the PWR packages are the hottest (98 to 99 °C) followed by the BWR packages (97 to 98 °C) and finally the HLW packages (95 °C). The presence of the drip shield can be inferred from Figure 5 by the temperature contours. While the temperatures under the drip shield vary significantly, the region outside the drip shield is at a relatively uniform temperature even with the large variation in waste package power. These temperatures depend on the 5-m rock boundary temperature, which is 77°C (350 K) in this simulation. If the boundary temperature is higher than 77°C (350 K), the waste package temperatures will be hotter than the temperatures given above.

The results at 300 years with a temperature tilt look practically identical and are not shown. While the 5-m rock boundary has a temperature tilt, the temperature in the air in the drift does not directly reflect this variation due to the presence of large-scale convection cells that will be discussed later.

Figure 6 shows the temperature results at 10,000 Years for the no temperature tilt case. As expected, the temperatures are much lower than at 300 years and are within a few degrees of the assumed boundary temperature of 77°C (350 K).

Fig. 6 Centerline Temperatures for 10,000 Years with No Temperature Tilt

Fig. 7 Gas Velocities (m/s) 1 m from the end of the Drift for 300 Years with No Temperature Tilt

b. Gas Velocity

Gas velocities for 300 years with no tilt are shown in Figures 7-8. Figure 7 shows an end view 1 m from the end of the model, or over the end PWR package. A typical natural convection "kidney" shape is seen both inside and outside the drip shield.

Figure 8 shows the centerline gas velocity above the 3 (PWR), 4 (BWR), and 5 (BWR-Adj.) waste packages on the model centerline. As can be seen, the gas velocity above the middle package (BWR) is essentially vertical. The packages to each side essentially "pair off", setting up local natural convection recirculation zones.

Fig. 8 Centerline Gas Velocity (m/s) over the 3 (PWR), 4 (BWR), and 5 (BWR-Adj.) Packages at 300 Years with No Temperature Tilt

Comparable results at 300 years with a temperature tilt are shown in Figures 9-10. Figure 9 shows the end view of the gas velocities similar to Figure 7. There is some difference in the

Fig. 9 Gas Velocities (m/s) 1 m from the end of the Drift for 300 Years with Temperature Tilt

velocities in the upper part of the "kidney" in the outer part of the flow. This difference is caused by global natural convection flow in the model (as opposed to local natural convection flow). With no temperature tilt, packages tend to "pair off" as seen in Figure 8 shown earlier. With a temperature tilt, global flow in the entire model is noted as seen in Figure 10. A distinct horizontal velocity from left to right is noted in Figure 10. This velocity causes increased mixing and dispersion as will be noted later.

Fig. 10 Centerline Gas Velocity (m/s) over the 3 (PWR), 4 (BWR), and 5 (BWR-Adj.) Packages at 300 Years with Temperature Tilt

Figures 11 and 12 show the gas velocities at 10,000 years. The values are similar in shape to those at 300 years with somewhat lower velocity values.

Fig. 11 Gas Velocities (m/s) 1 m from the end of the Drift for 10,000 Years with No Temperature Tilt

Fig. 12 Centerline Gas Velocity (m/s) over the 3 (PWR), 4 (BWR), and 5 (BWR-Adj.) Packages at 10,000 Years with No Temperature Tilt

c. Dispersion Calculations

Dispersion coefficients have been calculated by the FLUENT model for subsequent use in water vapor and trace gas transport calculations. To generate a dispersion coefficient, the concentration gradient and flux of the gas phase must be calculated by the model. A second air species (air2) was introduced in the model, and this air species was assigned identical physical properties to that of air. The concentration air2 was set to be 0.01 mass fraction on one side of the drift segment and 0.02 on the other side of the drift segment. From continuity, the mass fraction of air was 0.99 and 0.98 since the mole fractions must sum to 1.0 on both surfaces. The choice of using a second air component was made to eliminate any mass-based buoyancy effects in the model.

The mass dispersion coefficient, D , can be defined using the following relationship for mass flux.

$$Q/A = \rho D \nabla C \quad (\text{Eq. 1})$$

where Q is the mass flow rate [kg/s], A is the cross section area [m^2], D is the dispersion coefficient [m^2/s], ρ is the density [kg/m^3], and ∇C is the mass fraction gradient [$1/\text{m}$]. Solving for the dispersion coefficient, D :

$$D = Q / (A \rho \nabla C) \quad (\text{Eq. 2})$$

Two dispersion coefficients are found, one for the region inside of the drip shield and one for the region outside of the drip shield. The ends of the air regions at the two sides of the model are modeled as a thermally insulated, no-slip, constant mole fraction wall. Because the presence of the wall will alter the flow locally, this section of the model is eliminated from the region over which the dispersion coefficient is calculated. There are 13 waste packages (13 full- and 2 half-packages) in the model. The CFD model is composed of air regions that correspond to volumes around the waste packages as well as the gaps between the waste packages. There is an air gap 13.2 meters from the ends of the model in between the third and fourth waste packages and in between the twelfth and thirteenth waste packages. For this model, the concentration of air2 used

