Coupled Hydrothermal-Ventilation Studies for Yucca Mountain
Annual Report For April 2002—March 2003

NWRPO-2003-05

Prepared for
Nye County Department of Natural Resources and Federal Facilities,
Nuclear Waste Repository Project Office, Grant No. DE-FC28-02RW12163

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December 2003

DISCLAIMER

EXECUTIVE SUMMARY

This annual report summarizes the results of the coupled hydrothermal-ventilation studies conducted to support the evaluation of the design and performance of the high-level radioactive waste repository at Yucca Mountain, Nevada. This work was performed for the Nye County Nuclear Waste Repository Project Office during the period of April 15, 2002 through March 31, 2003 by Dr. George Danko, Professor, University of Nevada, Reno. Dr. John Walton, Professor, University of Texas at El Paso, also under contract to Nye County, provided an independent numerical code verification test problem and results and performed technical review of the work.

The following three independent tasks were performed:

- Task 1: A numerical verification test of the correctness of the coupled hydrothermal-ventilation model and software MULTIFLUX (2003).
- Task 2: A numerical study of temperature and relative humidity variations with time and location in a proposed, conceptual, high-level nuclear waste repository at Yucca Mountain.
- Task 3: A numerical study of relative sensitivities in the critical temperatures and relative humidities with respect to site properties and other input characteristics.

TASK 1

The purpose of Task 1 was to compare MULTIFLUX results with known analytical solutions to a quasi-three-dimensional convection-conduction ventilation problem. Four solutions were compared, as follows:

- A MULTIFLUX calculation with the Lawrence Livermore National Laboratory flow and transport rock-based software model NUFT (2000), using 137 time divisions.
- A MULTIFLUX calculation with a rock model applying an analytical-based, Carslaw and Jaeger (1986) reference solution with first-kind boundary condition and 35, 69, and 137 time divisions.
- An approximate, analytical calculation using a Carslaw and Jaeger (1959) solution with third-kind (i.e., convective) boundary condition, superposition, and numerical integration with 500 time divisions.
- A reference calculation generated by John Walton, Professor, University of Texas, El Paso, using the same Carslaw and Jaeger (1959) analytical solution without numerical integration. This analytical solution is assumed to be the most accurate solution.

A comparison of the four solutions showed excellent agreement. It was therefore concluded that the MULTIFLUX software was capable of correctly modeling the time-dependent, coupled convection-conduction problem without moisture.

TASK 2

The purpose of Task 2 was to analyze temperature and relative humidity variations in a conceptual, ventilated nuclear waste repository at Yucca Mountain. The drifts were assumed to be mechanically ventilated for 25 years with a forced, constant air flow rate of 15 m^3/s for 25 years, then ventilated from year 25 until year 300 under natural buoyancy pressure driving force through an open system and, finally, naturally ventilated by air infiltration through backfilled intake and exhaust shafts and tunnels from year 300 until year 5,000. The hydrothermal-ventilation software MULTIFLUX provided balanced results for air, heat, and moisture flows. A balanced solution between the pressure loss and pressure gain due to buoyancy was achieved in 15 total system iterations. The natural ventilation was found to adequately keep temperatures below boiling for the 25- to 300-year time period. The air flow rate decreased only moderately when the fans were removed in year 25. The backfill of the access shafts and tunnels at year 300 decreased, but did not eliminate, natural ventilation that is beneficial to controlling temperatures and relative humidities. The trend of the post-closure natural air flow rate variation with time indicated that natural ventilation may continue for much longer time periods. The relative humidity levels were found consistently lower than those expected in some of the current corrosion and performance assessment studies at Yucca Mountain.

TASK 3

The purpose of Task 3 was to study the sensitivity of temperatures and relative humidities to the variation of selected input properties and ventilation parameters at Yucca Mountain. The perturbed site input properties included rock heat conductivity, thermal diffusivity, and heat transfer coefficient on the drift surface. The ventilation air flow rate, input air temperature, areal thermal heat load, and average water percolation rate due to precipitation were also varied as input parameters. The temperatures and heat removal rates by ventilation were found to be most sensitive to the thermal conductivity, exceeding 100 percent at low ventilation rate. This finding underlines the importance of the thermal conductivity values for Yucca Mountain, since any input percentage error in conductivity may affect the predicted temperature fields by a higher percentage error. High sensitivities were also obtained to the intake air temperature, underlining the importance of studying seasonal temperature and possible future climate changes in the repository design.

