EVALUATION OF LARGE-SCALE TEMPERATURE GRADIENTS TO SUPPORT ASSESSMENT OF CONVECTION AND COLD-TRAP PROCESSES IN HEATED DRIFTS

Randall W. Fedors
CNWRA—Southwest Research Institute®
San Antonio, Texas

Chandrika Manepally
CNWRA—Southwest Research Institute
San Antonio, Texas

Lauren B. Browning
CNWRA—Southwest Research Institute
San Antonio, Texas

George R. Adams
CNWRA—Southwest Research Institute
San Antonio, Texas

Steve T. Green
Southwest Research Institute
San Antonio, Texas

ABSTRACT

This paper provides estimates of large-scale temperature gradients that can be used to support modeling of natural convection and cold-trap processes in thermally perturbed drifts. Temperature influences estimates of the quantity and chemistry of water contacting engineered components (e.g., drip shields and waste packages) in a potential high-level waste repository at Yucca Mountain, Nevada. Temperature gradients drive natural convection and cold-trap processes, which could affect the distribution, quantity, and chemistry of liquid-phase water contacting drip shields (waste packages). The confluence of high temperatures, liquid-phase water, and high chloride may lead to corrosion of drip shields and waste packages. An overview of the evolution of environmental conditions in thermally perturbed drifts is presented to provide a context for the estimates of temperature gradients.

A mountain-scale conduction-only model is used to estimate temperature gradients and temperature differences for a drift located at the center of a potential repository. Thermohydrologic models and heat transfer algorithms are used to evaluate the reasonableness of the conduction-only results. Estimates of temperature using an in-drift heat transfer algorithm account for the possibility of drift degradation and formation of a rubble pile on the drip shield. Temperature differences between the center and ends of the drift are estimated to rapidly increase to 80 °C soon after repository closure. That temperature difference decreases over time to 15 °C after 10,000 years. Local temperature gradients are generally estimated to be less than 0.2 °C/m, though the gradients can be much larger near changes in lithology and near the end of the drift. The estimates of temperature gradients do not account for intermediate- and small-scale variations, such as those influenced by differences in heat loads between waste packages, intra-layer variations in thermal properties of the surrounding fractured rock, or localized drift degradation.

INTRODUCTION

The quantity and chemistry of water contacting waste packages to be stored underground in drifts are important factors for determining the performance of a potential high-level waste repository at Yucca Mountain, Nevada. Environmental conditions surrounding waste packages located in drifts, however, are difficult to estimate because of complex relationships between thermal, hydrological, and chemical processes. Identifying the source, distribution, and magnitude of water contacting waste packages is important for estimating the chemistry of water that may contact and potentially lead to corrosion of drip shields and waste packages. If waste packages fail, characterization of the moisture movement is also important for estimating transport rates of radionuclides into the natural system below the repository.

A potential source of water contacting waste packages with markedly different chemistry compared to seepage or refluxed water is condensed water. The water may condense directly on the waste package, or may condense on other in-drift features prior to dripping onto the drip shields and waste packages. Increases in relative humidity caused by mixing associated with convection may lead to liquid-phase water on surfaces because of the phenomena of deliquescence. Moisture may be redistributed along drifts because of convection driven by axial temperature gradients, hence, in-drift convection must be understood for the design configuration. Understanding of external influences on in-drift temperature gradients is important for simulating natural convection and moisture redistribution.

Computational fluid dynamics (CFD) modeling is typically used to simulate airflow. Companion manuscripts by Green, et al. (2004) and Walter, et al. (2004) discuss the CFD modeling associated with this project. CFD models, however, generally have limited spatial extent due to the computational effort required. Furthermore, inclusion of the surrounding porous media in CFD models makes the computational effort excessive and requires undesirable simplifications. Whereas CFD modeling can address moisture redistribution driven by thermal gradients along drifts, thermal and thermohydrologic porous media models are needed to address temperature variations across the repository driven by processes in the fractured wallrock.

This paper provides an overview of a conceptual model of evolution of in-drift environmental conditions in drifts. Next, estimates are presented of temperature gradients from large-scale models. These estimates could be used to support and constrain the CFD modeling of in-drift environmental conditions. The focus is on enhancing understanding of spatial and temporal variabilities of in-drift conditions, which are essential for estimating the long-term performance of a potential repository at Yucca Mountain.

OVERVIEW

Conceptualization of In-Drift Temperature and Moisture Redistribution

The current design is for waste packages to be emplaced in drifts with forced ventilation during the operation period of a potential repository (DOE, 2002). After closure of the repository, the early thermal period is expected to be marked by high temperatures. Evaporation and convection to and into the wallrock are expected to expand the dryout zone near the drift wall created by preclosure forced ventilation and also elevate saturation at the outer reaches of the developed reflux zone. For most of the repository, cross-sectional convective airflow is expected to enhance the heat and mass (water) transfer away from the engineered components. Along-drift, or axial, temperature gradients are expected to arise in a small zone close to the edge of the repository. Near the edge of the repository, temperatures are expected to stay below boiling, hence, no dryout zone is expected to be present. Axial convection may lead to condensation in the cool, wet zone at the edge of the repository. In the intermediate zone between the hot interior zone and the cool outer zone, conditions may exist conducive to corrosion of drip shields and waste packages.

