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March 18, 2004
Contract No. NRC–02–02–012
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U.S. Nuclear Regulatory Commission
ATTN: Mr. Jeffrey Pohle
Office of Nuclear Material Safety and Safeguards
Division of Waste Management
TWFN, Mail Stop 7-D13
Washington, DC 20555

SUBJECT: Thermal Effects on Flow KTI Intermediate Milestone 06002.01.091.410: Analysis of In-Drift Environmental Conditions—Letter Report

Dear Mr. Pohle:

Enclosed please find the report titled "Environmental Conditions In Drifts." This technical document fulfills the requirements for the subject milestone, which is due March 19, 2004.

The subject report provides estimates of waste package temperature and relative humidity along drifts for drift-degradation and no-degradation scenarios. These estimates include the effects of repository edge cooling and thermohydrology and are compared with estimates from basecase TPA Version 5.0 simulations. Results from repository edge cooling and thermohydrology lead to an earlier onset of conditions conducive to localized corrosion of Alloy 22, and therefore should be factored into the performance assessment. Drift degradation leads to a significantly greater peak waste package temperature but delays the onset of conditions conducive to localized corrosion of Alloy 22. Estimates of temperature gradients along open drifts (no-drift degradation) are then used in preliminary drift-scale modeling to assess the magnitude of temperature gradients needed to drive axial convection. Axial convection in drifts is a necessary condition for cold-trap condensation. Completed and ongoing laboratory experiments are briefly described.

If you have any questions, please contact Randy Fedors at 210-522-6818 or me at 210-522-5082.

Sincerely yours,

Gordon Wittmeyer

Gordon Wittmeyer, PhD
Manager, Hydrogeology

AHC/ph
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ENVIRONMENTAL CONDITIONS IN DRIFTS

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–02–012

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ABSTRACT

Estimates of in-drift environmental conditions are used as input to chemical, corrosion, and radionuclide transport models for the potential high-level waste repository at Yucca Mountain, Nevada. This report begins with an assessment of postclosure temperature and relative humidity for drift-degradation and no-degradation scenarios. Estimates are provided for the onset and duration of temperature conditions conducive to localized corrosion of waste packages. Drift degradation delays the onset time of conditions conducive to localized corrosion. Thermohydrological processes reduce the onset time of conditions conducive to localized corrosion. Thus, the effects of drift degradation and thermohydrology need to be factored into performance assessment analyses. Temperature gradients along drifts based on analytical and thermohydrological models are then evaluated to determine the potential areal extent of axial natural convection and to create input for preliminary computational fluid dynamics models of air flow and moisture redistribution in drifts. Simulations using three-dimensional drift-scale model are used to assess the magnitude of axial air flow along waste packages of uniform heat loads. It is shown that axial flow patterns would not be impeded by the strong cross-sectional flow patterns imparted by the heat rising directly off the waste package. This means that axial convection and the cold-trap process will not be limited to the extreme ends of each drift. Also, comparison of results using properties of dry air and water vapor indicate future modeling need not consider changes in fluid (air) properties as a function of vapor content. Simulations of the benchtop laboratory experiments assess the importance of including the moisture model in reproducing realistic values of relative humidity near the heat source. Two ongoing laboratory experiments are briefly described; a condensation cell and 20-percent scale model of the draft. The U.S. Department of Energy has not decided how the issue of natural convection and the cold-trap process will be addressed in any license application for Yucca Mountain as a potential storage facility for high-level waste. The options are to include the effects of convection and the cold-trap process in performance assessment analyses, or, to provide a basis for excluding these processes.

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ACKNOWLEDGMENTS

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: Original CNWRA-generated data contained in this report meet quality assurance requirements described in the CNWRA Quality Assurance Manual. Sources for other data should be consulted to determine the level of quality for those data. The work presented in this report is documented in CNWRA Scientific Notebooks 432, 536, and 576.

ANALYSES AND CODES: MULTIFLO version 1.5.2 and the commercial package FLOW–3D® Version 8.2 were used to generate results for this report and are controlled in accordance with the CNWRA software procedure TOP–018.

References:

Flow Science, Inc. "FLOW–3D® User's Manual." Version 8.1.1. Sante Fe, New Mexico: Flow Science, Inc. 2003.

Painter, S., P. Lichtner, and M. Seth. "Multiflo User's Manual: Two-Phase Nonisothermal Coupled Thermal-Hydrologic-Chemical Flow Simulator Multiflo." Version 1.5. San Antonio, Texas: CNWRA. 2001.

1 INTRODUCTION

Temperature and moisture levels in the drift environment can have a significant impact on waste package integrity at the potential high-level waste repository at Yucca Mountain, Nevada. The need to understand the combined effect of fundamental processes involved in the movement of moisture driven by convection necessitated the development of laboratory, analytical, and numerical models. Individually, the heat-transfer processes of conduction, convection, radiation, and latent heat are reasonably well understood. The combined effects of all heat-transfer processes in geometrically complex environments, however, are difficult to model. The approach taken in this report is to estimate temperature gradients using analytical heat transfer and thermohydrologic porous media models. Then, use those results to constrain two- and three-dimensional computational fluid dynamics models to identify important characteristics of air flow and moisture redistribution patterns that need to be considered in performance assessment.

The need to understand drift-scale {i.e., 1 km [0.6 mi]} and local-scale [i.e., <100 m [330 ft]} temperature variations may be important for performance of the potential repository. Drift-scale temperature gradients may drive axial convection cells that move water in the vapor phase to locations where condensation could occur. Heat transfer caused by natural convection along drifts will affect the onset and duration of environmental conditions conducive to corrosion of the engineered barrier subsystem. Local-scale convection cells affected by the geometric arrangement of the engineered barrier components and emplacement strategy can create zones of reduced temperature, elevated relative humidity, and preferential condensation. Local-scale convection refers to axial and cross-sectional air flow patterns limited to sections of a drift. These air flow patterns can lead to nonuniform temperatures around and between waste packages because of convection beneath the drip shield, around the waste package stand, between individual waste packages, and between sections of waste packages. Besides variations in temperature caused by the geometrical arrangement of the engineered barrier subsystem, variations in temperature also are caused by variation in heat load between individual waste packages. These local zones around the complex geometry of the engineered barrier subsystem are not addressed in this report, but will be addressed in future studies.

Conductive, convective, thermal radiative, and latent-heat transfer processes all influence temperature estimates in the emplacement drifts of Yucca Mountain. Conduction is important in the solid portions of the engineered barriers and in the wallrock. Radiation is important across air spaces. Convection of air above and below the drip shield will lead to cross-sectional and axial air flow patterns that will enhance heat transfer away from waste packages. The U.S. Department of Energy (DOE) currently incorporates the effects of conductive and convective heat transfers in its total system performance assessment models through the use of effective thermal conductivity in porous media models (CRWMS M&O, 2001a). The convective heat transfer, however, is only incorporated in a cross-sectional sense (i.e., no axial heat transfer or moisture redistribution is incorporated). Although it is clear DOE has begun to assess the effect of the cold-trap process in separate process model calculations (Bechtel SAIC Company, LLC, 2003a,b), the decision to exclude or include moisture redistribution and the cold-trap process as a feature, event, and process in the performance assessment has not yet been made.

This report presents in-drift temperature and relative humidity estimates for two scenarios, drift degradation and no-drift degradation. Environmental conditions along a typical drift are assessed to support estimates of the onset and duration of conditions conducive to corrosion in

Chapter 2, and to provide input for computational fluid dynamics models of in-drift air flow and moisture redistribution in Chapter 3.

1.1 Background

Temperature gradients along drifts may drive axial convection cells that move water in the vapor phase to locations where condensation could occur. The edge effect, differential heat loading between sections of a drift, and lithological variations along the drift would all act to create repository-scale temperature gradients. The edge effect is the phenomenon where cooler temperatures are experienced at the ends of drifts relative to the centers because of the influence of the cooler rock beyond the edge of the repository. The specific heat load imposed on a drift is subject to emplacement strategies and different thermal history profiles for various waste types. A strategy to lessen the edge effect is to place hot waste packages at the ends of drifts and cool waste packages in the center. No strategy will eliminate temperature gradients entirely. Lithological changes affect thermal properties along the drift (e.g., the lower lithophysal unit of the Topopah Spring Tuff has larger saturated thermal conductivity than the middle nonlithophysal unit, and hence, would conduct heat away from the drifts at a faster rate). An approach for estimating temperature gradients along drifts, and the portions of drifts affected by those gradients, was described in Manepally and Fedors (2003). Complementing that approach, the work in this report delves further into the study of large-scale gradients and also focuses on the effect of natural convection on in-drift environmental conditions.

The proposed emplacement of high-level waste in drifts will significantly elevate the temperatures of the drift environment. Temperature gradients along drifts will lead to the movement of air and vapor in natural convection cells. In the cold-trap process, water evaporates at hotter locations, is carried in the vapor phase by convective air flow, and condenses at cooler locations. Elevated relative humidity combined with deliquescence may lead to liquid-phase water contacting waste packages in peripheral zones of the repository where wallrock temperature may not exceed the boiling point or in internal zones of the repository when the thermal pulse is dissipating. The geometry of the components of the engineered barrier subsystem (e.g., waste package and support, drip shield, and invert) and interaction with the wallrock adds complexity to the problem of simulating air flow and condensation associated with the cold-trap process.

Natural convection and the cold-trap process are expected to modify environmental conditions in drifts from those calculated using models that assume no convection. These modifications potentially could lead to the presence of liquid water and enhanced localized corrosion of some waste packages. For extended periods, benign in-drift conditions are likely to occur. Aggressive conditions, however, may exist in portions of the drifts for shorter periods of time and are dependent on a confluence of temperature, condensation, and chemistry. The waste package outer layer, Alloy 22, may be susceptible to localized corrosion in the presence of liquids with high halide content. The chemistry of water associated with the cold-trap process will differ markedly from that of ambient percolation and thermally refluxed water. The chemistry of condensed water also may vary markedly along the drifts or in the microenvironments of the engineered barrier subsystem because of variations in reactivity with the substrates (e.g., rock bolts, drip shield, and wallrock) on which condensation occurs. Interaction with dust or evaporative residues also will significantly modify the chemistry of the condensate. The cold-trap process will elevate relative humidity in the vicinity of waste packages earlier than the time estimated neglecting convection. The elevation of relative humidity, which may lead to the presence of liquid-phase water, may lead to localized corrosion of waste packages when temperatures are above 80 °C [176 °F] (Brossia, et al., 2001; Dunn, et al., 2003). At this time, the degree to which natural convection and the cold-trap process will modify temperature, relative humidity, and presence of liquid water in drifts, however, cannot be assessed quantitatively with much reliability because of the lack of measured data available to constrain models.

There are two situations that natural convection and the cold-trap process may play a prominent role in repository performance. Cross-sectional flow patterns driven by the heat load from eccentrically located waste packages in the drifts may be strong enough to impede the large-scale axial-flow patterns. The cross-sectional flow patterns also will lead to a nonuniform distribution of temperature around the engineered barrier subsystem. Temperatures on the outside of the waste package are not expected to be uniform because of the combined influence of conduction (to the waste package supports), convection, and thermal radiation. Specific locations where the relative humidity will be elevated near the waste packages, thus increasing the likelihood of condensation, will be controlled by convection in the microenvironments of the engineered barrier subsystem.

1.2 Technical Agreements

Two U.S. Nuclear Regulatory Commission (NRC) and DOE technical agreements were generated about the cold-trap process.

Agreement TEF.2.04: "Provide the Multi-Scale Thermohydrologic Model AMR, Rev. 01. The DOE will provide the Multi-Scale Thermohydrologic Model AMR (ANL–EBS–MD–00049) Rev 01 to the NRC. Expected availability is FY 02."

Agreement TEF.2.05: "Represent the cold-trap effect in the appropriate models or provide the technical basis for exclusion of it in the various scale models (mountain, drift, etc.) considering effects on TEF and other abstraction/models (chemistry). See page 11 of the Open Item (OI) 2 presentation. The DOE will represent the "cold-trap" effect in the Multi-Scale Thermohydrologic Model AMR (ANL–EBS–MD–00049) Rev 01, expected to be available in FY 02. This report will provide technical support for inclusion or exclusion of the cold-trap effect in the various scale models. The analysis will consider thermal effects on flow and the in-drift geochemical environment abstraction."

At the Thermal Effects on Flow Technical Exchange and Management meeting (Reamer, 2001) the presentation on resolution of the cold-trap process noted DOE would consider the cold-trap effect and would incorporate important effects in the thermohydrological model for performance assessment. DOE discussed possible approaches for modifying the drift-scale and mountain-scale models. To support these modifications, DOE intended to use a computational fluid dynamics approach for independently assessing heat and mass transfer in the emplacement drifts.

DOE released Bechtel SAIC Company, LLC (2003a), in part, to satisfy technical agreement TEF.2.04. However, it was not clear from the presented discussion how natural convection and moisture redistribution were incorporated in the Multiscale Thermohydrologic Model or the Total System Performance Assessment. Or, for an alternative approach, no basis was presented to exclude the cold-trap process and its associated processes of natural convection and moisture redistribution. Bechtel SAIC Company, LLC (2003a) noted that a new analysis model report on natural convection and condensation (Bechtel SAIC Company, LLC, 2003b) was being developed with a release date scheduled for the summer of 2004. CRWMS M&O (2001b) concluded that vapor might condense beneath the drip shield. Furthermore, Danko and Bahrami (2004) concluded that a significant amount of water will condense along drift segments due to axial convection based on simulations using MULTIFLUX.

1.3 Risk-Informed Aspects

The uncertainty of moisture movement in drifts associated with the cold-trap process is part of the more general concern of how water enters the drifts and how the water pathway dictates the chemistry of liquids contacting the engineered barriers. The chemistry of water contacting waste packages when waste package temperatures are above 80 °C [176 °F] is important for localized corrosion. Uniform and localized corrosion rates of the titanium drip shield are being extensively studied. Drift degradation will have a prominent effect on environmental conditions in the drifts, though it likely would dampen axial convection in the drifts, particularly above the drip shield.

1.3.1 Waste Package Corrosion

From a risk-informed perspective, it is important to quantify factors that affect the onset and duration of the window for localized corrosion of Alloy 22 and the processes by which water contacts the waste containers. Because the propagation rate of localized corrosion of Alloy 22 is fast, the onset of conditions conducive to corrosion is more important than duration as long as the duration is past a specified length of time. Based on parameters in the TPA Version 5.0 code, this length of time is approximately 80 years. Localized corrosion for Alloy 22 is most likely to occur between approximately 80 and 140 °C [176 and 284 °F], when liquid water may occur in dust or residue on the waste package surface. Within this temperature window, Alloy 22 may be susceptible to localized corrosion in the presence of solutions with high halide content (e.g., chloride) (Brossia, et al., 2001; Dunn, et al., 2003). Below the temperature window for localized corrosion, generalized corrosion can occur and would be dependent on the water flux contacting the drip shield and waste package. During the performance period, generalized corrosion is not expected to be important, however, the uncertainty of localized corrosion plays a prominent role in the uncertainty of dose (Mohanty, et al., 2002a).

The period encompassing the temperature window has been predicted to span several hundred to several thousand years depending on thermohydrological model inputs and assumptions (CRWMS M&O, 2001a; Manepally and Fedors, 2003; Fedors, et al., 2003a). During the window of localized corrosion, the physical process by which water comes in contact with the waste container must be understood well enough to support estimation of the chemistry of the liquid phase contacting the waste container. Hydrological processes by which water enters and redistributes in drifts, possibly coming in contact with the waste packages, include seepage and dripping, uniform condensation, cold-trap movement of moisture within a drift, and film and rivulet movement of liquid phase water on the engineered barrier. Assuming the integrity of the drip shield is maintained, natural convection associated with the cold-trap process could elevate the relative humidity near the waste packages. One possible mechanism to elevate the relative humidity beneath the drip shield is evaporation from the invert. Redistribution of water in the invert and evaporation beneath the waste package will lead to an elevation of vapor pressure. A dry invert may be rewetted by drainage condensation on the drift wall and drip shield on the invert. Deliquescence enables liquid phase water to form on waste package surfaces at relative humidity values well below the saturated vapor pressure. Because it is an important input to corrosion models, the uncertainty in timing and magnitude of relative humidity in the vicinity of waste packages, with and without considering the effect of the cold-trap process, requires further analysis.