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ACRONYMS AND ABBREVIATIONS

ρ	density
α	thermal diffusivity
°C	degree centigrade
AFR	air flow rate
AMR	analysis model report
ATL	areal thermal load
BSC	Bechtel SAIC Company, LLC
c	specific heat
CFD	computational fluid dynamics
CJ	Carslaw and Jaeger
DOE	U.S. Department of Energy
h	heat transfer coefficient
J	joule
K	degree Kelvin
k	thermal conductivity
kg	kilogram
m	meter
MF	MULTIFLUX
MTU	metric tonne of uranium
NTCF	numerical transport code functionalization
NUFT	non-equilibrium unsaturated-saturated flow and transport
NWRPO	Nuclear Waste Repository Project Office
PA	performance assessment
Pa	pascal
p_{sat}	saturated vapor pressure
p_v	partial vapor pressure
REKA	rapid evaluation of K and alpha
S	second
UNR	University of Nevada, Reno
W	watt
YM	Yucca Mountain

1.0 INTRODUCTION

The Nye County Nuclear Waste Repository Project Office (NWRPO) is independently evaluating the conceptual design of the Yucca Mountain (YM) high-level radioactive waste repository currently being developed by Bechtel-SAIC Company, LLC (BSC) for the U.S. Department of Energy (DOE). One major NWRPO interest is the use of ventilation in the repository design to enhance performance and thereby minimize long-term health and environmental impacts to southern Nye County. The NWRPO is specifically interested in the potential use of ventilation to keep repository temperatures below 100 degrees centigrade (ºC) and relative humidity below 100 percent, and to identify the safest, smallest portion of the mountain for long-term isolation of the nuclear waste.

The NWRPO, other stakeholders, and numerous independent reviewers believe that keeping repository temperatures below 100 ºC and relative humidity below 100 percent can reduce uncertainties in performance assessment (PA) models, improve the safety case, and ultimately benefit citizens living downgradient of YM. Many of these same entities believe that minimizing the total storage area will help ensure that waste is emplaced in the most stable, and therefore safest, area available.

Since the mid-1990s, the NWRPO has conducted independent modeling studies to analyze the feasibility and potential benefit of long-term ventilation (NWRPO, 2001). From April 2002 to March 2003, Nye County contracted the University of Nevada, Reno (UNR) to conduct hydrothermal-ventilation modeling using a code called MULTIFLUX (MF) (MULTIFLUX, 2003). This annual report describes the work performed.

MF was developed at UNR and applies the non-equilibrium, unsaturated-saturated, Lawrence Livermore National Laboratory flow and transport rock-based software model (NUFT) as a module for simulating heat and moisture flows in the rock domain (NUFT, 2000), and a computational fluid dynamics (CFD) module for the simulation of transport processes in the airway system, including the waste packages. The two modules are coupled on the rock-air interface until the heat and moisture flows are balanced at the common surface temperature and partial vapor pressure at each surface node and time instant. In case of natural ventilation, MF also balances the air flow rate, iteratively equating the pressure loss through the system with the buoyancy driving pressure difference caused by differences between the intake and exhaust air temperatures. For integrated pre- and post-closure hydrothermal simulations, MF applies a three-dimensional, combined canister- and mountain-scale rock mass model, based on NUFT. A detailed description of MF is presented in Section 3.2.

MF has been designed to avoid many of the limitations of the DOE hydrothermal-ventilation modeling approach. For example, the ventilation model used by BSC includes dry, conduction-only processes (BSC, 2002). In addition, the BSC model can assume only line-averaged heat load during pre-closure. Therefore, the BSC model cannot be used to study localized hot-spots due to individual, high heat-load waste containers. This modeling deficiency may be detrimental to evaluating necessary blending and/or waste aging.