After peak temperatures have occurred and as the thermal pulse dissipates, the zone of conditions conducive to corrosion is expected to migrate inward along the drifts. In areas where dryout has occurred, little moisture is expected in the drifts at peak temperatures. Preferential flow along fractures, however, may breach the dryout zone and lead to seepage into the drifts. As the thermal pulse dissipates, two other sources of water may lead to elevated relative humidity near the engineered components: moisture may be carried in the return flow of axial convection cells from the cooler zones to hotter zones, and the drift wall is expected to rewet because of collapse of the reflux zone and a return of ambient percolation.

Environmental conditions described above may be modified by the possible occurrence of drift degradation. Drift degradation may gradually lead to partial or complete coverage of the drip shield with natural backfill during peak temperatures and early stages of the cool-down period. A preliminary estimates is that drifts may fully degrade in about 1000 years (Gute, et al., 2003). Modeling with finer spatial resolution likely would result in a variable extent of degradation along the drifts. Drift degradation is expected to lead to increased temperatures compared with those estimated for the no-degradation assumption; the magnitude of increase is dependent on the timing of drift degradation.

Relation of Chemistry and Corrosion to Moisture Redistribution and In-Drift Temperature

The expected lifetimes of drip shield and waste package materials in an underground nuclear waste repository at Yucca Mountain are strongly dependent on the anticipated temperature, chemistry, and presence of liquid-phase water. Conditions are conducive for localized corrosion of waste packages within a temperature range of 80–120 °C (Dunn, et al., 2003; Brossia, et al., 2001). The upper bound may be higher and is dependent on the potential for liquid-phase water to be present. Elevated concentrations of certain dissolved species have been demonstrated to enhance aqueous corrosion—promoting specific corrosion modes, either uniform corrosion or localized corrosion, and accelerating corrosion rates. Alloy 22, for example, the material proposed for the outer container of the waste package, is susceptible to localized corrosion when exposed to solutions with high hydrogen and chloride ion concentrations (Dunn, et al., 2003). Titanium alloy (Ti Grade 7), the material planned for the drip shields that would cover the waste packages, may be susceptible to generalized corrosion in solutions with high concentrations of fluoride ions (Brossia, et al., 2001). Some types of anionic species, such as nitrate ions, may counterbalance the effects of deleterious species by inhibiting localized corrosion, if they are present in sufficient concentrations (Dunn, et al., 2003).

The composition of dripping water is expected to vary with time and location in the in-drift environment as a result of site heterogeneity and coupled thermal-hydrological-chemical processes. Pure condensed water is not expected to contribute to drip shield or waste package corrosion, unless its pH is extremely low. Water condensed in an engineered geologic repository, however, may interact chemically with the drift wallrocks and other types of engineered materials present inside the drifts, and/or mix with seepage waters, evolving rapidly to a more complex chemical composition. High concentrations of potentially corrosive species may result from the evaporation of seepage waters, even if those waters initially were dilute (Brossia, et al., 2001). If evaporation is significant, salts are expected to precipitate directly on drip shield and waste package surfaces.

Most inorganic salts are hygroscopic and will absorb moisture from humid air, generating small volumes of potentially corrosive brines at a threshold relative humidity, known as the deliquescence point or deliquescence relative humidity (Tang and Munkelwitz, 1993). The deliquescence relative humidity of salt mixtures depends on the mixture composition and temperature. The composition of the salt mixtures largely depends on the initial composition of the evaporating waters.

Variations in temperature and relative humidity across the repository footprint could affect the timing, mode, and rates of drip shield and waste package corrosion, even if the composition of salt mixtures present in those environments was identical. The composition of salt mixtures formed in a complex geologic and engineered repository is more likely, however, to vary with location. Spatial heterogeneity in the chemical environment may reflect the extent to which seepage waters mix with condensed waters. The quantity of condensate present at different drift locations over time could significantly modify the seepage water compositions or affect the timing and extent of salt dissolution.

Relation to Experiments and CFD Modeling of In-Drift Processes to Moisture Redistribution and In-Drift Temperature

Temperature gradients in the drifts are expected to promote natural convection. Heat transfer and water redistribution will be associated with the convection. Natural convection and the associated cold-trap process involve temperature gradient-driven airflow with evaporation from warm areas, movement of vapor driven by thermal gradients, and condensation on cool or hygroscopic surfaces. Estimating moisture movement associated with natural convection and the cold-trap process is complex. Axial drift convection and latent heat transfer both attempt to dampen axial temperature gradients. Offsetting that dampening is the effect of heat flux out the drift and thermal radiation, which serve to sharpen the temperature gradient between hot and cold locations. Natural convection, when acting in concert with thermal radiation, conduction, and latent heat transfer in drifts, is poorly understood.

The primary need for CFD modeling is to help understand the extent and magnitude of axial convection. In addition, assessing small-scale spatial variations of temperature around the engineered components requires computational fluid dynamics modeling of airflow. Fine-scale convection around the engineered barriers may be important for assessing the nonuniformity of temperature and relative humidity and for assessing the potential dispersion of acidic gases formed from evaporation of concentrated water.