Different modes of water movement lead to markedly different chemical conditions. Evaporated and initially condensated water is relatively dilute and will likely have a low pH. Interaction of the condensed water with the surface material on which it condenses, including any dust or residual mineralization left by previously evaporated water, will prominently alter the chemistry of the liquid phase water. Refluxed water that flows across a residue in fractures of the wallrock likely will be highly concentrated and possibly highly corrosive. Inadequate knowledge of the relative portions of ambient seepage, refluxed, and condensed water entering the drifts would lead to uncertainty about the chemistry of solutions contacting the waste container.

1.3.2 Transport

Current DOE models predict that a dryout zone in the invert and below the drift will serve as a significant natural barrier to radionuclide transport (Bechtel SAIC Company, LLC, 2001). Dripping, along-wall seepage, and condensation from the cold-trap process can accelerate rewetting of the invert in cooler locations. Increased wetness of the invert and the wallrock below the drift will increase radionuclide transport rates if breaching of waste packages occurs. The DOE models used for performance assessment (CRWMS M&O, 2001a), however, do not currently account for condensation, dripping, and along-wall seepage in the evolution of the drift shadow.

1.3.3 Effect of Drift Degradation

Current Center for Nuclear Waste Regulatory Analyses (CNWRA) estimates of drift degradation based on thermal-mechanical modeling suggest all the repository drifts will likely be backfilled within 1,000 years after closure because of drift degradation processes (Gute, et al., 2003). Drift degradation is modeled as a stochastic process. Drift degradation will lead to a rubble pile (natural backfill) gradually covering the drip shield during postclosure time. The time when drift degradation starts and the extent of degradation are important parameters for estimating temperatures at the waste package. Fedors, et al. (2003a) described the approach for linking drift degradation and estimates of temperature. In a sensitivity study, Manepally, et al. (2003) evaluated the importance of some assumptions inherent in the simple network algorithm that linked temperature to drift degradation. The timing and degree of natural backfilling control the magnitude of increased temperatures estimated for the waste packages for the drift-degradation scenarios when a rubble pile covers the drip shield.

Convective heat transfer and moisture movement along the length in a backfilled drift will likely be reduced than in the open drift with only a drip shield. If the drip shield remains intact below the rubble pile, convective heat transfer and moisture movement could occur beneath the drip shield and in the air pocket above the rubble pile. Convection through the rubble pile will likely occur and is expected to be greater than natural convection through the intact fractured wallrock, although it is expected to be much less than that through the open air space of the drift.

Nonuniformity of drift degradation also may increase the local-scale temperature gradients capable of causing increased convective air and moisture transfer along the drift between waste packages or zones of waste packages. Localized zones of degradation may act to bound separate zones of axial convection, with the highest temperatures occurring where rubble piles cover the drip shield. Models of air flow can bound the effects of different drift-degradation scenarios without further refinement of geomechanical models (e.g., Gute, et al., 2003). The magnitude of possible convection in the nonuniform drift-degradation scenario is not assessed in this report.

2 ENVIRONMENTAL CONDITIONS IN DRIFTS

Estimates of temperature and relative humidity are needed to support estimates of liquid water in the drifts and the potential for corrosion of engineered barrier components. Temperature estimates also are needed to describe temperature gradients along drifts because they are expected to promote natural convection. Natural convection and the associated cold-trap process involve temperature gradient-driven air flow with evaporation from warm areas, movement of vapor driven by thermal gradients, and condensation on cool or hygroscopic surfaces. The question then becomes, what temperature gradients may occur in the drifts of a potential repository?

Several combinations of different analytical and numerical thermohydrological porous media models are used in this chapter to

- Estimate in-drift environmental conditions along a drift, specifically temperature and relative humidity, and identify the onset of conditions conducive to localized corrosion of Alloy 22 for drift-degradation and no-degradation scenarios

- Identify extent and timing of significant temperature gradients along drifts to understand the magnitude of areal extent relevant for axial convection

- Estimate temperature boundary conditions along a drift and representative thermal properties of the wallrock for the drift-scale computational fluid dynamics modeling of in-drift natural convection and moisture redistribution described in Chapter 3

This chapter is divided into two parts, one part is about in-drift temperature and relative humidity estimates, and the other part is about in-drift estimates of temperature gradients. In the first part, the drift-degradation and no-degradation scenarios are considered. In the first section, an abstracted model is used to estimate time-dependent temperature and relative humidity for the repository center and edge locations of a typical drift. Then, results from a detailed thermohydrological model are linked to an in-drift heat transfer algorithm to evaluate temperature estimates previously obtained using the efficient abstracted model. Onset and duration of environmental conditions conducive to localized corrosion are extracted from the temperature and relative humidity estimates for the drift-degradation and no-degradation scenarios. In the second part, the most computationally efficient model (i.e., conduction-only) for temperature is used to estimate temperature gradients. Results from a three-dimensional thermohydrological model are used to evaluate the results of the conduction-only model. All results presented in this section are for the postclosure period, but postclosure temperature estimates account for the effect of preclosure forced ventilation.

2.1 Temperature and Relative Humidity

An in-drift heat transfer algorithm is used to estimate waste package and drift wall temperature for the drift-degradation and no-degradation scenarios. The in-drift heat transfer algorithm uses drift wall temperature estimates provided by either a mountain-scale conduction-only or thermohydrological model. Once the temperature has been estimated, the relative humidity can be estimated using simple assumptions.

For the repository design (DOE, 2002), cylindrical waste packages are to be eccentrically emplaced in a 5.5-m [18.0-ft] 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 (see Figure 2-1). The effect of drift degradation and formation of a rubble pile covering the drip shield can be factored into an in-drift heat transfer algorithm. This analysis assumes the drip shield remains intact, although the elevated temperatures from natural backfill may affect drip shield mechanical integrity.

The mountain-scale conduction-only model is an analytical, three-dimensional 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 Mohanty, et al.,[1] Claesson and Probert (1996), and Carslaw and Jaeger (1959). In-drift processes are modeled as conduction (i.e., the drift volume is modeled as an extension of the tuff wallrock). At any one location, the superposition principle is used to combine the effect of heat transfer from all nearby drifts and to approximate the effect of lithologic variations along a drift. Effective or representative thermal properties must be used in the conduction model; for example, thermal conductivity varies widely with saturation of the rock, but a single representative value must be used in the conduction equation. An alternative to using temperature estimates from the mountain-scale conduction-only model as the outer boundary condition in the heat transfer algorithm is to use those from the thermohydrological model described in Manepally and Fedors (2003). By linking thermohydrological model results extracted from Manepally and Fedors (2003), improved estimates of waste package temperature are produced because the in-drift heat transfer algorithm approximates the processes of convection and radiation better than the thermohydrological model.

The multimode algorithm for in-drift heat transfer processes is used to estimate waste package surface temperature. The algorithm 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 not included in this analysis. The in-drift, multimode algorithm uses the rock temperature estimated either from the conduction-only or thermohydrological model as an outer boundary condition at the drift wall. Hence, mountain-scale processes are decoupled from the in-drift processes. Figure 2-1 shows a schematic of the thermal network algorithm. The multimode algorithm allows fast analyses of new design features or different scenarios.

The multimode algorithm for estimating waste package temperatures is based on the following equation.

$$Q_p = \left\{ G_{inv} + \left[\frac{1}{G_{cpd} + G_{rpd}} + \frac{1}{G_{bf}} + \frac{1}{G_{cbw} + G_{rbw}} \right]^{-1} \right\} \left(T_p - T_w \right) \tag{2-1}$$

[1]Mohanty, S., G. Adams, and J. Menchaca. "An Abstracted Model for Estimating Temperature and Relative Humidity in the Potential Repository at Yucca Mountain." *Proceedings of the 2004 ASME Heat Transfer/Fluid Engineering Summer Conference, Charlotte, North Carolina, July 11–15, 2004.* American Society of Mechanical Engineers. Submitted for publication (2004).

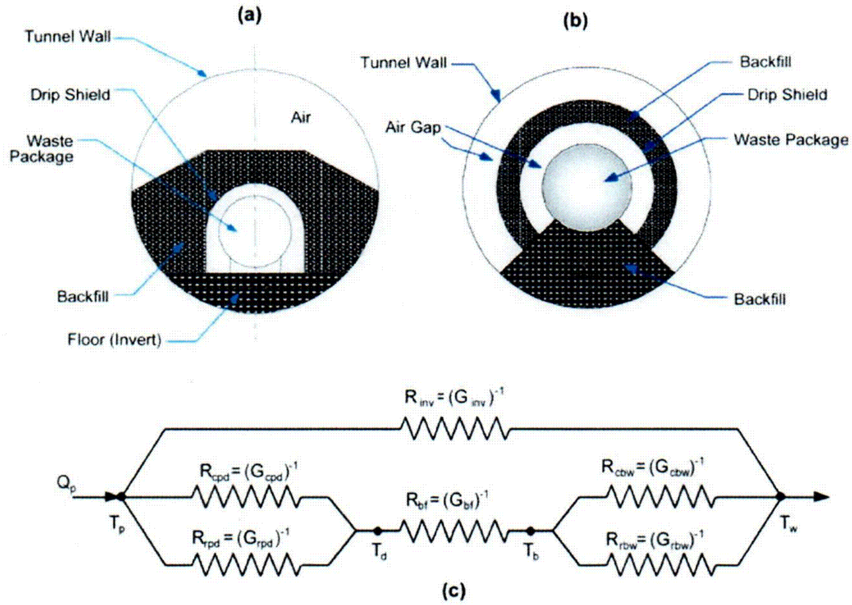

Figure 2-1. (a) Engineered Barrier Components, (b) Radial Approximation, and (c) Schematic of Network for Estimating Temperature from In-Drift Thermal Processes with Linkage to Drift Degradation. R Is the Thermal Resistance, Which Is the Inverse of the Conductance, G.

where

Q_p	—	time-dependent heat supplied by the waste package
G	—	refers to the conductance terms, which are the inverse of the resistance
inv	—	invert
cpd	—	convection between the waste package and the drip shield
rpd	—	radiation between the waste package and the drip shield
bf	—	conduction through the natural backfill (if present)
cbw	—	convection between the drip shield or backfill and the drift wall
rbw	—	radiation between the drip shield or backfill and the drift wall
T_p	—	temperature at the waste package
T_w	—	time-dependent temperature in the rock, outer boundary condition

C01

T_w is the boundary condition for the in-drift algorithm, and it is obtained from either the mountain-scale conduction-only model or the thermohydrological model results. Note the value of T_w for the boundary condition in the former case 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 (Figure 2-1). Expressions for each conductance term follow the development presented in Fedors, et al. (2003a), which followed the general methodology in Mohanty, et al.[2] Whereas heat storage in the wallrock is accounted for explicitly in the estimate of the outer boundary condition, heat storage in the drift is not considered in the equilibrium relation in Eq. 2-1. Slowly changing heat load is assumed to reduce the effect of ignoring in-drift heat storage, particularly for the rubble pile.

The linkage of temperature and drift degradation follows the approach presented in Fedors, et al. (2003a). The in-drift heat transfer algorithm was linked to the drift degradation model of Gute, et al. (2003). Their analysis stochastically estimated the drift degradation extent across the repository. For the analyses presented in this report, the mean 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 some air space above the rubble pile may be present. Convection and radiation in the air spaces below the drip shield and above the rubble pile are included in Eq. 2-1. Only results for the postclosure period are presented throughout this report.

2.1.1 Temperature Estimates

Waste package temperature estimates for early degradation, basecase degradation, and no degradation are presented in Figure 2-2. The early degradation scenario is considered an upper bound for temperature estimates. For the early degradation scenario, the drifts are presumed to degrade immediately after closure of the repository. The early, basecase, and no-drift degradation scenarios would lead to a peak temperatures of 362 °C [684 °F], 236 °C [457 °F], and 171 °C [340 °F]. The more likely scenario would be for nonuniform degradation, thus producing zones of higher and lower temperatures along the drift. The methodology employed in this report is not amenable to simulating the temperature changes along a drift with nonuniform drift degradation. These temperature estimates presume the entire drift uniformly degrades.

Basecase thermal properties from the TPA Version 5.0 code are used in these analyses {i.e., a thermal conductivity value of 1.59 W/m-K [22.0 BTU/ft–h-°F] is used for the wallrock}. The thermal conductivity of the rubble, however, is not yet part of the TPA Version 5.0 code (Mohanty, et al., 2002b). A thermal conductivity value of 0.27 W/m-K [3.75 BTU/ft-h-°F] is used for the analyses presented in this report based on the value used for the invert in TPA Version 5.0 code basecase. Fedors, et al. (2003a) and Manepally, et al. (2003) showed that there was a large sensitivity of temperature to the thermal conductivity value used for the rubble

[2]Mohanty, S., G. Adams, and J. Menchaca. "An Abstracted Model for Estimating Temperature and Relative Humidity in the Potential Repository at Yucca Mountain." Proceedings of the 2004 ASME Heat Transfer/Fluid Engineering Summer Conference, Charlotte, North Carolina, July 11–15, 2004. American Society of Mechanical Engineers. Submitted for publication (2004).

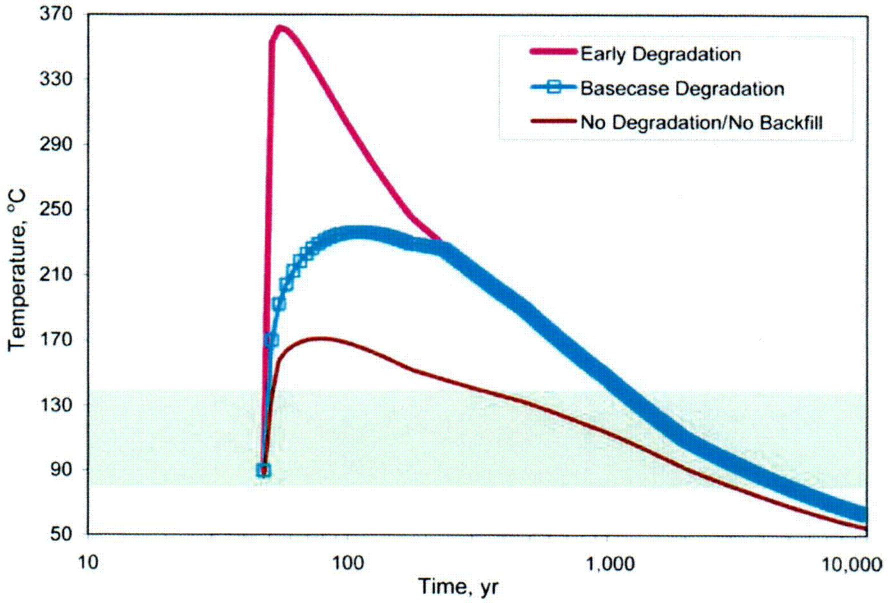

Figure 2-2. Waste Package Temperature Estimates for Early Drift Degradation, Basecase Drift-Degradation, and No-Degradation Scenarios Using Conduction-Only Model Results as the Boundary Condition for the In-Drift Heat Transfer Algorithm. Shaded Area Marks Zone of Temperature Conditions Conducive to Corrosion [°F = (1.8 × T °C + 32)].

pile. The thermal conductivity value for the rubble pile is highly uncertain; no supporting basis has been found in the general literature.

Temperature as a function of time at the center of the repository does not adequately reflect environmental conditions in drifts. Figure 2-3 illustrates the bounding waste package temperature profiles for a drift; all temperature conditions between the profiles (center and edge) occur at some location along the drift. The host rock properties are assumed constant along the drift for these estimates of the temperature profile.