The first NWRPO task with MF was a code verification activity designed to demonstrate MF's capability to accurately solve a time-dependent, coupled convection-conduction problem. Section 2.0 summarizes this code verification activity, which showed that MF modeling results closely matched those obtained from a known textbook analytical solution. Section 3.0 describes a 5,000-year MF hydrothermal modeling analysis to evaluate the effects of forced and natural ventilation on repository temperatures and humidities, assuming a conceptual high-heat-load repository design. Section 4.0 describes a numerical study of relative sensitivities of critical temperatures and relative humidities to selected site properties and other input characteristics.

2.0 COMPARISON OF MULTIFLUX AND ANALYTICAL SOLUTIONS IN A CONVECTION-CONDUCTION PROBLEM (TASK 1)

The purpose of Task 1 was to compare MF results with known analytical solutions to a quasi-three-dimensional convection-conduction ventilation problem. The method compared solutions to the test problem that used MF (i.e., Solutions 1 and 2) with analytical-based solutions that did not (i.e., Solutions 3 and 4). Solution 4 is assumed to be the most accurate, correct, or true solution.

- Solution 1: MF calculation with a NUFT-based rock model (NUFT, 2000) and 137 time divisions.
- Solution 2: MF calculation with a rock model, using an analytical-based reference solution (Carslaw and Jaeger [CJ], 1986) with a first-kind boundary condition and 35, 69, and 137 time divisions.
- Solution 3: Approximate, analytical calculation using a solution (CJ, 1959) with a third-kind, convective boundary condition, superposition, and numerical integration, and 500 time divisions.
- Solution 4: Reference calculation generated by John Walton, University of Texas, El Paso, Texas, using Solution 3 (CJ, 1959) but without numerical integration. This solution is assumed to be the reference standard by which to judge the accuracy of the others.

2.1 Problem Description

The test case, a convection-conduction problem, is shown on Figure 2-1 and presented in Appendix A. Rock and air properties assumed for this test case are summarized in Table 2.1. This problem was a quasi-three-dimensional heat transfer problem with no moisture involved. Air flowed in the positive y direction along a duct that was 500 meters long. The air entered the duct at 21 ^{o}C and flowed at a rate of 0.1 kilograms per second (kg/s) over a 1-meter (m) section in the z direction. The air was in convective contact with the solid wall; the other boundaries were insulated. The solid, representational rock was assumed to be anisotropic with a thermal conductivity of 2 watts per meter per degree Kelvin (W/m/K) in the x direction and zero thermal conductivity in the y direction. The initial temperature of the rock was 20 ^{o}C. The heat transfer coefficient was 2 W/m^{2}/K on the air-rock interface. The thermal diffusivity in the rock was 0.85 x 10^{-6} m^{2}/s. The specific heat of the air and water were 900 and 1,000 joules per kilogram per degrees Kelvin (J/kg/K), respectively. The simulation time was 0 to 3 years. The rock was infinite in the x direction; however, for the assumed parameters, the rock appeared infinitely thick as long as the thickness was greater than 40 m. Heat conduction in the z direction was not modeled. Adiabatic boundary conditions were present around the rock domain except for the air-rock interface.

Heat-conduction rock models were used in each of the solutions identified in this section. In Solution 1, MF used NUFT Version 3.0s in the rock domain for modeling heat and moisture transport, a predominantly heat-conduction process. The NUFT input parameters are summarized in Table 2-2.

Solutions 2 through 4 in this section used rock models based on CJ analytical solutions (1959 and 1986). The input parameters for these rock models corresponded to those found in Table 2.1.

2.2 Approach

Details of a required preliminary inverse solution, plus Solutions 1 through 4, are described in the following.

- Preliminary Solution: The purpose of this solution was to justify the use of porous media input parameters for approximating a conduction-only material. An inverse modeling technique (Danko et al., 2002) was used. The thermal properties shown in Table 2.2 were used in a 3-by-3-by-9-m^3 block, modeled using NUFT Version 3 with a dual porosity option. The qualified rapid evaluation of K and alpha software (REKA) Version 1.1 (REKA, 2001) was used to identify the thermal conductivity and diffusivity of the block based on the NUFT simulation. The REKA evaluation software is based on matching a measured temperature field generated by a probe's heater with a conduction-only model solution. The REKA results are shown in Table 2.3.