Laboratory experiments and CFD modeling are being performed to help address the potential effects of heat and moisture redistribution associated with axial convection in heated drifts. The cold-trap process has been evaluated in a 1-percent scaled (benchtop) laboratory model of a heated drift (assuming no drift degradation) using thermocouples, relative humidity probes, and anemometers to measure environmental conditions. Laboratory data and initial modeling results are reported in Fedors, et al. (2003a), and sensitivity analyses are reported in Walter, et al. (2004). The initial work illustrates the importance of including latent heat transfer and the associated evaporation and condensation processes. Green, et al. (2004) reported on development of an evaporation and condensation module for the CFD code. A temperature gradient in the benchtop experiment, when scaled to the emplacement drifts, is approximately 0.03 °C/m. This gradient is calculated using temperature differences from the zone of the benchtop experiment where most of the condensation was simulated to occur (see Figures 3-22 through 3-24 in Fedors, et al., 2003a). The question then becomes, what temperature gradients may occur in the drifts of a potential repository?

LARGE-SCALE TEMPERATURE GRADIENTS

A model that addresses in-drift and wallrock thermohydrologic processes in their entirety is beyond our computational capabilities, except possibly on a small scale. The approach in this paper is to evaluate axial gradients using a conduction-only model (conduction-only), and then evaluate the effect on the gradients when the effects of hydrology, in-drift heat transfer processes, and drift degradation are included. Implicit in this description is the in-drift and mountain-scale process models are decoupled.

Mountain-Scale Conduction

A mountain-scale conduction equation is used to evaluate the magnitude of repository-scale temperature gradients that reflect the edge cooling effect and the changes in lithology along a drift. Increased heat transfer at the edge of the repository leads to the edge cooling effect. Changes in thermal properties occur because emplacement drifts cross geologic unit boundaries. For the repository outline shown in Figure 1, there are three geologic units with different thermal properties. Most drifts pass through two of the units, but some will pass through all three units.

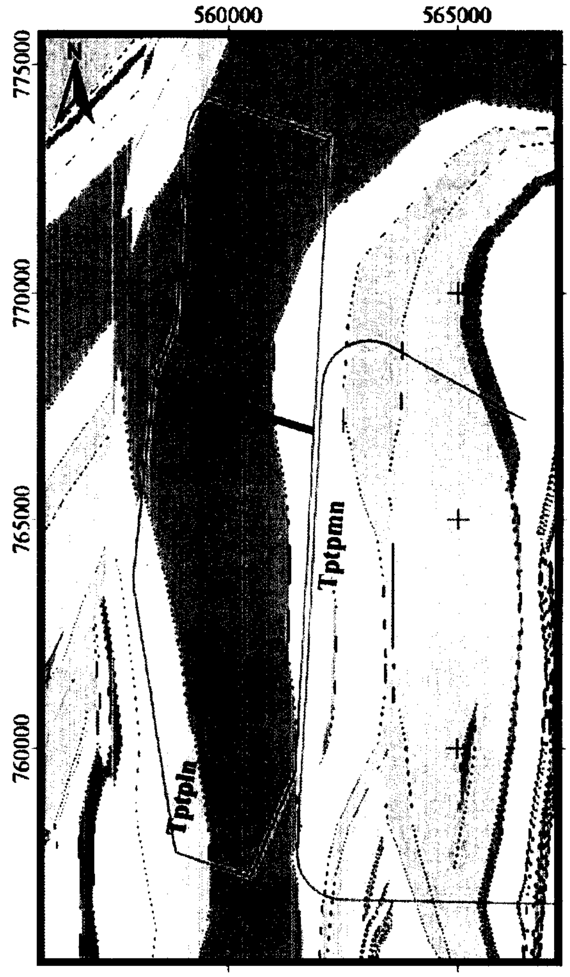

Figure 1. Geologic units along a potential repository horizon (outline shown, with Exploratory Studies Facility tunnel). The labeled geologic subunits of the Topopah Spring Unit are the middle nonlithophysal (Tptpmn), lower lithophysal (Tptpll), and lower nonlithophysal (Tptpln). State Plane (m) coordinates are used.

The mountain-scale model is an analytical, three-dimensional, conduction-only model for heat transfer that uses a line-source for a heat load to represent waste packages in each drift. The approach follows the methodology of Fedors, et al. (2003b), Mohanty, et al. (2002), Clausen and Proberts (1996), and Carslaw and Jaeger (1959). In-drift processes are ignored; the drift volume is modeled as an extension of the fractured tuff. To determine the evolution of temperature in the wallrock at any location in the repository, the superposition principle is used to incorporate the contribution of all the drifts and to approximate the effect of lithologic variations.

The conduction-only model is used to estimate temperatures along a drift located in the middle of the repository. The effect of drift degradation, thermohydrology, and in-drift heat transfer are not included in the conduction-only model results. In Figure 1, Drift 25 is shown to lie in two geologic units, the Topopah Spring middle nonlithophysal unit (Tptpmn) in the east and the Topopah Spring lower lithophysal unit (Tptpll) in the center and west. Thermal conductivity values of 1.945 W/m-K (26.98 BTU/ft-h-°F) and 1.61 W/m-K (22.3 BTU/ft-h-°F) are used for the two units to estimate temperatures along the drift at the driftwall. These driftwall temperature estimates can be used to evaluate the repository edge cooling effect by analyzing the temperature difference between the center and the edge locations (Figure 2a) and the local temperature gradient (Figure 2b). Using data only from the eastern half of Drift 25, which includes a change in lithology, Figure 2 shows two perspectives on temperature gradients that could affect along-drift convective airflow. The portion of the drift that exhibits the effect of edge cooling increases with time, though the temperature difference and the local temperature gradient decrease with time. Near lithologic changes, elevated local gradients persist beyond 2000 years, suggesting areas near lithologic changes may require increased emphasis when assessing natural convection and the cold-trap process.