The center and edge profiles are said to bound the conditions in a drift because, if profiles for every location were plotted in Figure 2-3, the curves would completely populate the zone between the center and edge temperature profiles. For example, at the peak temperature in the drift-degradation scenario, there is a temperature range along the drift from 150 °C [302 °F] at the edge to 236 °C [457 °F] at the center. Similarly at 1,000 years, there is a temperature range along the drift from 97 °C [207 °F] at the edge to 146 °C [295 °F] at the center. Thus, there is a zone of the drift where temperature conditions are conducive to localized corrosion early in the performance period that would be missed if the center location was considered representative of the entire repository. For the basecase drift-degradation scenario (Figure 2-3a), 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. Similar conclusions can be drawn for the profiles presented in Figure 2-3b for the no-degradation scenario.
The drift-degradation and no-degradation scenarios lead to markedly different temperature profiles across the engineered barrier subsystem and into the wallrock. For the no-degradation

C02

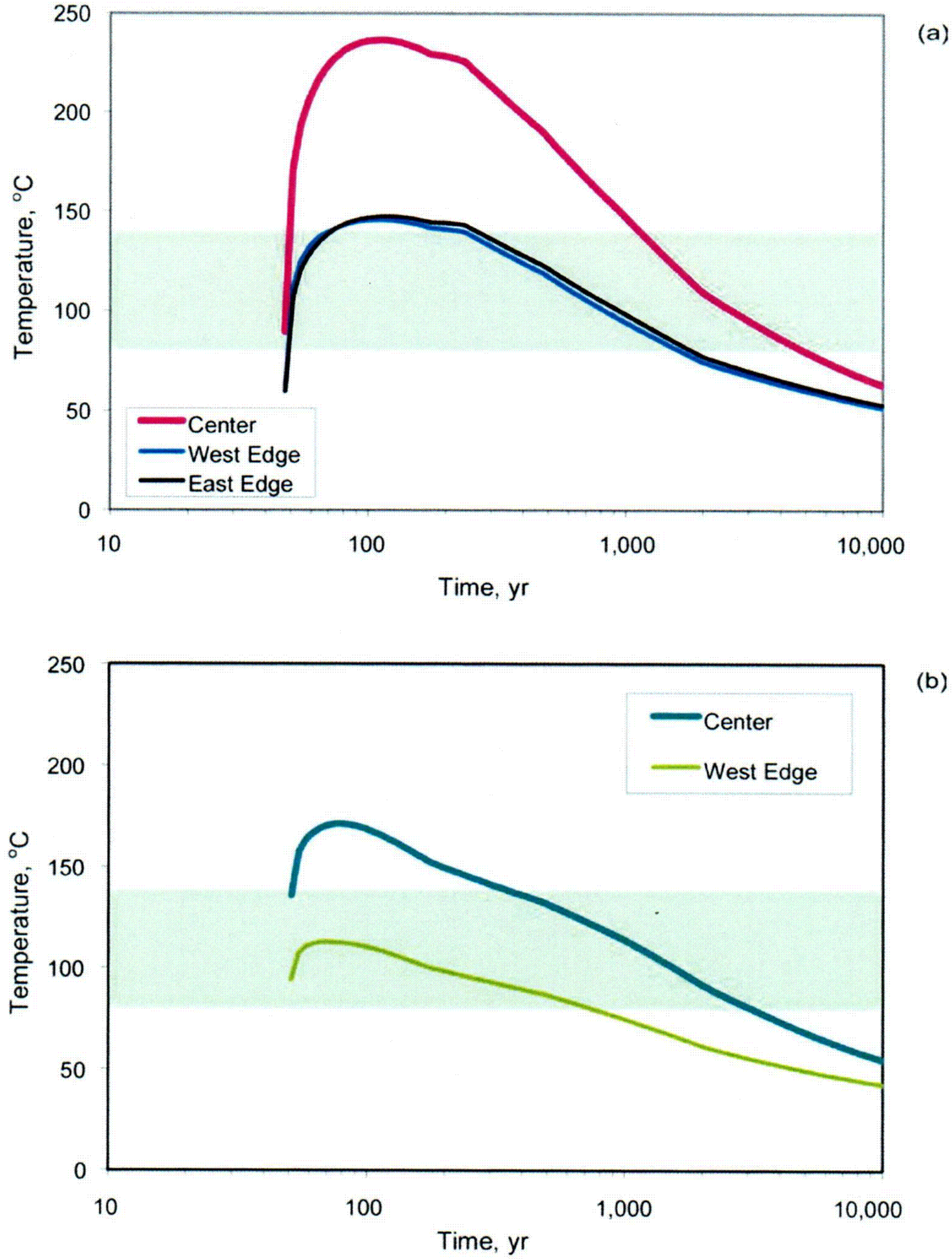

Figure 2-3. Waste Package Temperature Estimates at Center and Edge Locations for (a) Basecase Drift-Degradation and (b) No-Degradation Scenarios Using Conduction-Only Model Results as the Boundary Condition for the In-Drift Heat Transfer Algorithm. Shaded Areas Mark Zone of Temperature Conditions Conducive to Corrosion [°F = (1.8 × T °C + 32)].

C03

scenario, radiation and natural convection are effective and efficient for transferring heat from the waste package to the wallrock. Estimates of temperature differences between the waste package and the wallrock are approximately 10 °C [18 °F] for the no-degradation scenario at the time of peak temperature. This temperature difference decreases as the thermal pulse dissipates.

For the drift-degradation scenario, there is a large difference in the temperature at the waste package and that at the drift wall. Figure 2-4 illustrates the temperature profile across the engineered barrier subsystem at a center location. The temperature difference of 86 °C [187 °F] between the waste package and the drift wall illustrates how conduction through the rubble pile dominates the estimate of temperature in the drift-degradation scenario. As will be shown in the next section, the large temperature difference in the drift-degradation scenario serves to keep the relative humidity at a low value near the waste package.

2.1.2 Relative Humidity Estimates

The temperature difference between the waste package and the drift wall is an important factor for estimating relative humidity at the waste package. The temperature of the drift wall also is important because the supply of water comes from the drift wall (assuming no in-drift moisture redistribution due to axial convection). The estimate of relative humidity near the waste package assumes well-mixed air in the drift and uses the drift wall and waste package temperatures. The calculation of relative humidity differs depending on the temperature of the drift wall being above or below boiling.

Below boiling, the relative humidity is defined as the actual mole fraction of water vapor in the air divided by the mole fraction when the air is saturated with water vapor at the same temperature. For above boiling conditions, it is assumed vapor partial pressures cannot exceed the atmospheric pressure in drifts (i.e., there is no pressure buildup in the heated drifts). Thus, for above boiling, it is assumed the amount of water vapor held in the air phase at the boiling temperature remains constant for all temperatures above the boiling temperature. Also, by definition, the relative humidity has to be 100 percent at the boiling temperature for pure water not held by capillary tension.

At the elevation of the repository, total pressure dictates that the boiling temperature is between 96 and 97 °C [204.8 and 206.6 °F]. The assumptions are that capillarity does not affect the boiling temperature, and pore water is pure water. Capillarity and high concentrations of ions in solution will serve to elevate the relative humidity estimated at the drift wall. Higher boiling point temperatures at the drift wall will increase estimates of relative humidity for above-boiling conditions.

The definition of relative humidity used by hydrologists differs slightly from that used by chemists. Pabalan, et al. (2002) define relative humidity as the lowering of vapor pressure caused by ions. This vapor pressure lowering is called the deliquescence. This definition implies the gas phase is holding the maximum amount of moisture it can physically hold. Furthermore, liquid phase solutions on a surface will exist below the deliquescence point.

In the drift environment, relative humidity is estimated for the drift-degradation and no-degradation scenarios using two simple assumptions. The first assumption pertains to the definition of relative humidity above the boiling temperature. The estimate of relative humidity

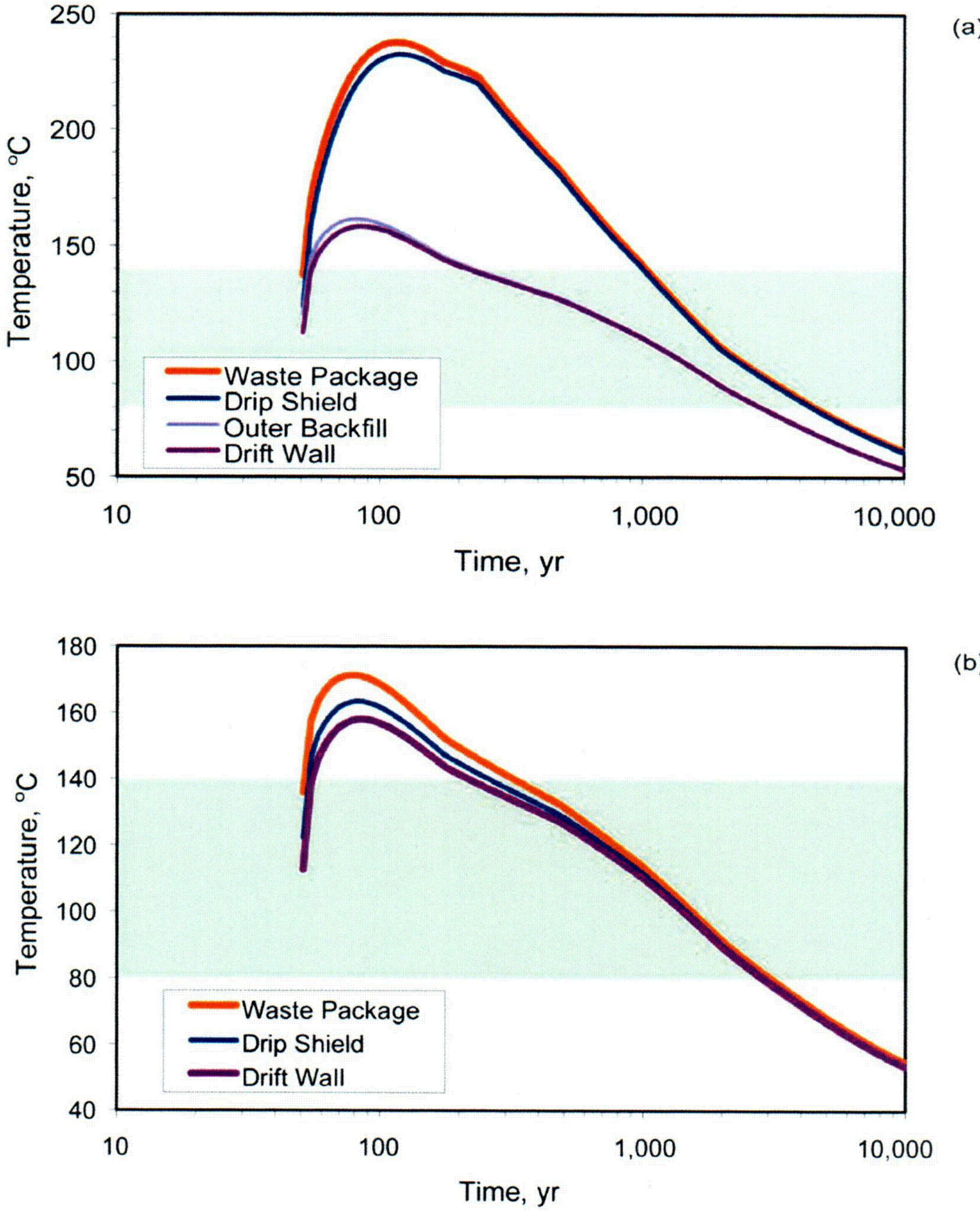

Figure 2-4. Waste Package Temperature Estimates Across the Engineered Barrier Subsystem for the (a) Basecase Drift-Degradation and (b) No-Degradation Scenarios Using Conduction-Only Model Results as the Boundary Condition for the In-Drift Heat Transfer Algorithm. Shaded Areas Mark Zone of Temperature Conditions Conducive to Corrosion [°F = (1.8 × T °C + 32)].

C04

uses a ratio of saturated vapor pressures with the numerator dependent on the temperature at the drift wall. The denominator for this definition of relative humidity is always the saturated vapor pressure at the temperature of the waste package. Saturated pressures of water vapor are approximated here using the Keenan, Keyes, Hill, and Moore formula (American Society of Heating Refrigeration and Air Conditioning Engineers, Inc., 1977). If the temperature at the drift wall is below boiling, the numerator is saturated vapor pressure at the temperature of the drift wall. If the temperature at the drift wall is above boiling, the numerator is the saturated vapor pressure at boiling. Intuitively, this definition of relative humidity is reasonable because at boiling, the relative humidity is 100 percent. Above boiling, no additional water can be added to the gas phase because the vapor pressure should not exceed the total pressure, which remains at the local atmospheric pressure. Hence, the moisture content of the gas phase remains constant for all temperatures above boiling.

For the second assumption, the rubble pile is assumed to contain large open-space voids and thus does not impose a strong capillarity pull on the moisture like a typical porous media. In essence, the rubble pile still allows for a well-mixed gas phase throughout the drift opening. With drift degradation, estimates of relative humidity values are lower and remain lower much longer than those of the no-degradation scenario.

Relative humidity estimates for center and edge locations are plotted in Figure 2-5 for the drift-degradation and no-degradation scenarios. For the no-degradation scenario, the relative humidity values revert to high values (above 80 percent) shortly after closure. Although not accurately represented in the models, the dryout from preclosure forced ventilation will delay the return to high relative humidity values at edge locations by a number of years. The preclosure values of relative humidity for all scenarios should be approximately 5 percent, which is a function of the 30-percent relative humidity of the intake air for ventilation and temperature increases at the waste package. For the drift-degradation scenario, estimates of the relative humidity remain low until beginning to rise at 100 years. The relative humidity rises above the deliquescence lower bound in TPA Version 5.0 code beyond 200 years.

Use of the vapor pressure at boiling temperature to define the numerator for the relative humidity estimate has a theoretical ramification. The balloon analogy indicates that, as the boiling isotherm expands and contracts, there is no exchange of vapor across the boiling isotherm. The volume in the balloon varies, but the pressure inside the balloon does not change. Moisture cannot enter the balloon from outside the boiling isotherm because it would evaporate and return to the reflux zone, thus lowering the temperature inside the boiling isotherm. Another view is that mountain-scale circulation of gas or diurnal pressure fluctuations can induce pressure differences that lead to air exchange. For this second view, there is the potential for lower relative humidity values to occur than those values estimated in the balloon analogy.