- Solution 1: The coupled convection-conduction model was solved using MF and applying the NUFT rock model. The following steps were taken to accomplish the task.

  Step 1: The NUFT rock model was configured for the geometry of this test case, shown on Figure 2-1. Since the model is adiabatic in all directions except in the x direction, a one-dimensional rock model was applied to determine rock-model numerical transport code functionalization (NTCF) matrices. Further details regarding NTCF matrices are presented in Section 3.2.2. The NUFT input deck is presented in Appendix B.

  Step 2: The input deck was prepared for the NTCF module of MF. This input file is presented in Appendix C. The NTCF input deck was described in detail in the software documentation. In order to determine a start-up boundary temperature, an approximate CJ solution was used. It will be demonstrated herein that the start-up assumption is ambivalent to calculation precision in this linear case. The CJ macro used (i.e., MATLAB) is presented in Appendix D. The MF directory structure was set up in accordance with the software documentation and the medium-level NTCF module nmain2d.m was executed in order to obtain the NUFT rock-model NTCF matrices required by MF.

  Step 3: The CFD model of MF was configured using the macro utility presented in Appendix E.

  Step 4: The MF coupler configuration files were prepared and MF was executed.

- Solution 2: Another rock model based on an analytical solution given in CJ (1986) for a first-kind boundary condition was used to generate another MF solution. The MATLAB macro (Appendix D) was used to calculate the NTCF matrix according to the CJ analytical solution. The NTCF rock matrices are the only new components in this solution.

- Solution 3: An approximate analytical-numerical solution to the test problem, based on the 1959 CJ analytical solution described in Solution 4, applied a third-kind boundary condition with superposition and numerical integration along the air flow direction. This approximate solution was used for auxiliary comparisons only.

- Solution 4: This solution was a 1959 CJ analytical solution for heat conduction into a semi-infinite domain with a convection heat-transfer boundary condition and an arbitrary time-variant boundary condition. This analytical solution is assumed to be the most accurate of the four and the reference standard for determining the accuracy of the others. The details of this solution are presented in Appendix F.

2.3 Results and Discussions

As shown in Table 2-3, inverse-evaluated properties from NUFT agreed closely with the desired conduction-only properties.

Figures 2-2 and 2-3 show temperature distributions in time and space for the air and rock surfaces based on the NUFT rock model in Solution 1. Figure 2-4 shows air temperature history comparisons at 1 m, 250 m, and 500 m along the airway of Solutions 1 through 4. Figure 2-5 shows the wall surface temperature at the same airway locations for Solutions 1 through 4. The excellent agreement between Solutions 1 and 2, which used MF, and Solutions 3 and 4, the approximate and accurate analytical solution, respectively, demonstrated that MF was capable of correctly modeling the time-dependent, coupled convection-conduction test problem.

Figures 2-6 through 2-11 show rock temperature distributions in time and space at 1 m, 250 m, and 500 m distance along the airway, respectively, using the NUFT-based rock model (i.e., Solution 1).

The excellent agreement in the temperature history results obtained with three different NTCF rock matrices shown in Figures 2-12 and 2-13 proved that the NTCF rock model was linear, and that the NTCF matrix can be obtained using the temperature at any location for matrix preparation. There was no need to reiterate the NTCF matrix in this case. The NTCF matrix depended only on rock properties and time discretization, and was independent of the temperature history. Therefore, the technique eliminated the need for recalculating the rock domain numerically at each airway length position. In this example, the gain was a 500-fold reduction in computational time for the rock domain, and additional time reduction during the iteration of balancing between the NTCF (i.e., rock) and CFD (i.e., air) modules, since the matrix equation was an order of magnitude faster to evaluate than the numerical recalculation of the rock domain.

Finally, it can be seen from Figure 2-14 that the MF results with Solution 2 converged to Solution 4 as the number of time divisions increased. Moreover, Solution 3, the approximate analytical solution, nearly replicated Solution 4, the accurate analytical solution.