The portions of the half-drift with specific temperature differences (relative to the center location) and specific local temperature gradients are plotted as a function of time in Figure 3a. A similar analysis for the western half

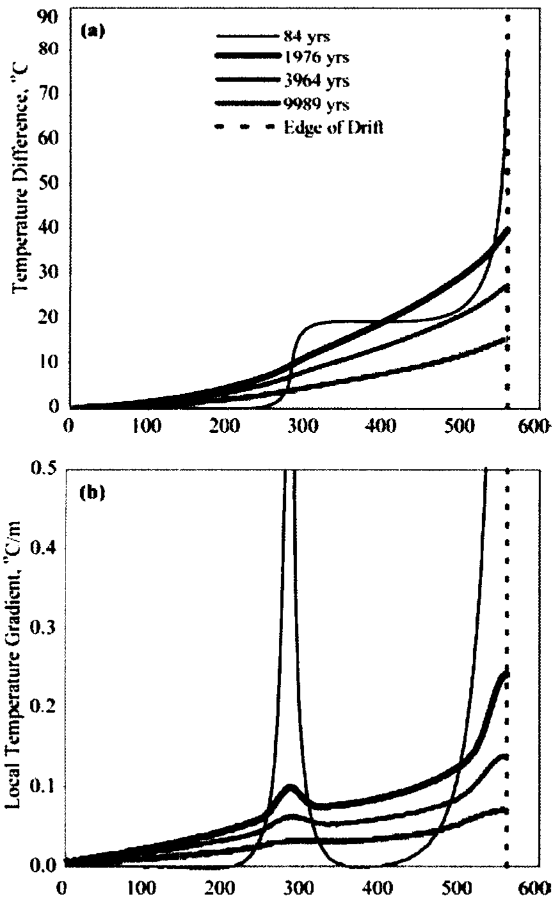

Figure 2. (a) Temperature differences and (b) local temperature gradients along eastern half of Drift 25, which includes a lithologic change at a distance of 284 m from the center.

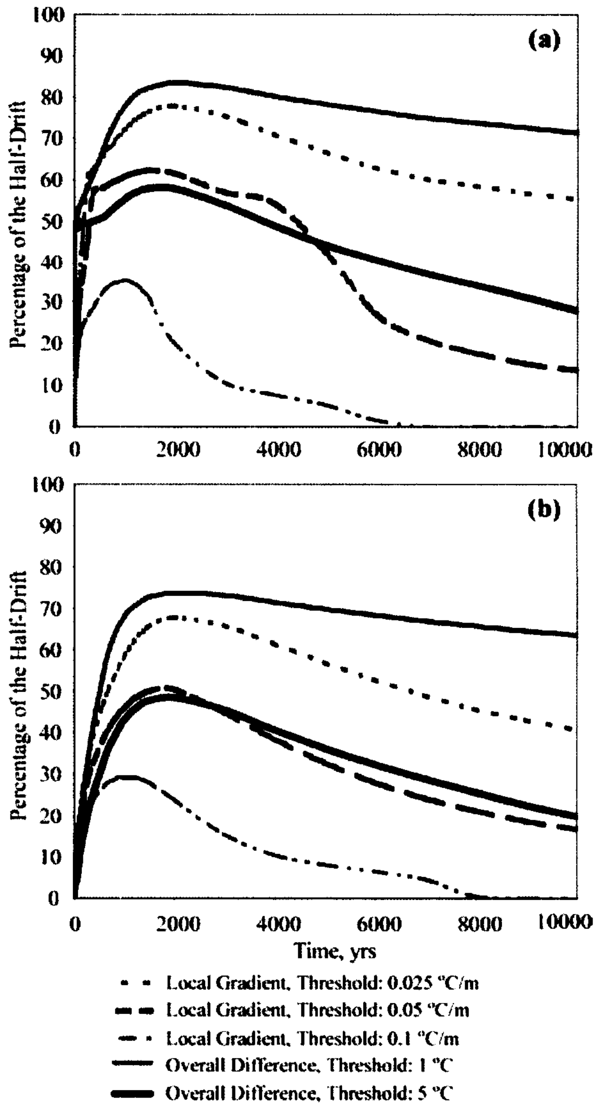

Figure 3. Portions of the (a) eastern half and (b) western half of Drift 25 where significant local gradients (dashed and dotted lines) and temperature differences (solid lines) occur. The eastern half (a) of Drift 25 includes a change in lithology.

of Drift 25, which has no change in lithologic units, is presented in Figure 3b. The threshold for temperature differences or local temperature gradients needed to drive natural convection along a drift is not known, though the magnitude of temperature gradients should correlate with the magnitude of axial airflow rates. The values of local temperature gradient in Figure 3 bound the value derived from the benchtop laboratory experiment where condensation from the cold-trap process was demonstrated to occur. A threshold likely occurs, however, because cross-sectional convective cells from the eccentrically located waste packages may constrain axial convection. Future CFD modeling will address the topic of cross-sectional versus axial convection.