2.1.3 Effect of Thermohydrology on Temperature and Relative Humidity Estimates

A linkage of thermohydrological model and the in-drift heat transfer algorithm is used in this report to assess the abstractions used in the TPA Version 5.0 code. Simulating the effects of

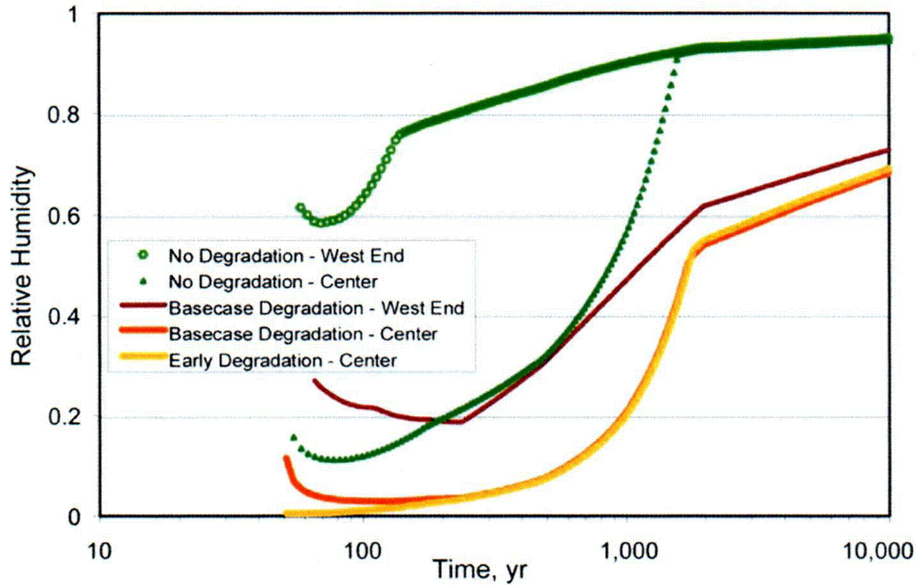

Figure 2-5. Waste Package Relative Humidity Estimates at Center and Edge Locations for the Basecase Drift-Degradation and No-Degradation Scenarios

thermohydrology on estimates of temperature and relative humidity using complex dual-permeability codes cannot directly be used for Monte Carlo simulations using the TPA Version 5.0 code. Use of the conduction-only model in conjunction with the in-drift heat transport algorithm lends itself readily to use in abstracted approaches for stochastic performance assessments. Previously, Manepally and Fedors (2003) evaluated the effect of thermohydrology on waste package temperature estimates by linking a mountain-scale conduction-only model to a detailed process model using MULTIFLO Version 1.5.2 code. The process model was a thermohydrological, dual-permeability representation of the fractured porous media that included the effect of climate change. In this report, instead of using a temperature estimate from a conduction-only model as a boundary condition, a temperature estimate from a two-dimensional thermohydrological model is used for the boundary conditions in the in-drift heat transfer algorithm. The results are shown in Figure 2-6.

Because spatial and temporal variations in water content will affect the thermal properties of the wallrock, the thermohydrological model should provide more reliable temperature estimates. The thermohydrological model is able to account for variations in percolation rates and thermal conductivity. Because the latter is a function of saturation and lithology, it varies in space and time. Both matrix and fracture continua are included in the thermohydrological model. The two-dimensional model is perpendicular to the drift and extends from the drift center to the centerpoint between drifts. The domain extends from the ground surface to the water table, and there is significant grid refinement in the vicinity of the drift. Because the model is two dimensional, it only can provide results at a specified position along a drift. To incorporate the effect of mountain-scale thermal processes, the heat load is scaled for locations based on distance from the center of a drift using results from the mountain-scale conduction-only model. A climate change model is used of modern climate for 600 years, followed by 1,400 years of

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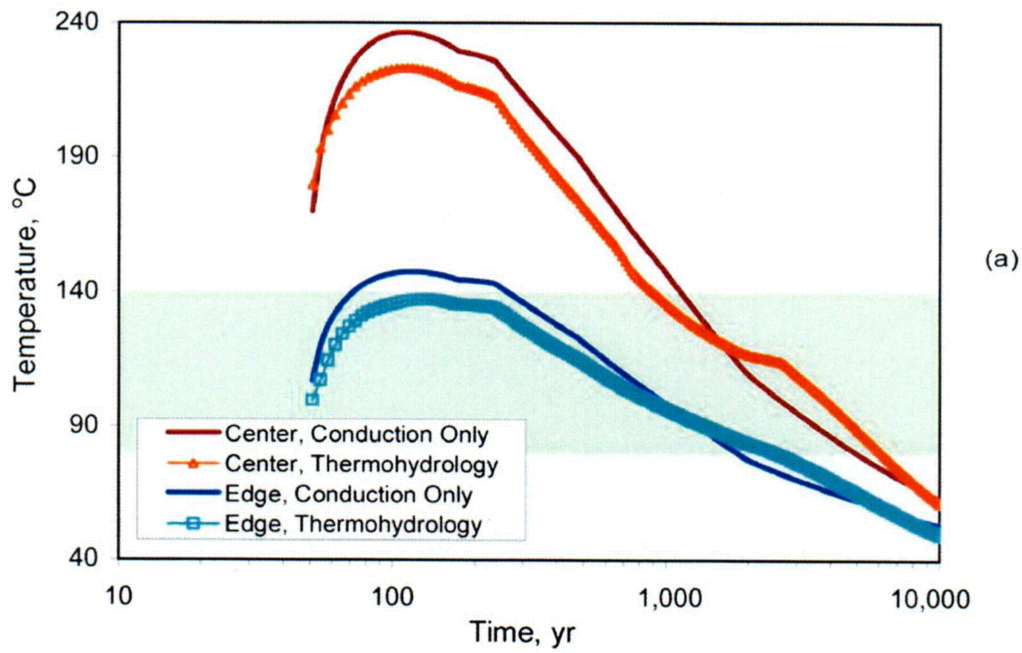

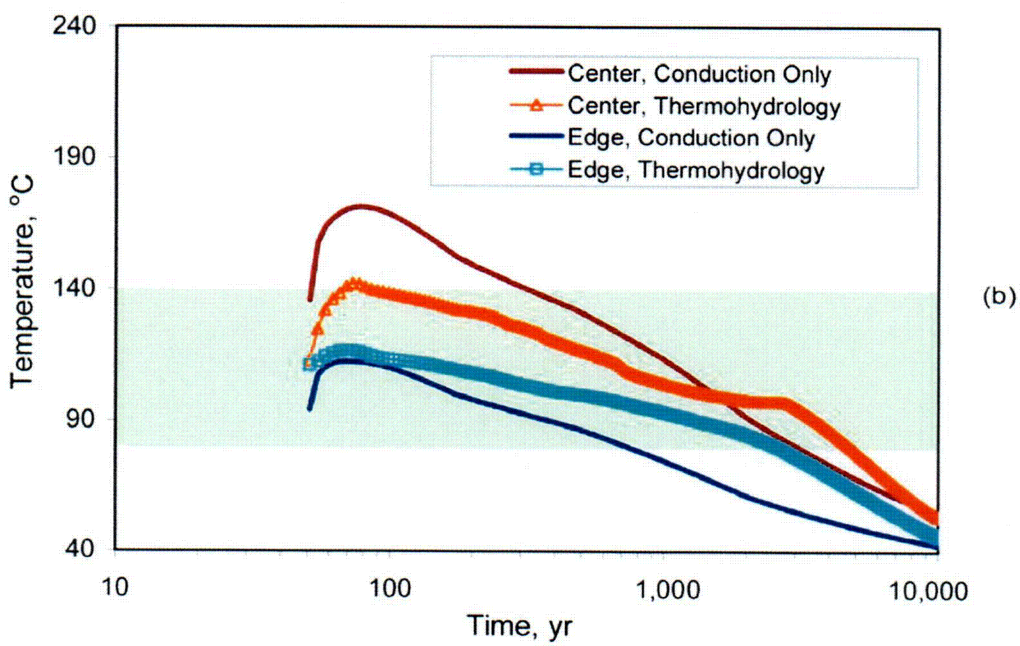

Figure 2-6. Waste Package Temperature Estimates at the Center and Edge of a Typical Drift for the (a) Basecase Drift-Degradation and (b) No-Degradation Scenarios Using Conduction-Only and Thermohydrological Model Results as the Boundary Condition for the In-Drift Heat Transfer Algorithm. Shaded Areas Mark Zone of Temperature Conditions Conducive to Corrosion [°F = (1.8 × T °C + 32)].

C06

monsoonal climate, then a glacial transition climate for the remainder of the performance period. More details about the thermohydrological model can be found in Manepally and Fedors (2003). The temperature estimates of Manepally and Fedors (2003) are used as boundary conditions in the in-drift heat transfer algorithm. The in-drift heat transfer algorithm represents in-drift conduction, convection, and radiation in a more physically realistic manner than the thermohydrological model.

Figure 2-6a illustrates the effect of thermohydrology on waste package temperature estimates for the degradation scenario, and similarly, Figure 2-6b for the no-degradation scenario. Early in the thermal period, the effective thermal conductivity is near the saturated value. As the thermal pulse dries out the wallrock, however, the effective thermal conductivity decreases until approaching the dry thermal conductivity value when the rock is nearly completely dried out. The overprint of climate change is evident in Figure 2-6, particularly for the change to a glacial transition climate at 2,000 years.

Relative humidity in Figure 2-7 is calculated using the temperature estimates at the waste package derived from the in-drift heat transfer algorithm that used the thermohydrological model-derived boundary conditions. Using thermohydrological results, instead of conduction results, for the outer boundary condition in the in-drift heat transfer algorithm leads to a shift in the profile such that a value of 50-percent relative humidity is reach 389 years sooner (488 instead of 877 years) for the no-degradation scenario. The edge location remains above 50-percent relative humidity regardless the source of input for the temperature boundary condition. Because there are large differences in the wallrock and waste package temperature for the degradation scenario, there is little change in the relative humidity profile when thermohydrological results are used in the heat transfer algorithm instead of conduction-only model results.

2.1.4 Onset and Duration of Temperature Conditions Conducive to Corrosion

The onset and duration of waste package temperature conditions in the range 80–140 °C [176–284 °F] are important for determining the potential for localized corrosion of the engineered barrier subsystem. The upper bound for the temperature window of 140 °C [284 °F] is chosen because the corresponding maximum relative humidity would be 24.7 percent, which is approximately the lower bound for deliquescence relative humidity used in the TPA Version 5.0 code (Mohanty, et al., 2002b). The lower bound of approximately 80 °C [176 °F] is chosen based on the suggestion of Dunn, et al. (2003) and Brossia, et al. (2001) that localized corrosion of Alloy 22 is highly unlikely. Because the propagation rate of localized corrosion of Alloy 22 is fast once initiated, the onset time is more important than the duration. Based on parameter values used in the TPA Version 5.0 code, the duration only is important if it is less than approximately 80 years.

Table 2-1 presents results for the basecase degradation and no-degradation scenarios at the center and end of a typical drift in the middle of the repository. The onset and duration of conditions in Table 2-1 are relevant to the waste package environment and are based on an instantaneous emplacement strategy. The drift-degradation scenario leads to a later onset of temperature conditions conducive to corrosion of waste packages, which suggests that emplaced backfill might be an advantageous strategy. Furthermore, when the effect of

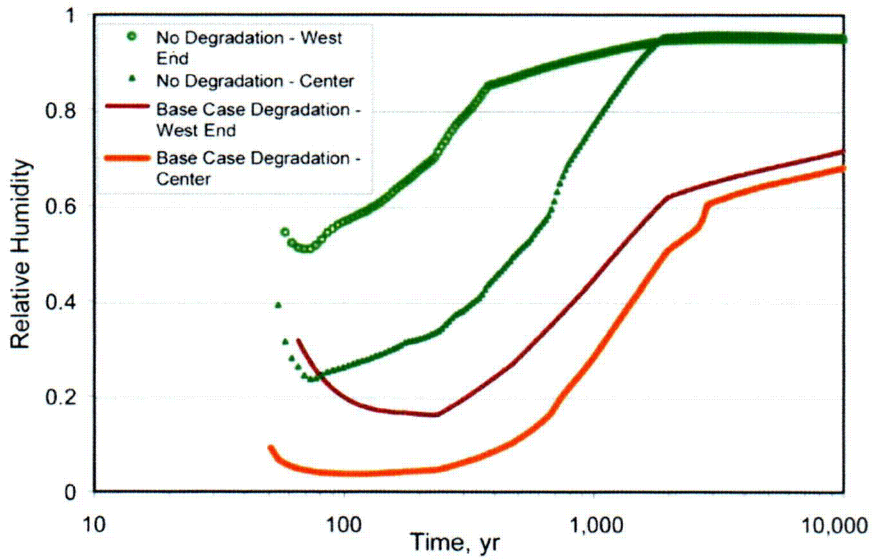

Figure 2-7. Waste Package Relative Humidity Estimates at Center and Edge Locations for the Basecase Drift-Degradation and No-Degradation Scenarios Using Thermohydrological Results As the Boundary Condition for the In-Drift Heat Transfer Algorithm

thermohydrology is incorporated in the heat transfer algorithm, the onset is earlier at the center locations for either scenario than when thermohydrology is not considered.

2.2 Drift-Scale Temperature Gradients in Open Drifts

To evaluate the effect of axial natural convection on temperature and relative humidity estimates, the influence of the porous media needs to be used as input to computational fluid dynamics models of in-drift air flow. Estimates of drift-scale temperature gradients derived from processes acting in the porous media are discussed in this section. Chapter 3 introduces drift-scale modeling of natural convection using computational fluid dynamics models. Only the no-degradation scenario is considered; therefore, the results are relevant for convection in open drifts (e.g., only waste package and drip shield are present).

A model that addresses in-drift and wallrock thermohydrological processes in their entirety is beyond our computational capabilities, except possibly on a small scale. The approach in this section is to evaluate axial gradients using the computationally efficient conduction-only model, and then evaluate the effect on the gradients when the effect of hydrology is included through the use of a three-dimensional thermohydrological model of half a drift.

2.2.1 Gradients Based on Conduction-Only Model

A mountain-scale conduction-only 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

C07

Table 2-1. Onset and Duration of Temperature Conditions Conducive to Localized Corrosion When the Temperature Boundary Condition for the In-Drift Heat Transfer Algorithm Is Based on the Conduction-Only or Thermohydrological Model						
Scenario	Peak Temperature, °C*		Duration of Number of Years within 80 < T °C < 140		Onset Year of Temperature Window	
	Conduction Only	Thermohydrologic	Conduction Only	Thermohydrologic	Conduction Only	Thermohydrologic
Center, No Degradation	171	142	2,751	4,722	325	86
West Edge, No Degradation	113	117	684	2,543	51	51
Center, Basecase Drift Degradation	236	223	3,814	5,403	1131	900
West Edge, Basecase Drift Degradation	146	137	1,395	2,429	232	51
*NOTE: [°F = (1.8 × T °C + 32)]						

cooling effect. The conduction-only model is used to estimate temperatures along a drift located in the middle of the repository. This is the conduction-only model that provided outer boundary condition temperatures for the in-drift heat transfer algorithm in Section 2.1. The effects of drift degradation, thermohydrology, and in-drift heat transfer are not included in the conduction-only model results presented in this section.

The selected drift for these analyses is in the center of the repository, and it is referred to as a typical drift. This analysis focuses on half of a drift because, if there are no variations in lithology, the results for one half would mirror the results of the other half. For the selected drift, the lithology varies in the eastern half of the drift but not in the western half of the drift. The two lithologic units are the Topopah Spring middle nonlithophysal unit in the east and the Topopah Spring lower lithophysal unit 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 drift wall. These representative values of thermal conductivity are the average of the saturated and dry thermal conductivity for each of the lithologies.

The drift wall temperature estimates based on the mountain-scale conduction-only model can be used to evaluate the repository edge cooling effect by analyzing the temperature difference between the center and the edge locations (Figure 2-8a) and the local temperature gradient (Figure 2-8b). Using data only from the eastern half of the typical drift, which includes a change in lithology, Figure 2-8 illustrates the results using the two alternative perspectives on temperature gradients that could affect along-drift convective air flow.

The portion of the drift that exhibits the effect of edge cooling increases with time, although the temperature difference and the local temperature gradient decrease with time. Near lithologic changes, elevated local gradients persist beyond 2,000 years. This persistence suggests that areas near lithologic changes may be zones of elevated axial air flow and condensation.

The portions of the half drift with specific temperature differences (relative to the center location) and specific temperature gradients are plotted as a function of time in Figure 2-9a. A similar analysis for the western half of the typical drift, which has no change in lithologic units, is presented in Figure 2-9b.

The threshold for temperature differences or temperature gradients needed to drive natural convection along a drift is not known, although the magnitude of temperature gradients should correlate with the magnitude of axial air flow rates. Thus, curves are presented for a range of thresholds for temperature differences and gradients. The magnitude of cross-sectional convection that will constrain axial convection is not known. Computational fluid dynamics modeling in Chapter 3 addresses the issue of cross-sectional air flow hindering axial convective patterns. Even using the most stringent threshold presented in Figure 2-9, approximately 30 percent of each half drift will have local temperature gradients potentially capable of driving axial convection and moisture redistribution.