2.4 Conclusions

- MF with the NUFT rock model (i.e., Solution 1) closely matched MF with the 1986 CJ rock model (i.e., Solution 2). This agreement was significant because it implicitly validated the NUFT model configuration against a textbook result.
- MF with the 1986 CJ rock model (i.e., Solution 2) closely approximated the 1959 CJ solution (i.e., Solution 4) with an increasing number of time divisions. A slightly higher number of time divisions appeared to be needed in Solution 2 for achieving the accuracy of Solution 4.
- A great many time divisions appeared necessary for achieving good agreement in all solutions, which underlined the importance of a time-division sensitivity evaluation for each application.
- The approximate analytical solution with superposition (i.e., Solution 3) agreed very well with the reference solution (i.e., Solution 4). Any difference may have been caused by the difference in the number of time divisions.
- Temperature variations at 1, 250, and 500 m do not affect the numerical values of the NTCF rock matrices. Therefore, in this dominantly linear case, the selection of the start-up (i.e., central) temperature variation necessary for the NTCF process did not affect the results.

3.0 POWERED AND NATURAL PASSIVE VENTILATION AT YUCCA MOUNTAIN (TASK 2)

3.1 Introduction

The site recommendation design of the proposed repository at YM includes continuous emplacement drift ventilation for up to 300 years (BSC, 2002). Ventilation fans are assumed to be used to maintain air flow in the drifts at a rate of 15 cubic meters per second (m^3/s) for the low thermal (i.e., cold) operating mode, in which the drift wall temperatures are kept below 95 ^oC, the approximate boiling-point temperature at YM.

In order to use the repository emplacement area efficiently, there is an advantage in using the highest-possible areal waste mass load density for a given maximum target operating temperature. Continuous ventilation reduces temperatures; therefore, it is beneficial to increase the allowable mass load density for a given temperature.

A frequent question is whether a hot or a cold repository should be designed. Current PA results indicate that there is no significant difference in long-term safety performance between the hot and the cold design options (Boyle, 2002). However, the PA analyses did not provide evaluation for each of the hot and the cold options with and without ventilation. In general, since little is known about repository ventilation, partially due to lack of a qualified hydrothermal-ventilation code, the assumptions in the PA models are over-simplified. For example, the relative humidity history given in a corrosion analysis (Gordon, 2002) is approximately 300 percent higher than in the draft ventilation model prepared for the YM Project (BSC, 2002).

A hot repository with a high air flow may be significantly different in performance from one with the same maximum temperatures but no ventilation and a low areal heat load density. When the two cases are compared, for example, the hydrothermal processes and dry-out conditions will be different. It may be necessary to include these variations in the future PA studies in order to achieve more specific evaluations comparing not only hot and cold, but also hot and ventilated-hot, or cold and ventilated-cold options. It is especially important to address these scenarios in order to gain a better understanding of how a flexible design option with various rates of ventilation may affect the safety of the repository.

Long-term ventilation of several hundred years is quite feasible using fans; however, the use of fans for the entire time period may not be necessary. A better understanding is needed of the role that natural, buoyancy-driven ventilation may have in the design to achieve optimum drift and waste package layout for 1) maximizing safety, 2) maximizing the use of the available emplacement area, and 3) minimizing the cost of construction and operation. In addition, natural ventilation for several hundred years may assist in achieving a high mass-load density, but below-boiling temperature operation that has several advantages, including 1) increased drift roof stability, 2) better predictability of performance with close-to-linear rock properties, and 3) decreased variation in the hydrologic conditions, with no water accumulation over the repository horizon. Continuous ventilation may help provide the advantages of lower temperatures while achieving a high mass and associated high thermal load.

After permanent closure at year 300, natural air infiltration will take place through the backfill and the natural fracture and faults system at YM. Moist air flow will be driven through the mountain by a buoyancy pressure generated by the density difference between the incoming cold and dry air and exiting hot and humid air. The effects of such hydrothermal-driven air infiltration have not yet been studied and included in the process models used by the DOE. The air infiltration may be engineered for maximum efficiency in order to achieve a favorable, benign psychrometric waste container environment for several thousands of years.

The purpose of the Task 2 study was to analyze the temperature and relative humidity variations along a 600-m emplacement drift for 5,000 years under the following ventilation conditions:

- The drift is ventilated with a forced, constant air flow rate of 15 m^3/s for 25 years, using a fan.
- With the fan(s) off, the drift is ventilated without interruption from year 25 until year 300 under a natural buoyancy pressure driving force.
- With the access shafts and tunnels backfilled, the drift is naturally ventilated until the end of the study time period.