Effect of Hydrology

The mountain-scale conduction-only model does not include the effect of hydrology. Spatial and temporal variations in water content will affect the thermal properties of the wallrock. The required assumption for the conduction-only model is that representative values of thermal properties can be used to adequately estimate temperature profiles. Thermal conductivity is the most sensitive thermal property needed for the model.

A two-dimensional drift scale thermohydrologic model is coupled to the mountain-scale conduction model. The conduction-only model is used to determine reduction factors used in the thermohydrologic model for the heat load at locations not at the center of the repository. The two-dimensional drift scale thermohydrologic model is developed using the two-phase mass and energy transport (METRA) component of MULTIFLO v 1.5 (Painter, et al., 2001). The dual-permeability approach is used to characterize the flow of heat and moisture through the fractured rock. Temporal variations in thermal properties of the rock will result from changes in saturation caused by the thermal pulse and by climate variations. Ambient percolation rates above the drifts are also expected to vary with climate scale during the 10,000-year performance period of a potential repository. The effect of climate change is incorporated by step increases in net infiltration for monsoonal and glacial-transition climates at 600 and 2000 years.

Figure 4 illustrates the effect of hydrology on temperature estimates at the center of a drift and at the end (edge of repository). The conduction-only model uses a constant value for thermal conductivity whereas the thermohydrologic model varies thermal conductivity as a function of saturation. Early in the thermal period, the thermal conductivity is near the saturated value. As the thermal pulse dries out the wallrock, the thermal conductivity approaches the dry value. Later, as ambient conditions return, the percolation flux from a future, glacial transition climate leads to thermal conductivity values near the wet thermal conductivity value. After the thermal peak passes, the zone with elevated saturation will begin to collapse inward, and supported by ambient percolation, the drift walls will begin to rewet. Rewettting

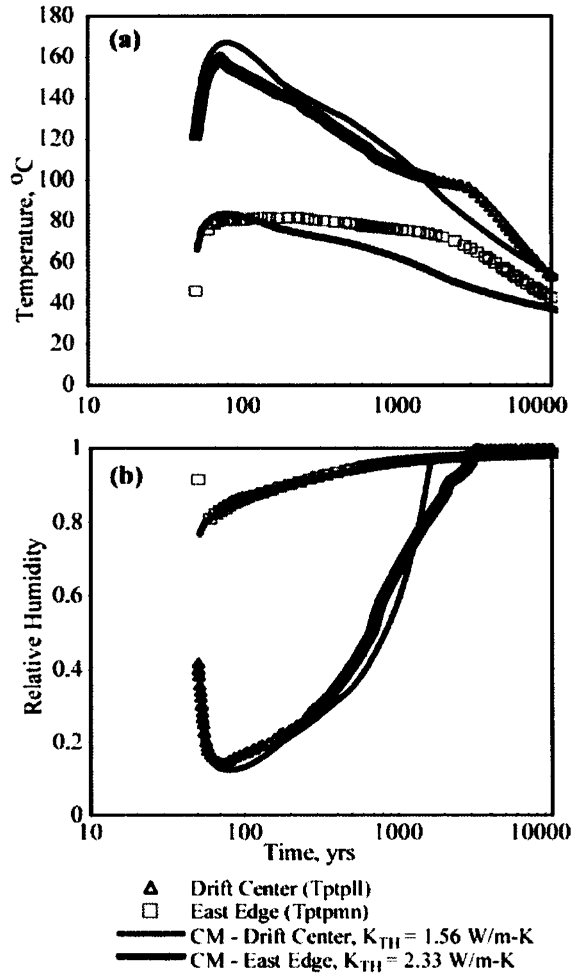

Figure 4. Waste package (a) temperature and (b) relative humidity estimates for center and edge of Drift 25 using thermohydrologic model (symbols) and conduction-only model (CM, lines). For relative humidity, the CM assumes no change in vapor pressure with time. K_{TH} is the effective thermal conductivity used in the conduction-only model.

of the wallrock will lead to increases in the relative humidity and the increased likelihood for liquid-phase water to occur on the drip shields and waste packages. For the Tptpll unit, the wet and dry values for thermal conductivity used in this modeling are 2.02 and 1.2 W/m-K. Other model parameters are consistent with those described in Fedors, et al. (2003b).

Figure 4 also illustrates the temperature and relative humidity differences between the center and repository edge along Drift 25 using the thermohydrologic model. Compared to the conduction-only model, the temperature difference between the center and edge decreases during the cool-down period. Considering the time when the waste package temperature is estimated to be above boiling, the temperature difference between the center and edge is maintained for a longer time using the thermohydrologic results than when using the conduction-only results. In addition, the duration of time that waste packages may be in the temperature range 80–120 °C is greater when the effect of hydrology is included.

Effect of In-Drift Processes

Given the design geometry, an evaluation is needed to determine if the conduction-only mountain-scale and thermohydrologic models adequately represent the effect of the in-drift heat transfer processes. In the EDA-II repository design (CRWMS M&O, 2000), cylindrical waste packages are to be eccentrically emplaced in a 5.5-m diameter drift. The waste packages will be placed on a stand supported by invert material at the bottom of the drift. A drip shield may cover the waste package, with air space above and below the drip shield. In addition, the effect of potential drift degradation and formation of a rubble pile covering the drip shield can be factored into an in-drift heat transfer algorithm. The analysis presented here assumes the drip shield remains intact, though the elevated temperatures from natural backfill may affect drip shield mechanical integrity.