2.2.2 Effect of Thermohydrology on Temperature Gradients

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

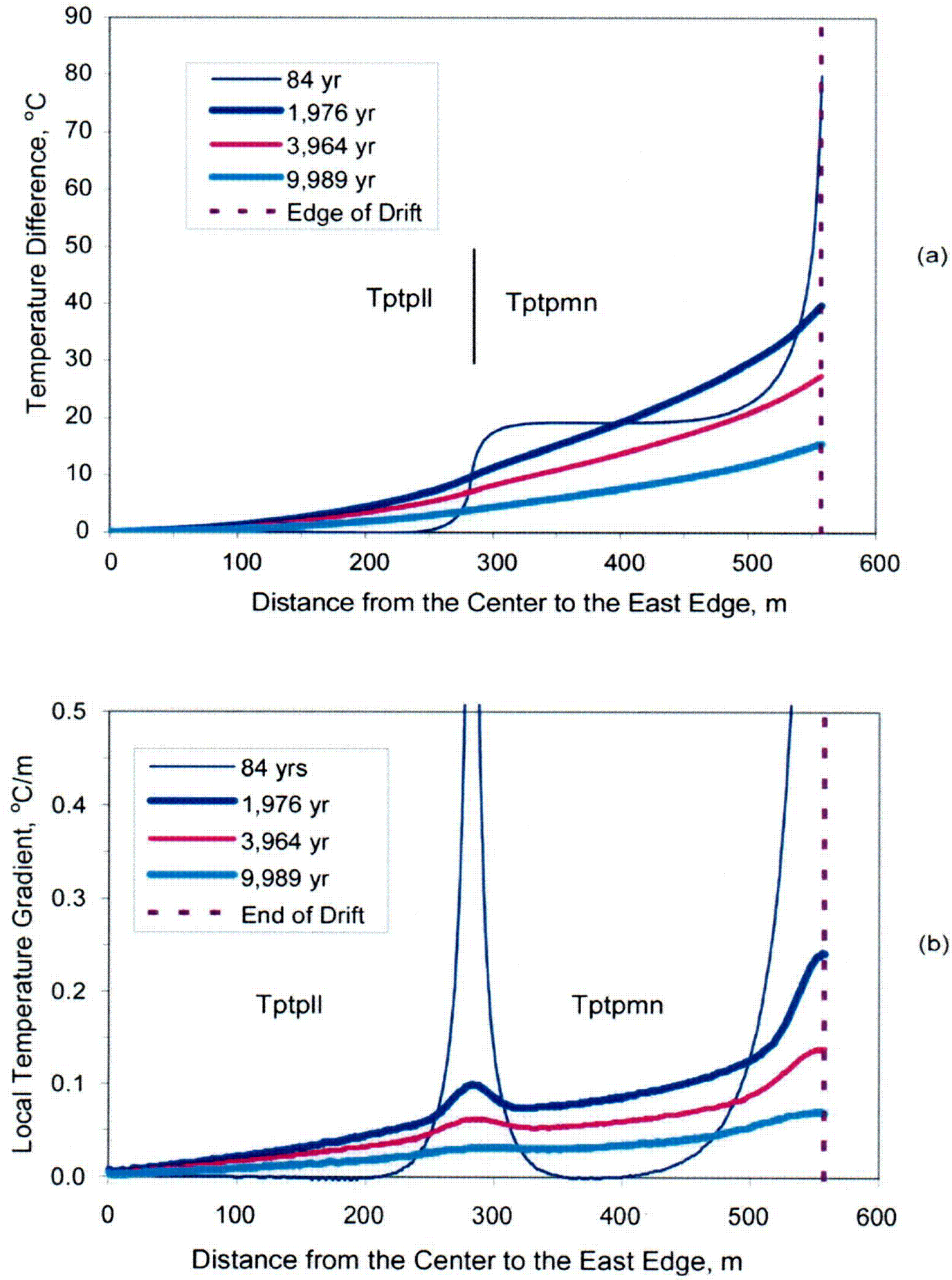

Figure 2-8. Estimated (a) Temperature Differences and (b) Local Gradients Along the Eastern Half of a Typical Drift. The Specified Times Include the 50-Year Preclosure Period [°F = (1.8 × T °C + 32); 3.3 ft = 1; 1.82 °F/ft = 1 °C/m].

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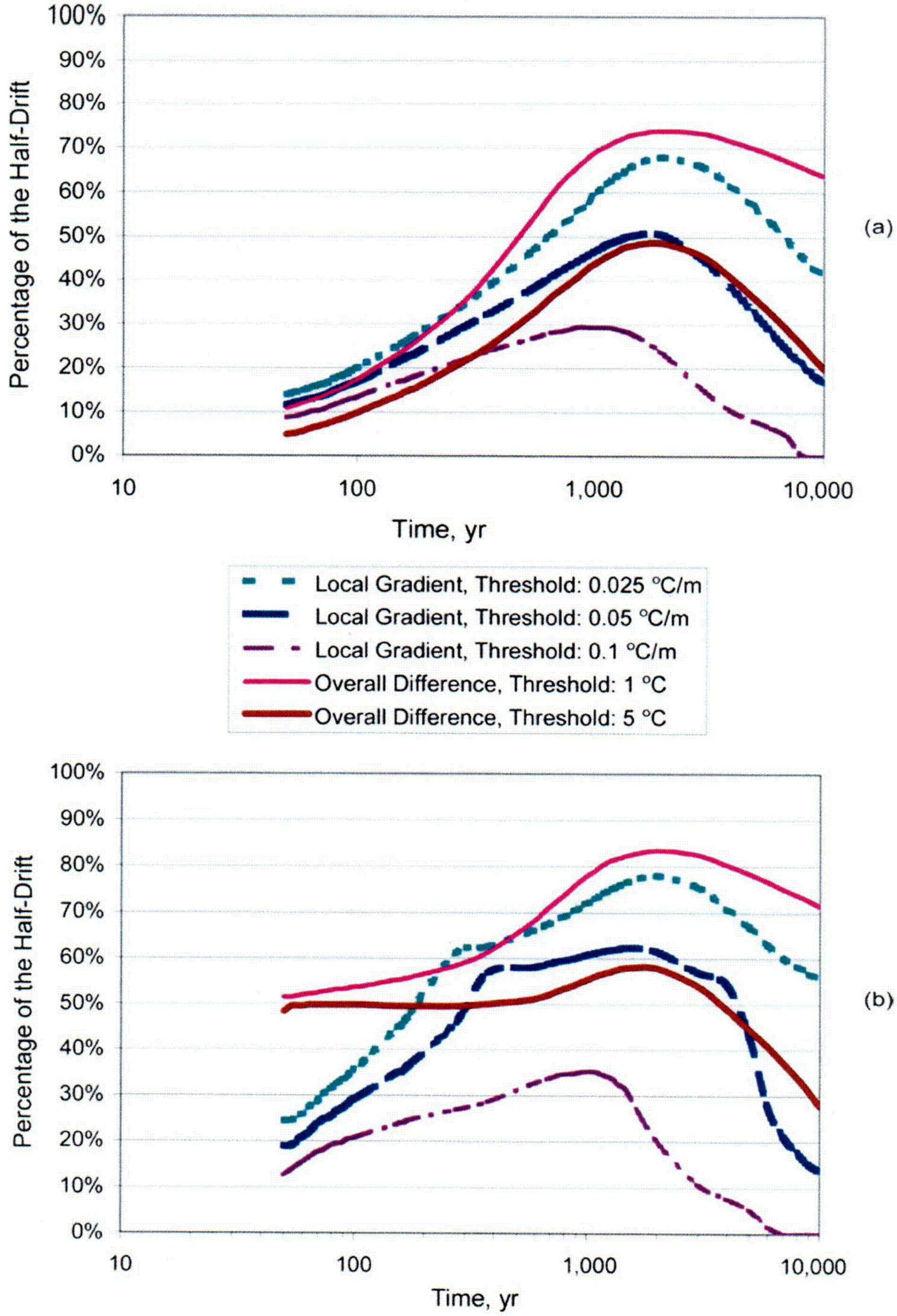

Figure 2-9. Estimated Portions of the (a) East and (b) West Portions of a Typical Drift with Temperature Differences and Local Gradients for the Specified Threshold Values [1 °F/ft = 0.55 °C/m; 1.8 °F =1 °C]

C09

properties can be used to adequately estimate temperature profiles along a drift. Effective thermal conductivity is the most sensitive thermal property needed for the conduction-only model. Because dual-permeability models implicitly account for the variations in thermal conductivity as a function of space and time, they can be used to confirm reasonableness of effective thermal conductivity estimates used in the conduction-only model. Computationally efficient two-dimensional dual-permeability thermohydrological models were developed for selected locations along a drift. Because the assumption of two-dimensional heat transfer becomes more questionable farther from the drift center, a three-dimensional thermohydrological model was developed.

The estimates from conduction-only and thermohydrological models are expected to differ. The conduction-only model uses a constant value for thermal conductivity, whereas the thermohydrological model allows 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. 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. 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. Rewetting 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 Topopah Spring lower lithophysal unit, the wet and dry values for thermal conductivity used in this model are 2.02 and 1.2 W/m-K [28.0 and 16.6 BTU/ft-h-°F].

The three-dimensional model of half of a drift is able to incorporate lateral heat transfer, including hostrock processes of conduction, convection in gas phase, advection in liquid phase, and latent heat transfer. Whereas the two-dimensional thermohydrological model decouples the heat transfer processes from the dimensionality, the three-dimensional model is fully coupled.

The grid for the three-dimensional model is derived from that used in the ventilation study (Painter, et al., 2001). The model inputs were updated to include the TPA Version 5.0 code heat load and the active fracture implementation currently available in MULTIFLO Version 1.5.2 code. The modeled region is a slab that extends from the water table to the ground surface, though the type of boundary conditions used at the top and bottom limit the utility of the grid to early times (500–1,000 years) depending on the heat load and thermal properties. The grid includes one-half of an emplacement drift, thus taking advantage of the east-west symmetry of drifts. Symmetry also is used to reduce the grid domain in the other horizontal dimension by including a region from the center of the pillar between drifts to the center of the drift opening. The grid is unstructured with grid refinement near the drift opening. There is a total of 440 cells for each continua, matrix and fracture in each vertical slice of the grid. Twenty vertical slices comprise 30-m [98-ft] panels along the drift. A value of 10 mm/yr [9.39 in/yr] is used for mass flow at the top boundary. At all sides of the domain, a general temperature boundary condition is used (i.e., temperature is set to a constant value at some specified distance away from the computational domain).

The conduction-only results are compared with results from the two- and three-dimensional thermohydrological models in Figure 2-10. The two-dimensional thermohydrological results, simulated at five separate locations along the drift, were extracted from Manepally and Fedors (2003). The heat load reduction factors used in the two-dimensional model results were based

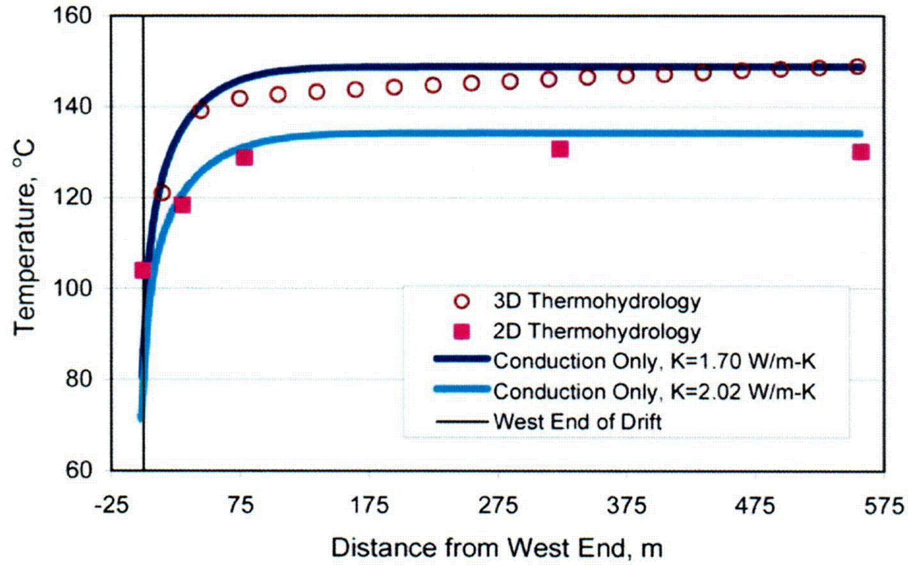

Figure 2-10. Drift-Wall Temperature Estimates from the Two-Dimensional (2D) and Three-Dimensional (3D) Thermohydrological Models Compared with Those from the Conduction-Only Model Using Two Different Values for Representative Thermal Conductivity at a Time of 109.1 Years. Vapor Phase Lowering Was Not Used [°F = (1.8 × T °C + 32); 3.3 ft = 1 m; 1 BTU/ft-h-°F = 13.9 W/m-K].

on conduction-only model results that used a saturated thermal conductivity value. The two-dimensional thermohydrological model results closely match the conduction-only results when the latter used a representative thermal conductivity value of 2.02 W/m-K [28.0 BTU/ft-h-°F], possibly reflecting a self-consistency rather than an accurate indication of the conditions. Two important differences are noted in Figure 2-10. One, the percolation rate of 6.0 mm/yr [0.24 in/yr] at early times in the two-dimensional model leads to temperatures lower than predicted by the conduction-only model. The lower temperature is likely caused by advection of heat in the liquid phase. The other difference is that the two-dimensional thermohydrological results estimate higher temperatures at the extreme end of the drift. This discrepancy may be caused by the no flux (heat and mass) on the lateral boundary of the domain, when clearly there will be some transfer of heat and mass along the axial direction of the drift.

The results of the three-dimensional thermohydrological model presented in Figure 2-10 and overlie the results from the conduction-only model when a representative thermal conductivity value of 1.70 W/m-K [23.6 BTU/ft-h-°F] is used in the latter model. The slope of the temperature profile along the drift for the three-dimensional thermohydrological model results indicates that axial heat transfer in the wallrock is caused by both lateral conduction (edge effect) and spatial changes in thermal conductivity due to changes in saturation along the drift. Other processes that may affect axial heat transfer include one or more of the following: (i) convection in gas phase, (ii) advection in liquid phase, and (iii) latent heat transfer. When the option in MULTIFLO Version 1.5.2 code to include vapor phase lowering is enabled, overall temperatures along the

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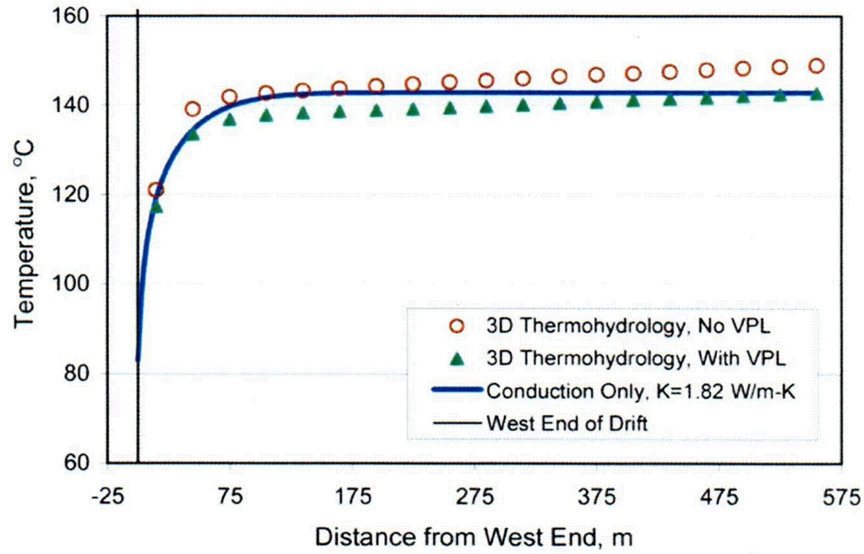

Figure 2-11. Comparison of Drift-Wall Temperature Estimates from the Three-Dimensional Thermohydrological Model with and without Vapor Phase Lowering (VPL) at 109.1 Years [°F = (1.8 × T °C + 32); 3.3 ft = 1 m; 1 BTU/ft-h-°F = 13.9 W/m-K]

drift are reduced (Figure 2-11). When vapor phase lowering is included, an effective thermal conductivity of 1.82 W/m-K [25.2 BTU/ft-h °F] is the appropriate value to use in the conduction-only model to replicate the thermohydrologic effects. It is not known if the difference in results between the conduction-only and thermohydrologic models are important for axial natural convection. Future computational fluid dynamics modeling will be needed to assess the significance of small differences in axial gradients.