in the calculation of the dispersion coefficient calculation is the volume averaged concentration in the air gap in between the third and fourth waste packages and in between the twelfth and thirteenth waste packages. The model z -locations for these two air volumes are 13.2 and 57.4 meters, or a difference of 44.2 meters. The magnitude of the mass flow rates of air2 at these monitoring locations can differ slightly so they are averaged to get the mass flow rate, $\dot{Q}$. The areas of the inner and outer air regions are 1.838 and 7.897 m^2 , respectively. The inner air region does not include the cross section area of the waste package. The density, ρ , is calculated internally by the FLUENT code and corresponds to the volume-averaged density of the volumes inside and outside of the drip shield. The equation above can then be written in terms of output from the FLUENT model as follows:

$$D = \frac{(\dot{Q}_{\text{inner}} + \dot{Q}_{\text{outer}})}{2} \left(\frac{C_{\text{air}2, z=13.2\text{m}} - C_{\text{air}2, z=57.4\text{m}}}{L_{\text{air}2, z=13.2\text{m}} - L_{\text{air}2, z=57.4\text{m}}} \right) \quad (\text{Eq. 3})$$

The variation in the cross-sectional average concentration for the no temperature tilt boundary temperature is shown in Figure 13. The results from all the various times are very similar except for the inner air at 10,000 years. There are steps in the concentration profiles. The larger jumps fall where there are three hotter packages in a row. These 3 package sequences tend to form a barrier to mass dispersion because they are the boundaries of larger convection cells as indicated in the velocity plots shown earlier.

Fig. 13 Cross-Sectionally Average Air2 Concentrations with No Temperature Tilt

The results from the simulations with a uniform temperature boundary condition are shown in Table 2. The inner dispersion coefficient ranged from 0.006 to 0.007 m^2/s for the four simulation runs. The outer dispersion coefficient ranged from 0.004 to 0.008 m^2/s . The diffusion coefficient for air for air/vapor mixture at STP is $2.13 \times 10^{-5} \text{ m}^2/\text{s}$ (Pmss

1987). Therefore, the calculated dispersion coefficients for these runs are several hundred times greater than for pure diffusion. The reason that the dispersion coefficient is higher than the diffusion coefficient is that buoyantly driven circulation cells develop within the model as shown earlier in Figure 8.

Table 2 Dispersion Coefficients (m^2/s) With No Temperature Tilt

	300 Yrs	1000 Yrs	3000 Yrs	10,000 Yrs
Under Drip Shield	0.007	0.006	0.007	0.006
Outside Drip Shield	0.008	0.004	0.004	0.004

A second set of simulations was run at the same four times except with the boundary temperature tilted linearly from one end of the drift segment to the other. This temperature tilt destroys the natural symmetry of the model and is a more realistic boundary condition for the edges of the repository, which are expected to be cooler than locations in the center of the repository. The temperature drop across the 71 meter length of the drift segment was 4K for the 300 year simulation, 3K for the 1000 year simulation, 2K for the 3000 year simulation, and 1K for the 10,000 year simulation. The average boundary temperature was kept at 350K for all runs so for the 300 year simulation, the temperature varied from 348K to 352K.

The variation in the cross-sectional average concentration for the no temperature tilt boundary temperature is shown in Figure 14. The hotter temperature is on the right side of the model. The results are significantly different than with no temperature tilt. The inner and outer region calculations are similar within each group but are significantly different from each other. The inner region values have a large jump at the location of the first three hot packages similar to Figure 13. However, there is no similar jump at the next two sets of three hot packages. This effect may be due to the temperature tilt that may break up the inner region into two separate convective cells. The outer region shows relatively uniform concentrations except near the hot end, where the concentrations increase significantly. This behavior is still being investigated.

Fig. 14 Cross-Sectionally Average Air2 Concentrations with Temperature Tilt

The simulation results are shown in Table 3. The dispersion coefficients are higher for these cases than for the uniform temperature cases. The inner dispersion coefficients ranged from 0.007 to 0.01 m²/s while the outer dispersion coefficients ranged from 0.03 to 0.1 m²/s, or up to 5000 times molecular. The inner values are slightly higher when compared with the previous simulations. The outer values are several orders of magnitude higher than for the uniform temperature case. Figure 10 given earlier shows the presence of global recirculation in the presence of temperature tilt, which leads to the significantly higher dispersion coefficient with temperature tilt compared to no tilt.

Table 3 Dispersion Coefficients (m²/s) With Temperature Tilt

	300 Yrs	1000 Yrs	3000 Yrs	10,000 Yrs
Under Drip Shield	0.007	0.007	0.009	0.01
Outside Drip Shield	0.1	0.1	0.1	0.03

SUMMARY AND CONCLUSIONS

FLUENT has been used to model the heat and mass transfer in Yucca Mountain Drifts during the post-closure period. There are significant differences in the waste package power at various times that leads to significant differences in waste package temperatures.

General natural circulation flow patterns are observed in the cross section. With no temperature tilt, the packages mostly "pair off" setting up local natural convection cells axially. When temperature tilt is added, larger scale convection cells are established.

The calculation of effective mass dispersion coefficients has been performed for various times with and without temperature tilt. The effective dispersion coefficients are from several hundred to several thousand times the molecular value. The value for the area under the drip shield is not significantly affected by time or the temperature tilt. The outer region dispersion coefficient is not a strong function of time, but it is significantly affected by the temperature tilt.

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