A multi-mode algorithm for in-drift heat transfer processes is used to estimate waste package surface temperature. The estimate uses thermal output from the high-level waste (heat load) and wallrock temperature and includes the in-drift thermal processes of thermal radiation, convection, and conduction. The effect of latent heat transfer is neglected in this analysis. The in-drift, multi-mode algorithm uses rock temperature estimated from the thermohydrologic model as an outer boundary condition at 5 m from the drift wall. Hence, mountain-scale processes are decoupled from the in-drift processes. The multi-mode algorithm allows for fast analysis of new design features or different scenarios.

The multi-mode algorithm for estimating waste package temperatures is based on the following equation:

$$Q_{wp} = \left\{ \left[\frac{1}{G_{inv}} + \frac{1}{G_{rk1}} \right]^{-1} + \left[\frac{1}{G_{cpd} + G_{rpd}} + \frac{1}{G_{bf}} + \frac{1}{G_{cdw} + G_{rdw}} + \frac{1}{G_{rk2}} \right]^{-1} \right\} \left(T_{wp} - T_{rk} \right) \qquad \textbf{EQN (1)}$$

where Q_{wp} is the heat supplied by the waste package, and efers to the conductance terms, which are the inverse of the resistance. The subscripts *inv* refer to the invert, *rk1* and *rk2* to conduction in the rock below the invert and above the drift, *cpd* and *rpd* to convection and radiation between the waste package and the drip shield, *bf* to conduction through the natural backfill (if present), and *cdw* and *rdw* to convection and radiation between the drip shield or backfill and the drift wall. T_{wp} and T_{rk} refer to temperatures at the waste package and in the rock. T_{rk} is the boundary condition for the in-drift algorithm and is obtained from either the mountain-scale conduction-only model or the thermohydrologic model results. Note the value (T_{rk}) for the boundary condition is approximate because it is estimated using the conduction-only model. A fraction is assigned that accounts for the portion following the two thermal network pathways; one pathway from the waste package through the invert and one pathway through the airspace, drip shield, and outward. Radial symmetry is assumed. Expressions for each conductance term follow the development presented in Fedors, et al. (2003b) and are similar to those in Mohanty, et al. (2002).

Radiation and convection are nonlinear processes. Eq. (1), however, uses linearized approximations for the convection and radiation terms. An effective thermal conductivity term for natural convection (K_{eff}) is assumed constant, regardless of the temperature difference across the gaps. Also, inherent in the temperature difference used in Eq. (1) and the expressions for the G is the assumption all radiation and convection terms can be calculated using only the heat load and the temperature wallrock (i.e., Q_{wp} and T_{rk}). An iterative, nonlinear algorithm iss developed for the thermal network described in Eq. (1) that uses the appropriate intermediate temperatures for estimating the G terms for radiation and convection. A comparison of the iterative and linearized results is presented in Figure 5. For the cases of drift degradation and no-drift degradation, the linearized solution is within 1 percent of the iterative result.

The range of values used for K_{eff} for the convection terms is also plotted in Figure 5. The values of K_{eff} used in the iterative algorithm were based on the approach described in Raithby and Hollands (1975). For comparison, values of K_{eff} from Francis, et al. (2003) (plotted in Figure 4b) are based on relations developed from CFD simulations supported by laboratory test data. Simulations using K_{eff} values at either end of the range shown in Figure 5 indicate that waste package temperature estimates are not sensitive to the value used for K_{eff}. Thus, further refinement is not warranted for estimates of the effective thermal conductivity accounting for the heat transfer of cross-sectional convection around eccentrically placed waste packages in drifts. CFD modeling would still be needed, however, to evaluate the effects of heat transfer heterogeneity around the engineered barriers, local moisture redistribution, and axial convection.

To assess the effect of drift degradation on the temperature difference over time between the center and end of Drift 25, the in-drift heat transfer algorithm was linked to the drift degradation model of Gute, et al. (2003). The analysis by Gute, et al. (2003) stochastically estimated the drift degradation extent across the repository. For the analysis here, the mean behavior drift degradation case leads to a rubble pile that covers the drip shield within 800 years. The air space between the waste package and drift shield remains open for convection, and