The results of this study were previously pblished by Danko and Bahrami (2003a).

3.2 Numerical Model Description

3.2.1 Conceptual Repository Arrangement

The conceptual repository arrangement follows the conceptual design developed by the DOE, assuming 178 emplacement drifts and 14 shafts, as well as peripheral tunnels for access and connections for ventilation. The geometry of the three-drift section used in the numerical study is shown on Figure 3-1. Two peripheral drifts located perpendicular to emplacement drifts act as manifolds to distribute and collect air flows for 26 emplacement drifts, of which only 3 are shown on Figure 3-1. Finally, two vertical shafts, an intake and an exhaust, are used to connect the peripheral drifts to the atmosphere, also shown on Figure 3-1. The airflow resistances of the peripheral drifts and the shafts are included in the numerical analysis.

3.2.2 Rock Domain Model

The rock domain was divided into 17 cells bounded with adiabatic surfaces on the vertical planes. One cell is depicted on Figure 3-1. The numerical model assumed a porous, wet, but unsaturated rock formation in which both heat and moisture transport were present and affected the thermal and psychrometric waste container environment. MF was configured to model the cells using NUFT as a module for simulating heat and moisture flows in the rock domain. NTCF was used in all versions of MF to compress and process the time-dependent heat and moisture responses from the hydrothermal process model into matrix equations. An experimental, preliminary, nonlinear NTCF processor was applied, using matrix polynomial equations for modeling heat and moisture fluxes on the boundaries in a wide range of temperature and partial vapor pressure variations with constant-coefficient matrices. The NTCF numerical model of the time-dependent heat and moisture transport on the rock-air interface of a model cell, shown on Figure 3-1, was a set of matrix equations with identified constant coefficients determined from NUFT runs.

The numerical discretization points on the drift wall were bundled into 21 averaged, independent surface nodes with respect to temperature and partial vapor pressure variations in the model. The NTCF rock model defined heat and moisture flux vectors as a function of the 21 time-dependent input vectors of surface temperature and partial vapor pressure boundary conditions. The 21 nodes represented the interface boundary at the points between a rock cell and the airway containing the waste packages. Conductive heat flow between neighboring rock cells was calculated using an experimental, mountain-scale model element.

3.2.3 Model of Airway with Waste Container

A lumped-parameter CFD model was used in MF to describe the air flow, heat, and moisture transport in the airway. Heat and moisture transport by laminar or turbulent convection were modeled on the drift and the waste container wall. Although no fan was used after 25 years to ventilate the storage system and the air flow was maintained only by natural buoyancy pressure difference, the air in each drift was forced to move by the system pressures known as the chimney effect. Natural, secondary flow may have been due to the local temperature differences and related local, superimposed natural convection. The heat and moisture transport coefficients in the annulus between the waste containers and the drift wall were calculated in MF using transport coefficients in the lumped-parameter CFD. A differential-parameter CFD model (Danko and Bahrami, 2002) can also be used in MF if refinement of the transport coefficients is needed; however, this option was not applied in Task 2. A direct thermal radiation between the waste containers and drift wall was also included in the model configuration.

The flow resistances in the airflow model included laminar or turbulent friction, and shock loss in the 5.5-m-diameter emplacement drifts, peripheral tunnels, and access shafts. The air flow resistances of the intake and the exhaust shafts were changed at year 300 to model the effect of a coarse backfill. The backfill resistance assumed a 40-percent available area of the original shafts, a 0.02-m hydraulic diameter of the flow channels, and a 50-percent increase in length in the rubble fill. In addition, 40 shock loss coefficients, each with a unitless value of 0.3, are assumed in series per unit length.

3.2.4 Total System Model

The NTCF and CFD modules were coupled on the rock-air interface by MF until the heat and moisture flows were balanced at the common surface temperature and partial vapor pressure at each surface node and time instant. In the period of natural ventilation between years 25 and 5,000, the air flow rate was also balanced, iteratively equating the pressure loss through the system with the buoyancy driving pressure difference caused by differences between the intake and exhaust air temperatures. The following three simplification assumptions were used to reduce the complexity of the task due to hydrothermal rock modeling.