2.3 Summary

An in-drift heat transfer algorithm is used along with either a mountain-scale conduction model or a thermohydrologic model to estimate temperature conditions at various locations along a typical drift. Relative humidity is estimated directly from the temperature estimates of the waste package and drift wall using some simple assumptions on the moisture content of the gas phase above and below the boiling point of pure water. The onset and duration of conditions conducive to localized corrosion are estimated for the drift degradation and no degradation scenarios. It was shown that the conditions conducive to localized corrosion {80<T °C<140 [176<T °F<284]} occur much earlier at locations that are not in the center of drifts. Since the TPA Version 5.0 code currently uses the center locations of subareas, its results may not be conservative. The effect of thermohydrology is shown to reduce the onset time and lengthen the duration of conditions conducive to localized corrosion, and therefore, should be factored into performance assessment analyses.

Next, the mountain-scale conduction-only model is used to define portions of a drift that are estimated to exhibit specified temperature gradients. Portions of a drift that exhibit temperature

C11

gradients vary widely with time, but appear to range from 20 to 65 percent during the times of interest for potential localized corrosion of Alloy 22. The uncertainty in the range is directly tied to the uncertainty in the threshold to use for temperature gradients. These estimates of the portion of a drift that exhibit the specified temperature gradient, however, do not include the effect of hydrology. Results from a three-dimensional model simulation using MULTIFLO are provided as a comparison to the estimates of temperature from the conduction-only model. The three-dimensional thermohydrological model accounts for the spatial and temporal variation in effective thermal conductivity. The thermohydrological results indicate a temperature gradient exists along the drift due to the variation in effective thermal conductivity and saturation; this gradient does not occur when using the conduction-only model. It is not known, however, what magnitude of temperature gradient would be important for axial convection and moisture redistribution. Thus, temperature variations along a drift also are developed to support computational fluid dynamics modeling of in-drift air flow and moisture redistribution.

Natural convection will affect temperature profiles along drifts and modify local temperature variations across the engineered barrier subsystem. Estimates of temperature and relative humidity presented in this section did not incorporate these effects. Chapter 3 specifically addresses issues related to natural convection and describes ongoing efforts to develop simulation tools and laboratory data needed to validate those tools.

3 MODELING NATURAL CONVECTION IN HEATED DRIFTS

The primary need for computational fluid dynamics modeling is to help understand the extent and magnitude of axial convection and moisture redistribution along drifts. Moisture movement from wet areas to areas previously dried out by the thermal pulse may elevate the relative humidity sooner than if no convection is considered. In addition, assessing small-scale spatial variations of temperature around the engineered components (e.g., waste packages, drip shields) requires computational fluid dynamics modeling of air flow. In addition, convection around the engineered barriers may be important for assessing the nonuniformity of temperature and relative humidity around waste packages and the drip shield and for assessing the potential dispersion of acidic gases formed from evaporation of concentrated water. These local zones within the complex geometry of the engineered barrier subsystem are not addressed in this report, but will be addressed in future studies.

Individually, natural convection, thermal radiation, conduction, and latent heat-transfer processes are reasonably well understood, however, the combined effects of all heat-transfer processes in geometrically complex environments are poorly understood and difficult to model. Axial drift convection and latent heat transfer 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. The intimate linkage of in-drift natural convection and condensation to heat and mass transfer in the host rock complicates modeling efforts because both porous media and computational fluid dynamics codes may be necessary. The need to understand the combined effect of fundamental processes involved in the movement of moisture driven by convection necessitated developing of laboratory, analytical, and numerical models.

Preliminary drift-scale computational fluid dynamics models are presented in Section 3.1. These models are used to assess two important aspects of natural convection in the heated drifts that, if shown to be unimportant, would simplify the modeling effort.

- Are variations in fluid (air and air plus water vapor) properties expected to significantly influence modeling results?

- At what temperature gradients do cross-sectional flow patterns limit axial convection cells?

In Section 3.2, simulation results are presented for a laboratory experiment using a porous ceramic cylinder surrounded by variably saturated sand to represent a drift located in fractured rock. A temperature gradient inside the drift was induced by placing a heater cartridge at one end of the cylinder and a heat sink at the other end. The variably saturated sand was intended as a source of water for inside the cylinder. This benchtop laboratory experiment has been completed and the final computational fluid dynamics simulation results are presented in this section. Previously, these simulations did not include the effect of phase change and latent heat transfer (Walter, et al., 2004; Fedors, et al., 2003b). This section also presents preliminary information on two other laboratory experiments currently ongoing. One experiment is designed to help understand moisture movement and condensation in a tightly controlled environment. The other experiment more closely matches the geometry of the emplacement drift, but at a 20-percent scale.

3.1 Drift-Scale Simulation with Single Component Gas

The simulation of the flow and heat transfer processes in a full-scale repository drift loaded with waste packages entails large-scale natural convection flow, water phase change at the walls, and thermal conduction in the walls. Temperatures along the drift are estimated to vary widely throughout the life of the repository; so, the gas in the drift can be a highly variable composition of air and water vapor. Before including the effects of evaporation and condensation on the flow field, it is beneficial to investigate the effects of a single component gas in the drift without the complications of the phase change process at the walls.

The first objective of this analysis is to compare the estimated flow velocities and temperature profiles of a repository drift in which the gas is either dry air or pure water vapor. This investigation will reveal the sensitivity of the fluid dynamics and the thermal response of the repository to water vapor concentration.

The second objective is to determine if the gas circulation and temperature vary significantly over a long section of drift. This investigation will reveal whether a full three-dimensional flow simulation is required or the drift can be simulated as independent two-dimensional flow fields in the cross section of the drift.

3.1.1 Drift-Scale Model Description

A 200-m [656-ft] length of drift from a closed end was simulated using FLOW–3D® using a three-dimensional mesh. The drift diameter is 5.5 m [18.0 ft], and a nonporous invert was modeled in the bottom of the drift. Waste packages are individually simulated in the outer 60 m [197 ft] of the drift segment. A line load is used instead of individual heat sources for the inner portion of the drift segment. Waste packages were simulated as 1.8-m [5.9-ft] diameter by 5.1-m [16.7-ft] long cylinders. The waste packages were placed at 6.1-m [20.0-ft] intervals. The waste package power output was specified as 2,150 W [7,338 BTU/h] per waste package, which is appropriate for the time of 109.1 years using TPA Version 5.0 code (Mohanty, et al., 2002b) parameters. A mesh spacing of 0.29 m [0.95 ft] was used near the closed end of the drift, and the mesh spacing expanded to about 3.9 m [12.8 ft] at the opposite end of the drift. A mesh-independence study was not performed, so results should be considered preliminary. The use of a no-flow boundary at the end of the hot end of the mesh is consistent with the attainment of a constant temperature (no edge effect) at this internal position of the drift.

A 1-m [3.3-ft] thickness of rock surrounding the drift was included in the simulation. The temperature at the outer surface of this rock layer was specified consistent with estimates from a conduction-only model using parameters from the basecase TPA Version 5.0 code for 109.1 years. Early in the postclosure period, temperature gradients near the edge of the repository are greater than at later times. Thus, the conditions at 109.1 years may be considered a bounding case for along-drift temperature gradients that drive axial convection. The rock surface temperature 1 m [3.3 ft] outside the closed end of the drift is specified as 80 °C [176 °F] and increases in a nonlinear fashion to 127 °C [261 °F] at a location 200 m [656 ft] from the closed end. The rock surface temperature is assumed to be circumferentially uniform at each axial location.

3.1.2 Drift-Scale Simulation Results

The simulations were run until the overall fluid kinetic energy and thermodynamic energy were varying less than 1 percent, indicating a nearly steady-state condition. The three-dimensional simulation results were processed to provide cross-sectional average values for the gas temperature and volumetric flow rate as a function of distance from the closed end.

The gas circulation rate is computing by integrating the fluid velocity of the cross section for all locations where the gas is moving away from the closed end of the drift. A closed boundary was assumed for these simulations; therefore, at any given cross section along the drift axis, the flow of gas away from the closed end of the drift is balanced by flow toward the closed end. Because a closed boundary is used, the effects of barometric pumping or natural convection through the surrounding fractured tuff cannot be simulated using this model. So, gas circulation rate is the volumetric flow of gas exchanged between volumes on either side of a plane at the specified axial location.

The calculated gas circulation rates for dry air and pure water vapor are compared in Figure 3-1. There are some slight differences between the two sets of results, however, the gas circulation rates for the two gas compositions are in close agreement. The circulation rate is strongest at the closed end of the drift where the gas circulates between the hot waste package and the relatively cooler end wall. The circulation rate decreases with the distance, but the circulation rate does not decrease to an insignificant value until the no-flow end is reached.

The axial fluid temperature profile is shown in Figure 3-2. Similar to the gas circulation rates, this graph shows the average temperature in the drift cross section is virtually identical for both dry air and pure water vapor. The cross-sectional mean temperature varies by only 5 °C [9 °F] along the drift, while the rock temperature increases approximately 47 °C [85 °F] along the drift. This temperature information indicates the gas circulation tends to mix the gas and decrease the effects of the axial variation in rock temperature.

There are axial variations not present from 60 to 200 m [197 to 656 ft] in the circulation rate and fluid temperature for locations less than 60 m [197 ft] from the closed end. These variations are indicative of the mesh expanding in the axial direction away from the closed end. The coarser mesh cannot resolve the geometric details around the waste packages that are greater than 60 m [197 ft] from the closed end. The computational fluid dynamics model in these locations is essentially for a 140-m [459-ft] long cylinder with a heat generation rate per unit length consistent with locations closer than 60 m [197 ft] from the closed end.

Two conclusions may be drawn from these computational fluid dynamics results. For the first conclusion, it is clear the temperature and circulation rates for pure air and water vapor are approximately equal. This implies the details of the gas composition do not strongly affect the overall simulation of fluid dynamics and heat transfer in the drift. The overall temperature and overall gas flow rates do not depend on the precision with which the composition is known. This means that the properties of the gas phase do not have to account for the variations in vapor mole fraction in future modeling efforts. The second conclusion is cross-sectional air flow patterns do not eliminate axial convection for conditions representing a time of 109.1 years in emplacement drifts. As noted earlier, temperature gradients are largest near the ends of drifts at early times. Temperature gradients from distances of 100 to 150 m [328 to 492 ft] are approximately 0.01 °C/m [0.005 °F/ft]. Thus, the conditions at 109.1 years represent a

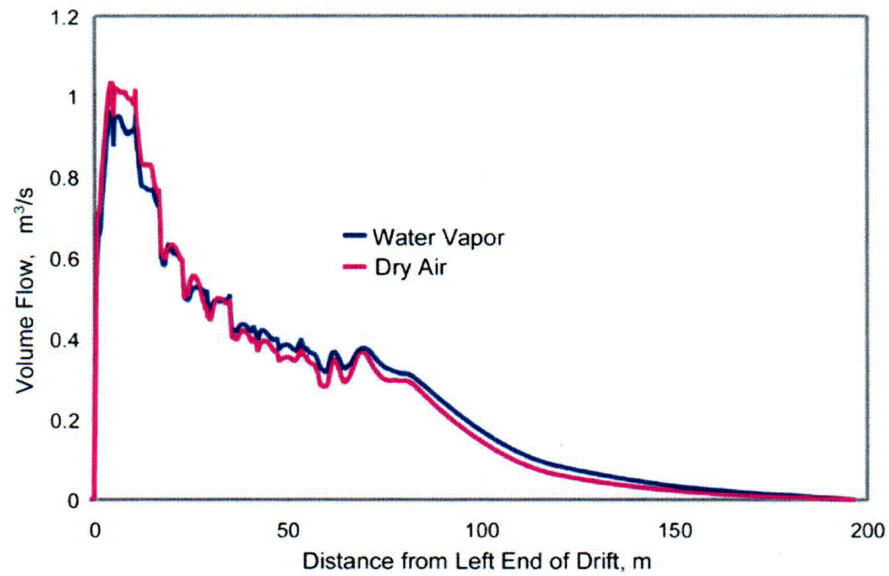

Figure 3-1. Estimated Axial Circulation (Gas Phase) Rate [3.3 ft = 1 m; 35.3 ft^3/s = 1 m^3/s]

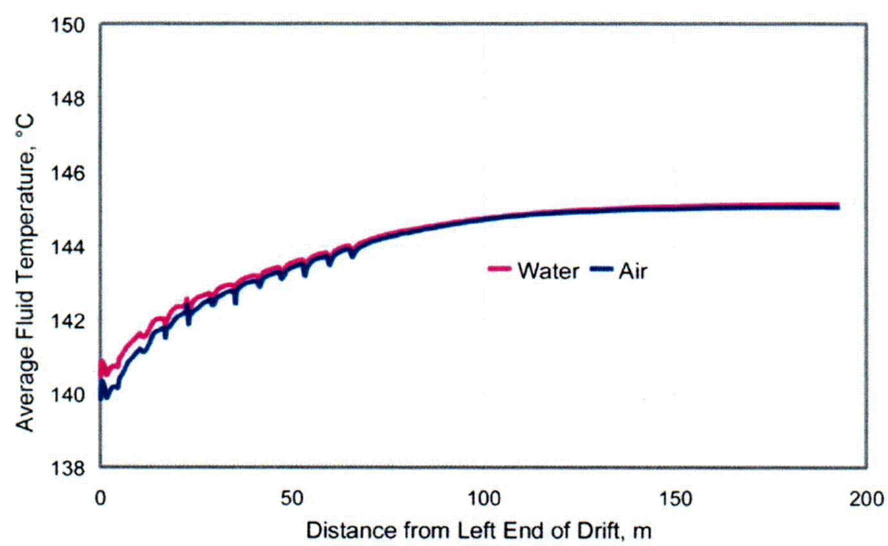

Figure 3-2. Estimated Axial Fluid (Gas Phase) Temperature Profile [3.3 ft = 1 m; °F = (1.8 × T °C + 32)]

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bounding case for evaluating the effect of cross-sectional air flow patterns on axial air flow. The axial flow decreases slightly more strongly than linearly but is significant enough far away from the drift end to modulate the axial gas temperature variation.

3.2 Benchtop Experiment Simulation Results

A small, prototype laboratory-scale experiment was designed, assembled, and conducted to investigate vapor driven air movement and condensate formation induced by the cold-trap effect in a simulated emplacement drift. This 1:100 scale experiment (Figure 3-3) was modeled using a computational fluid dynamics code, FLOW–3D®, in an attempt to further understand the experimental results and to develop numerical modeling techniques that could be used to model larger scale experiments and the full-scale Yucca Mountain waste package emplacement drift. A description of the experiment and FLOW–3D® model inputs and mesh can be found in Walter, et al. (2004) and Fedors, et al. (2003b). This prototype laboratory experiment was useful for identifying numerical model features and property measurement needs to support a larger scale experiment and drift-scale modeling.

The initial modeling effort did not match the experimental results with a high level of accuracy (Fedors, et al., 2003b). One reason identified for the poor match between the model and the experiment was the lack of a phase change model in the computational fluid dynamics code. A phase change model was developed and implemented into FLOW–3D® that accounts for the mass transfer and latent heat transfer associated with the evaporation and condensation of water in the drift (Green, et al., 2004). The laboratory experiment was remodeled using this new model. A comparison of the phase change model results with the previous nonphase change model results is summarized in this section.