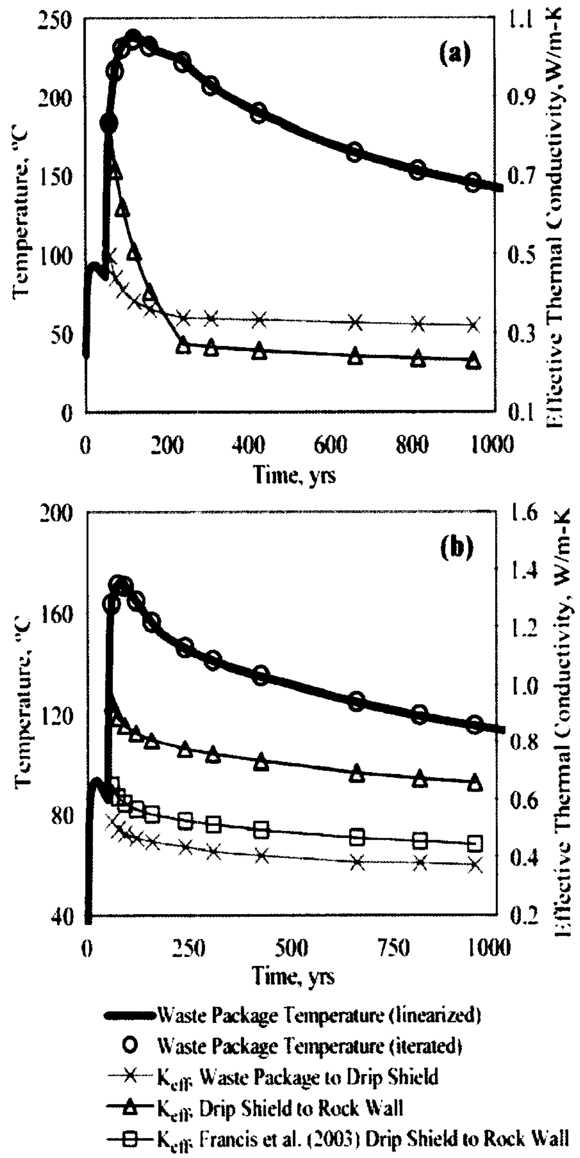

Figure 5. Effect of linearization of convection and radiation terms for estimating waste package temperatures for (a) drift degradation with natural backfill and (b) no-drift degradation scenarios. K_{eff} is the effective thermal conductivity for convection.

some air space above the rubble pile may be present. Figure 6 presents estimates of the temperature differences between the center and edges during time assuming drift degradation occurs uniformly along a drift. These estimates do not account for the change in the host rock (i.e., K = 1.56 W/m-K used for both locations). Temperatures at the drip shield are generally less than 10 °C cooler than those at the waste package at the peak of the thermal pulse. The temperature difference between the waste package and drip shield decreases as the thermal pulse dissipates. Temperature estimates for the east and west ends of the drift are nearly identical because conduction through the rubble pile dominates the heat transfer in the system.

Table 1 contains the in-drift heat transfer algorithm results with and without drift degradation compared to the mountain-scale conduction-only results. Compared to the in-drift heat transfer model fractured wallrock, the mountain-scale conduction-only model (i) underestimates temperature difference between the center and edge locations at the time of peak temperature, (ii) overestimates the temperature differences at 1000 years, and (iii) underestimates the duration of time when waste packages remain above 80 °C (the lower bound for potential localized corrosion of waste packages).

Table 1. Temperature differences (ΔT) between center and edge locations at selected times using two different models.

	ΔT at Peak	ΔT at 1000 yrs	ΔT When Center Reaches 80 °C
Conduction-Only Model	71 °C	46 °C	26 °C at 3960 yrs
Basecase Drift Degradation, In-Drift Algorithm and Thermohydrologic Model	86 °C	39 °C	20 °C at 6260 yrs

Missing from the analysis is the effect of spatial heterogeneity of drift degradation. Because drift degradation is unlikely to occur uniformly along a drift, rather to different degrees intermittently along the drift, the temperature differences in Figure 6 may not be the

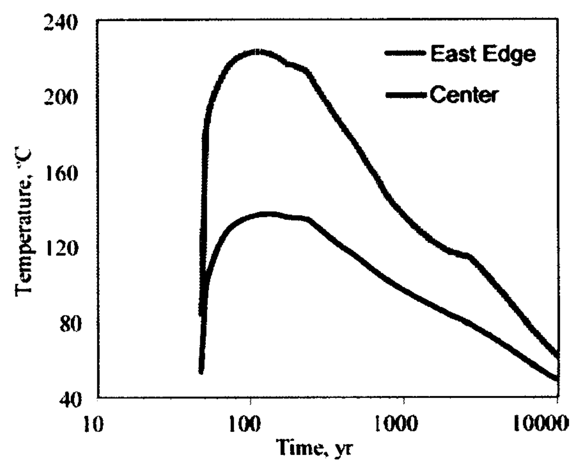

Figure 6. Waste package temperature estimates at center and east edge of Drift 25 for the mean case drift degradation scenario. Results from the thermohydrologic model were used as input for the outer boundary condition of the heat transfer algorithm.

most likely scenario to occur. Instead of the large-scale temperature differences, large temperature gradients for small spatial scales may occur. Figure 7 illustrates bounding calculations where early drift degradation would lead to peak temperatures up to 362 °C, mean expected degradation would lead to 236 °C, and no drift degradation would lead to 189 °C.