The comparison between the two models is made by analyzing the gradient of the average fluid temperature, the total air flow rate, and the net vapor flow rate along the drift. Figure 3-4 shows a comparison of the average fluid temperatures estimated by the two models. These temperature data were generated by calculating the area weighted average fluid temperature at each cross section along the drift axis.

The results show the phase change model had little effect on the temperatures except near the heater. The phase change model lowered the fluid temperatures in the region near the heater. The average temperature throughout the rest of the drift is nearly the same for the two models. Even in the heater region, the phase change model results are only approximately 1 °C [1.8 °F] lower than the nonphase change model results. These results are somewhat unexpected because it was anticipated there would be enough evaporation and, therefore, latent heat loss to lower the air temperatures significantly. These results indicate this latent heat effect, at least for this small-scale experiment, is not significant.

Figure 3-5 shows a plot of the total fluid flow rate and the net vapor transport rate for the two different models. The postprocessing methodology for the total air flow rate is identical for the nonphase and phase change model results. The total air flow is nearly identical for the two models except for the region near the heater, where the nonphase change results are slightly higher than the results from the model with phase change. The fluid flow rate is calculated by summing the product of the axial velocity, area, and density for all cells in each drift cross section. Because the simulations use an incompressible fluid model, the net air fluid flow at

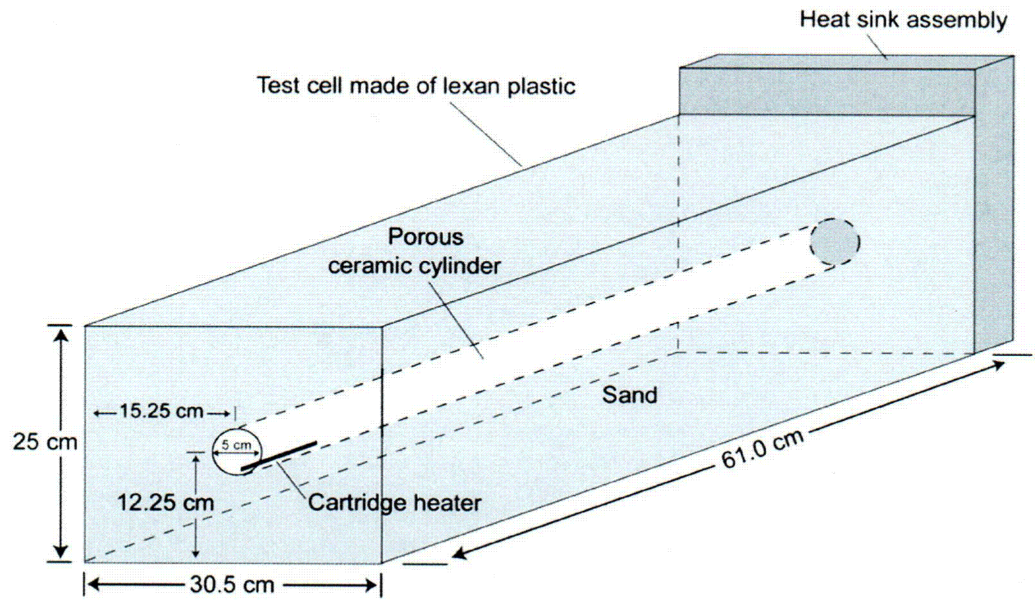

Figure 3-3. Schematic Drawing of Benchtop Cold-Trap Experiment [1 in = 2.54 cm]

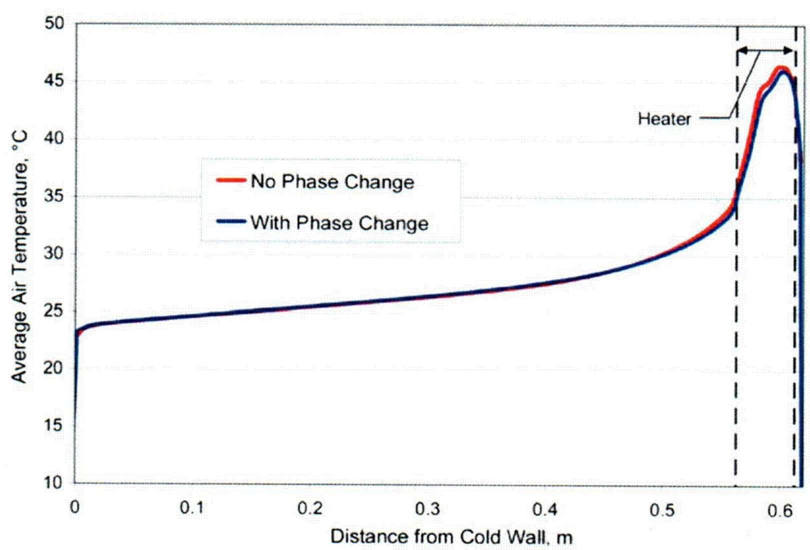

Figure 3-4. Average Fluid Temperatures Estimated with FLOW–3D® Models, with and without Phase Change [3.3 ft = 1 m; °F = (1.8 × T °C + 32)]

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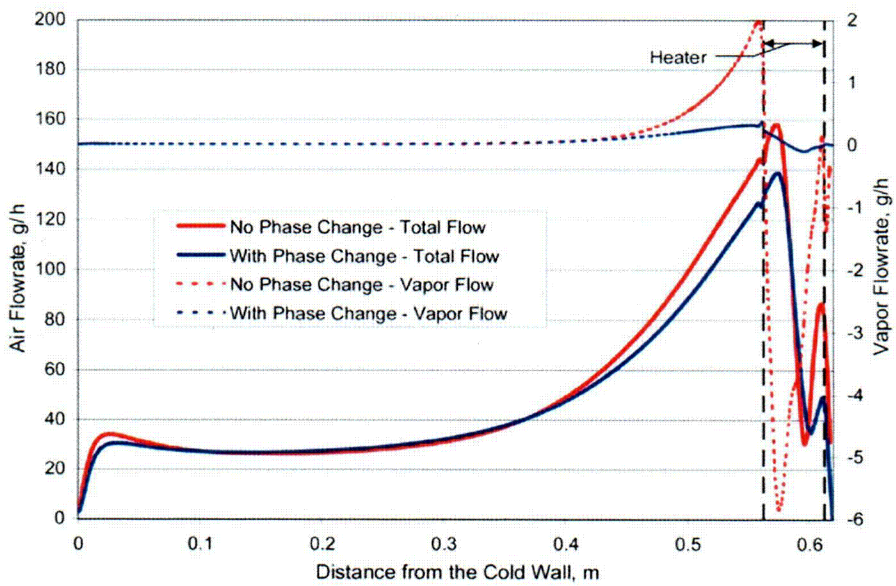

Figure 3-5. Estimated Bulk Air and Vapor Flow Rates Using FLOW–3D®, with and without Phase Change [3.3 ft = 1 m; 1 lb/h = 454 g/h]

each cross section is zero. The fluid flow rates shown in Figure 3-5 refer only to the component of flow moving from the cold wall end toward the heater.

The postprocessing calculations for the net vapor flow rate are unique for the two different models. For the model with nonphase change, the net vapor flow rate is simply the sum of the product of the mass flow rate and the vapor concentration for all cells in each drift cross section. For the nonphase change model, the vapor transport must be inferred from the dry air results. An assumption must be made that all the air in the drift is at saturated conditions, and the latent heat because of evaporation and condensation is negligible compared with the overall heat transfer rate. Assumptions are made that all the air in the drift is at saturated conditions and the latent heat because of evaporation and condensation is negligible compared with the overall heat transfer rate. With these assumptions, the vapor transport is determined by first calculating the saturated vapor concentration of each cell based on the cell fluid temperature. This concentration is then used to calculate the net vapor flow rate in an identical manner to that used for the phase change model results. Because the vapor flow rate is presented as a net value, it describes the difference in transport rates at a particular drift cross section of the moisture traveling both toward and away from the heater.

The total axial flow rate in the plane at the end of the heater is about 10 percent less for the case when phase change is included in the calculations. Variations in the cross sections containing the heater are greater than those away from the heater. At a position of 0.4 m [1.3 ft] from the cold end, however, the total axial flow velocity results are virtually identical for the two models. The net vapor flow rate results show a more significant variation between the two models than the total flow rate. The axial vapor flow rate in the plane at the end of the heater for the phase change case is approximately 15 percent of the case when vapor flow is inferred

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from the air-only calculations. In the heater region, the variation in the two sets of results is even more pronounced. The discrepancy is mainly because the assumption regarding completely saturated fluid is not valid, especially near the heater. These results show that there is much less vapor transport than if a fully saturated assumption is made.

Figure 3-6 further explains this conclusion by showing a contour plot of the relative humidity near the heater (results are from the model with phase change). The plot shows the air entering the heater region from the cold wall end (lower left hand region) is greater than or equal to 100-percent relative humidity. Supersaturated air is allowed in the model for fluid away from solid surfaces. As the heater raises the temperature of the air, the vapor diffusion rate is not adequate to keep the air saturated, thereby, causing the humidity to drop. As the air travels back toward the cold wall, it cools due to natural convection and picks up moisture due to diffusion and evaporation at the drift wall. Because of this prominent nonsaturated region near the heater shown in Figure 3-6, 100-percent relative humidity is not a valid assumption for the nonphase change model.

It is important to note these results and conclusions are based solely on computational fluid dynamics modeling. In this study, no attempt was made to make comparisons to the experimental results, because of the difficulty in matching the measured results described by Fedors, et al. (2003b). The small size (1-percent scale) of the benchtop experiment logistically precluded precise measurements later deemed important for computational fluid dynamics modeling. This prototype laboratory experiment did provide valuable insights to guide the study of convection and the cold-trap process in heated drifts.

These computational fluid dynamics results are adequate to draw two useful conclusions that will be helpful in future computational fluid dynamics modeling efforts. One conclusion, at least for this scale experiment, is the phase change model has little effect on the temperature and a moderate effect on the overall fluid flow. The other conclusion is that if information about the vapor transport rate is necessary, especially in regions where heat is added (like the heater region), the phase change model is necessary because the key assumption required for the nonphase change model is not valid.

3.3 Ongoing Laboratory Experiments

Besides the benchtop experiment described in Section 3.2, two other laboratory experiments are ongoing. These two experiments will provide measured data to support the parameters used in the computational fluid dynamics models. The first experiment is a small condensation cell that intends to provide data for moisture redistribution using a geometry that allows for tight control of conditions, although not necessarily a geometry analogous to the emplacement drifts. The second experiment is an approximate 20-percent scale model of the emplacement drift with up to four analog waste packages providing a heat source in a long pipe. The valuable insights learned from the prototype benchtop experiment guided many of the design features of the 20-percent scale experiment. Both ongoing experiments are briefly described next.

3.3.1 Condensation Cell

Laboratory tests with tightly controlled conditions are designed to validate the water transport models added to the FLOW–3D® computational fluid dynamics code. The code modules were added (with the assistance of Flow Science, Inc.) to simulate water evaporation at a heat source

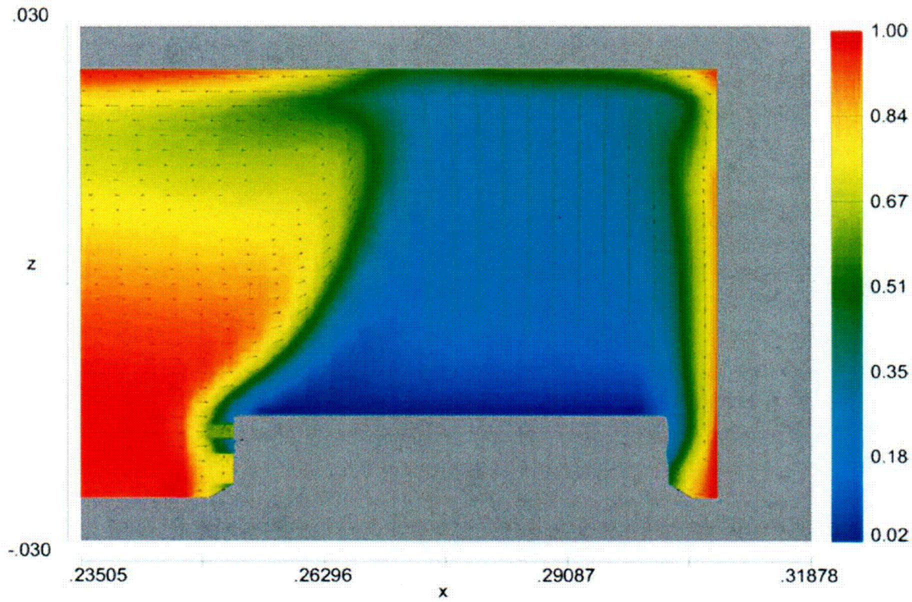

Figure 3-6. Relative Humidity Contour Plot in the Region near the Heater Estimated Using FLOW–3D® with Phase Change [3.3 ft = 1 m]

and water condensation on cool surfaces. Tests are being conducted to measure water evaporation and water condensation rates in a natural convection flow. Comparisons will be made between the measured water transport rates and the rates calculated by the computational fluid dynamics model. Tests are being conducted to measure the amount of water transported from the water source to the condensation plate. It is anticipated three tests will be conducted by varying the heat rate to the water source and measuring the steady-state temperatures and water transport rate.

Pretest computational fluid dynamics model simulations were used to determine the dimensions of the condensation cell to (i) ensure conditions in the cell were amenable to two-dimensional modeling; (ii) determine size of free water surface and power needed to heat that water; (iii) determine the size and operating temperature of the cold plate; (iv) define the operating conditions for testing; and (v) make sure the moisture transport rate would be high enough to be easily measured.

A schematic and photographs of the test rig are shown in Figure 3-7. The enclosure is made of polycarbonate sheet (clear) and aluminum. The cell is 53-cm long, 15-cm tall, and 30-cm deep [23-in long, 6-in tall, and 12-in deep]. Water is condensed and collected on the aluminum plate shown on the left side of the test enclosure. Water evaporates from the pan shown on the bottom-left of the enclosure. Instrumentation has been included to measure the evaporator (water) temperature, condenser temperature, air temperatures, water evaporation rate, and the water condensation rate.

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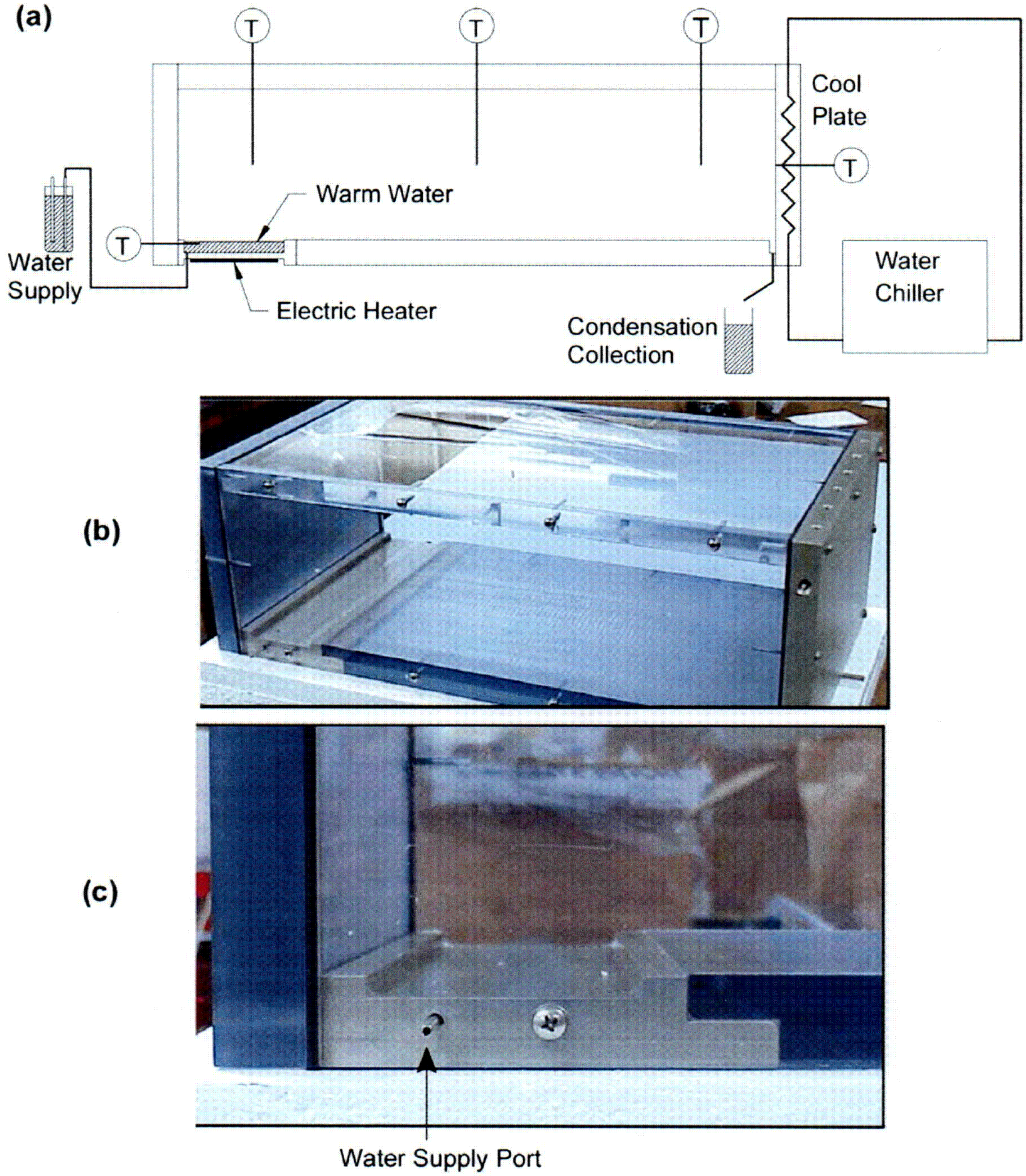

Figure 3-7. (a) Design Schematic of the Condensation Cell. Photographs of (b) Condensation Cell and (c) Water Supply Port and Depression Inside Cell [T = Thermocouple for Measuring Temperature]

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3.3.2 The 20-Percent Scale Experiment of a Drift

This section describes a large-scale laboratory experiment being developed to evaluate processes governing temperature and moisture redistribution in a heated enclosed tube scaled to approximately 20 percent of a proposed emplacement drift at Yucca Mountain. This experiment is not to replicate expected in-drift conditions at Yucca Mountain, but rather (i) develop a fundamental understanding of the cold-trap process and (ii) effectively represent the cold-trap process in numerical models used to simulate in-drift conditions during the postclosure period. Currently, an open-drift design has been implemented to simplify the range of processes occurring in the experiment. As testing proceeds, additional features such as a drip shield and natural backfill can be added.

A comprehensive approach is currently lacking of modeling the cold-trap process at Yucca Mountain and its impact on the performance of the potential repository is currently lacking. As noted by Fedors, et al. (2003b), "... the specifics of natural convection in emplacement drifts and its effects on moisture redistribution have not been sufficiently studied to assess the effect of the cold-trap process on the performance of the repository. Computational fluid dynamics codes are needed to simulate in-drift air-flow patterns, and experimental data are needed to support the numerical models developed using these codes." Fedors, et al. (2003b) further note "sub-scale laboratory models can be an efficient way to help in understanding the cold-trap process and its effect on environmental conditions in heated drifts. Experiments can be used to investigate natural convection heat transfer temperature distributions and air flow in several reduced scale models of a representative drift at Yucca Mountain under postclosure conditions. However, uncertainties in the direct scaling of results from small-scale to large-scale conditions in drifts at Yucca Mountain warrant careful attention."

Fedors, et al. (2003b) describe a bench-scale laboratory experiment designed to examine the cold-trap process and related processes in relation to Yucca Mountain. Their experiment was constructed to approximately 1 percent of the scale of an actual repository drift. Fedors, et al. (2003b) noted the bench-scale laboratory experiment may not adequately represent conditions in emplacement drifts. Two reasons were given: (i) it was not practical to include important details of the engineered barrier subsystem into the experiment, and (ii) considerable uncertainty existed in the scaling of processes and parameters between field-scale and laboratory-scale. Fedors, et al. (2003b) suggest the uncertainty related to scaling may be reduced by performing laboratory experiments at different scales and incorporating this information into numerical models to simulate conditions at Yucca Mountain. Considering the results from the prototype bench-scale laboratory experiment, a decision was made to perform a laboratory experiment at a much larger scale and to incorporate more features representative of Yucca Mountain drifts during the postclosure period.

3.3.2.1 The 20-Percent Drift-Scale Design

The 20-percent drift-scale experiment is currently being constructed and tested. The 20-percent drift-scale experiment was proposed as a means to gain additional insights into the cold-trap process that were not possible with the 1-percent bench-scale prototype laboratory experiment. In addition to its size, the new experiment incorporates an additional feature to replicate waste package heating during the postclosure period. It is assumed inclusion of these scaled features will support understanding the complex air flow and condensation patterns expected at Yucca Mountain during the postclosure period. Four heater canisters are proposed for the experiment to enable uniform and nonuniform heat loads along the pipe. Temperature and relative humidity distributions will be measured during the heating phase of the experiment. Measuring these two parameters will provide valuable insights into the cold-trap process. Although direct measurements of air flow would provide important information in support of the cold-trap process, the accuracy is low of devices available for measuring air flows at the expected low velocities. For this reason, direct measurements of air flow are not currently planned.

The experiment uses a polyvinylchloride pipe closed on each end to simulate the enclosed environment (Figure 3-8a). Because the physical and chemical properties of the pipe differ significantly from those of the repository walls at Yucca Mountain it is obvious the experiment will not serve as an exact analog for Yucca Mountain. The choice of the polyvinylchloride pipe was, in part, governed by the need to reduce complex boundary interactions (e.g., vapor and air diffusion across boundaries and water sorption along bounding walls) that would occur with other materials such as concrete, thereby reducing complex interactions that could complicate understanding the fundamental processes governing the cold-trap process. The internal diameter of the pipe is approximately 1.056 m [41.8 in], the external diameter is approximately 1.125 m [44.3 in], and the length is approximately 6.096 m [20 ft]. The end caps of the pipe are made of 6.4-cm- [0.25-in]-thick low thermal conductivity Lexan to minimize heat loss.

The simulated waste package is scaled to approximately 20 percent of the proposed waste package dimensions for Yucca Mountain. Four such aluminum canisters were constructed. Each canister is approximately 30.5 cm [12 in] in diameter and approximately 0.998 m [39.3 in] in length. Extending internally from one face of each canister is a heating rod. The rod will be heated in the presence of a vacuum in the canister such that the walls of the canister are heated by radiation. Figure 3-8b shows the fabricated canisters. The current design has the canisters aligned end-to-end but not touching and resting on stands.

3.3.2.2 System Monitoring

Temperature and relative humidity will be actively monitored during the experiment. Temperature monitoring will be performed using a series of nested calibrated thermocouples along the surfaces of the canisters, suspended in the air, and along the inner and outer walls of the pipe. The latter combination will support estimation of the heat flux across the pipe boundary. The relative humidity is monitored using a series of sensors placed at specified locations. The locations of the nested thermocouples and relative humidity sensors are based on the computational fluid dynamics simulations performed to date. Figure 3-8c shows some of the thermocouples installed in the pipe.

3.4 Summary

Natural convection will modify temperature gradients along drifts and within the complex engineered barrier subsystem. To assess the effect of natural convection and the associated cold-trap process, computational fluid dynamics simulations and laboratory experiments are being performed.

A three-dimensional drift-scale model of a 200-m [656-ft] drift segment was developed. For temperature gradients along drifts relevant for a time of 109.1 yrs, drift-scale computational fluid dynamics modeling concluded that axial air flow will occur in spite of strong cross-sectional air flow patterns. Although this indicates that further modeling is needed to assess the effects of

(a)

(b)

(c)

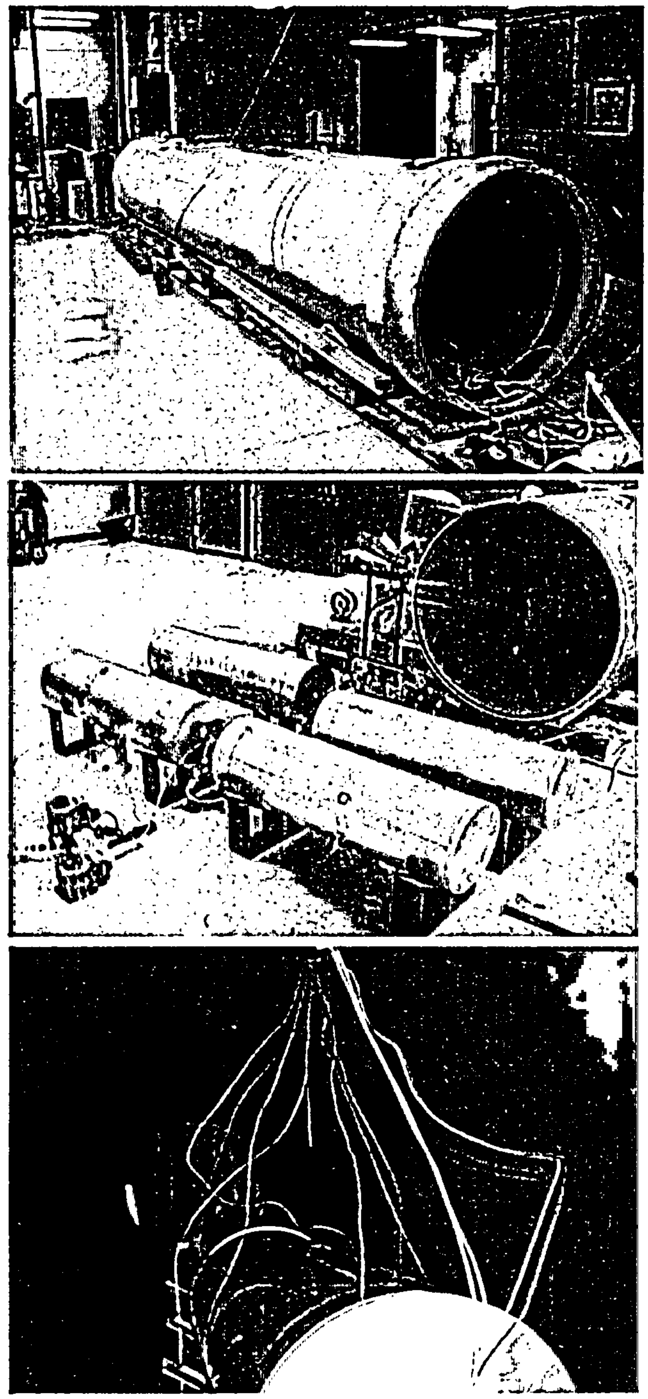

Figure 3-8. Photographs of the 20-Percent Drift-Scale Natural Convection and Cold-Trap Laboratory Experiment with (a) Polyvinylchloride Pipe, (b) Four Analog Waste Packages and Stands, and (c) Waste Packages Inside Pipe with Thermocouples for Preliminary Testing

axial convection and the cold trap process, it also indicates that two-dimensional cross-sectional models should not be used unless a new approach is developed to account for the three-dimensional effects. The three-dimensional computational fluid dynamics simulations also suggest that axial convection will occur along a line of uniformly heated waste packages when temperature gradients are as low as 0.01 °C/m [0.005 °F/ft]. Furthermore, it is shown that the variation in gas phase properties due to variations in moisture content need not be considered in future computational fluid dynamics modeling efforts.

There is no relevant measured data in the scientific literature to support models of air flow and moisture redistribution in heated tunnels. Thus, a prototype benchtop laboratory experiment was developed as previously described (Fedors, et al., 2003b). The benchtop experiment is a one-percent scale model of the proposed drifts for Yucca Mountain. In the previous modeling effort, the computational fluid dynamics simulations of the benchtop experiment did not include latent heat transfer. A module that includes evaporation, condensation, and latent heat transfer was linked to FLOW–3D® as described in Green, et al. (2004). Simulations with and without the moisture module illustrate the difference in vapor flow between the approaches. Results obtained using the moisture module better represent the expected relative humidity near the heat source. The low values of relative humidity near the heat source invalidate the assumption used prior to implementation of the moisture module.

Two ongoing laboratory experiments are expected to provide measured data to support computational fluid dynamics modeling of natural convection and cold-trap process. The first one is a tightly controlled condensation cell designed to validate the moisture module added to FLOW–3D®. The second ongoing laboratory experiment is a 20-percent scale model of a drift segment with four geometrically scaled waste packages. This second experiment is designed to provide data that is relevant to the geometry of the emplacement drifts. Drift degradation was not included in the design of the 20-percent experiment to simplify the experiment, although flow blockage above a drip shield may be an added feature for additional test phases. Both experiments are currently in the testing and data collection phase. As a result, no data are presented in this report.

4 CONCLUSIONS

Environmental conditions along a typical drift were estimated using an in-drift heat transfer algorithm with either a mountain-scale conduction model or a thermohydrological model being used to determine the temperature boundary condition in the wallrock. The onset of conditions conducive to localized corrosion of Alloy 22 for the drift-degradation and no-degradation scenarios occurs much earlier at locations that are not in the center of drifts. Since the TPA Version 5.0 code currently uses the center locations of subareas, its results may not be conservative. Also, the effect of thermohydrology is shown to reduce the onset time of conditions conducive to localized corrosion, and therefore, should be factored into performance assessment analyses.

The computationally efficient mountain-scale conduction-only model was used to define portions of a drift that are estimated to exhibit specified temperature gradients. Portions of drifts exhibiting specified temperature gradients exceed 30 percent. The magnitude of temperature gradients important for driving natural convection, however, is highly uncertain. Sensitivity analyses for different magnitudes of temperature gradients were provided to illustrate the effect on estimates of the portions of a drift. Preliminary drift-scale computational fluid dynamics modeling of convection suggests temperature gradients producing axial air flow approach the lowest values used in the sensitivity analyses. Since the conduction-only model does not include the effect of hydrology, results from a three-dimensional simulation using MULTIFLO are provided as a comparison. The thermohydrological results indicate a temperature gradient exists along the drift due to the variation in effective thermal conductivity and saturation; this gradient does not occur when using the conduction-only model. Temperature variations along a drift were also developed to support computational fluid dynamics modeling of in-drift air flow and moisture redistribution. Temperature gradients along drifts for the drift-degradation scenarios were not calculated, but may be inferred from temperature differences between the repository center and edge. During the temperature range of interest for localized corrosion, the temperature differences along degraded drifts are only slightly greater than those in open drifts. Heterogeneity of drift degradation, however, has the capability of significantly modifying axial temperature gradients and, thus, will be the focus of a future study.

Modeling of natural convection and the cold-trap processes in thermally perturbed drifts requires the use of computational fluid dynamics codes and measured data for validation of said models. Preliminary results of drift-scale modeling indicates that axial convection in drifts will be present in spite of strong cross-sectional flow patterns. Furthermore, it was shown that parameter inputs for the properties of the gas phase need consider the variation in moisture content across and along the drifts. While the first conclusion indicates that three-dimensional computational modeling (rather than two-dimensional cross-sectional modeling) is required, the second conclusion greatly simplifies the modeling effort. Two ongoing laboratory experiments, a condensation cell and a 20-percent scale model, are expected to provide data to support the assessment of natural convection and the cold-trap process. Drift degradation will not be incorporated into the computational fluid dynamics simulations until the simpler case of an open drift can be adequately simulated.

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