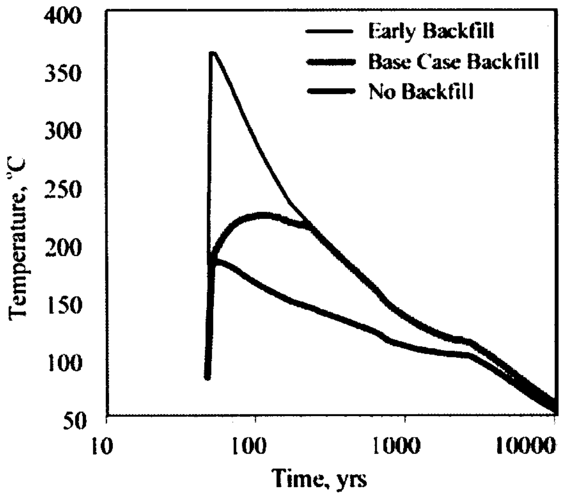

Figure 7. Comparison of waste package temperature estimates for early, basecase, and no drift degradation scenarios using thermohydrologic modeling results as input for the outer boundary condition of the heat transfer algorithm.

SUMMARY

Modeling of natural convection and the cold-trap processes in thermally perturbed drifts requires the use of CFD codes. The effects of large-scale processes such as mountain-scale thermohydrology and drift degradation along drifts are most efficiently represented by the indirect linkage of models.

Mountain-scale conduction-only models are used to estimate temperature gradients along the length of a drift. Assessments of the conduction-only model results using a model that integrates thermohydrology, drift degradation, and in-drift heat transfer processes show some important differences that need to be incorporated when assessing the effect of natural convection and the cold-trap processes on in-drift temperature and moisture conditions. Heterogeneity of drift degradation on axial temperature gradients has the capability of significantly modifying axial temperature gradients and, thus, will be the focus of future study.

ACKNOWLEDGMENTS

This paper was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC–02–02–012. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Waste Management. This paper is an independent product of CNWRA and does not necessarily reflect the view or regulatory position of NRC.

REFERENCES

Brossia, C.S., . Browning, L, Dunn, D.S., Moghissi, O.C., Pensado, O., and Yang. L., 2001, "Effect of environment on the corrosion of waste package and drip shield materials," CNWRA 2001-003, Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Clausen, T. and Proberts, J., 1996, "Temperature field due to time-dependent heat sources in a large rectangular grid–derivation of analytical solution," SKB96–12, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Carslaw H.S. and Jaeger, J.C., 1959, "Conduction of heat in solids," Oxford University Press, United Kingdom.

CRWMS M&O. 2000. "Site recommendation subsurface layout," ANL–SFS–MG–0001, Rev. 00, North Las Vegas, Nevada.

DOE, 2002, "Yucca Mountain science and engineering report, Rev. 1, DOE/RW–0539–1, Department of Energy, Office of Civilian Radioactive Waste Management, Las Vegas, NV.

Dunn D. S., Yang, L., Pan Y-M., and Cragnolino, G. A., 2003, "Localized corrosion susceptibility of Alloy 22," Corrosion 2003, Paper No. 03697, pp. 1–14.

Fedors, R.W., Walter, D.B., Dodge, F.T., Green, S.T., Prikryl, J.D., Svedeman, S.J., 2003a, "Laboratory and numerical modeling of the cold-trap process," Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Fedors, R.W., Adams, G.R., Manepally, C., and Green, S.T., 2003b, "Thermal conductivity, edge cooling, and drift degradation–Abstracted model sensitivity analyses for Yucca Mountain," Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Francis, N.D., Webb, S.W., Itamura, M.T., and James, D.L., 2003, "CFD Modeling of natural convection heat transfer and fluid flow in Yucca Mountain Project (YMP) enclosures," SAND2002–4179, Sandia National Laboratories, Albuquerque, New Mexico.

Green, S.T., Walter, D.B., Fedors, R.W., and Dodge, F.T., 2004, (these proceedings), "A model for moisture transport in a high-level radioactive waste repository drift," Society for Mining, Metallurgy, and Exploration Annual Meeting, February 23–35, 2004, Denver, Colorado.

Gute, G.D., Ofoegbu, G., Thomassy, F., Hsiung, S., Adams, G., Ghosh, A., Dasgupta, B., Chowdhury, A., and Mohanty, S., 2003, "MECHFAIL: A Total-System Performance Assessment Code Module for Evaluating Engineered Barrier Performance under Mechanical Loading Conditions," CNWRA 2003–06, Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Mohanty, S., McCartin, T.J., and Esh, D.W., 2002, "Total-system Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide," Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Painter, S., Lichtner, P.C., and Seth, M.S., 2001, "MULTIFLO User's Manual," MULTIFLO, Version 1.5: Two-Phase Nonisothermal Coupled Thermal-Hydrologic-Chemical Flow Simulator, Rev. 3, Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Raithby, G. D. and Hollands, K.G.T., 1975, "A general method of obtaining approximate solutions to laminar and turbulent heat transfer problems," T. F. Irvine, and J. P. Hartnett, eds, Advances in Heat Transfer, Vol. 11, Academic Press, New York, pp. 265–315.

Tang, I.N., and Munkelwitz, H.R., 1993, "Composition and temperature dependence of the deliquescence properties of hygroscopic aerosols," Atmospheric Environment, Vol. 27A, pp. 467–473.

Walter, D.B., Green, S.T., Fedors, R.W., and Hart, R.A., 2004 (these proceedings),"Modeling a Small Laboratory Cold-Trap Experiment," Society for Mining, Metallurgy, and Exploration Annual Meeting, February 23–35, 2004, Denver, Colorado.

Unit Conversions:

1 ft = 0.3048 m

°F = 1.8 x T °C+ 32

1BTU/ft-h-°F = 13.87 W/m-K