- The air mass flow rate is uniform in the 26 drifts.
- The intake and exhaust shafts are thermally insulated from the rock mass. In order to compensate for the possible loss in chimney efficiency due to heat exchange, a reduced height of 250 m was used in the simulation.
- The emplacement panel is infinite in the lateral direction, eliminating mountain-scale heat and moisture flows between the repeating parallel drifts across the pillars; however, mountain-scale heat flow along the length of the drifts in the rockmass was iteratively modeled by MF.

The NTCF modeling technique with nonlinear processing was an efficient way to reduce the necessary number of NUFT runs during the iterative numerical calculations, incorporating the following five nested iteration loops:

- NTCF model re-functionalization with NUFT.
- Buoyancy pressure and air flow iteration for 26 drifts.
- Mountain-scale heat flow correction iteration between cells along the drifts.
- Heat balance iteration in each cell between NTCF and airway CFD models
- Moisture balance iteration in each cell between NTCF and airway CFD models.

As the outside loop, one set of NUFT runs and NTCF model preparations served four internal, nested iteration cycles, minimizing the number of time-intensive NUFT runs.

3.2.5 Input Data

The input data used in the calculation essentially agreed with those used in the draft BSC ventilation model (BSC, 2002), referred to as the ventilation AMR Rev 01D in the following. The main input parameters are as follows:

- Rock input data: NUFT input deck specified in the ventilation AMR Rev 01D. The spatial rock domain is represented by 17 NUFT cells; one cell is shown on Figure 3-1.
- Drift dimensions: 600-m long and 5.5 m in diameter.
- Ventilating air: 25 ^{o}C intake temperature with 30 percent relative humidity.
- Air flow rate: 15 m^3/s at intake properties until year 25; variable, balanced value afterward.
- Waste packages: Eight waste packages in a repeating drift segment of 35.5 m as shown on Figure 3-1.
- Waste mass load: 85 metric tonnes of uranium per acre (MTU/acre).

Each of the required MF input decks for the Task 2 simulations are included in Appendices G through J (i.e., NUFT), Appendix K (i.e., NTCF), and Appendix L (i.e., CDF).

3.3 Results

The fully-balanced calculation results for temperatures and relative humidity in the central, representative drift are shown on Figures 3-2 through 3-7 as a function of time and drift length. Results for the waste package surface are shown on Figures 3-2 and 3–3, the ventilating air on Figures 3-4 and 3-5, and the wall surface on Figures 3.6 and 3-7. The pressure loss and buoyancy driving pressure difference across the total system that included the intake shaft, peripheral intake manifold drift, peripheral exhaust manifold, and exhaust shaft, are shown on Figure 3-8. The ventilating air flow rate variation with time in the emplacement drift is shown on Figure 3-9.

Fifteen iteration steps were needed to achieve balancing within a 10-pascal (Pa) pressure error. During the course of the balancing calculations with the five previously described nested iteration loops, MF used each NTCF model approximately 3 times for moisture and 50 times for heat balance iterations in each rock cell, repeated 17 times along the drift length. The total number of 2,550 runs with each NTCF model was further multiplied by 12 mountain-scale heat flow correction iterations and 15 buoyancy pressure balancing iterations, totaling 459,000 hydrothermal model runs, each with a different boundary condition variation for the entire time interval of 5,000 years.

The NTCF modeling technique reduced the number of necessary NUFT runs, making it feasible to complete the complex calculations in two months in spite of the total number of nearly one-half-million iterations with the hydrothermal model. For comparison, a single NUFT run with one set of boundary condition variations for 5,000 years for the rock cell took 2.5 hours. Comparing run times between MF with the NTCF method and a hypothetical case without the NTCF method indicated that replacing the NTCF method with direct NUFT runs and assuming the same number of balancing iterations would take a minimum of 131 years of non-stop computation to complete.

3.4 Discussion

The numerical results demonstrated that temperature and relative humidity could be controlled around the waste containers for a long period of time using natural ventilation. The waste container surface temperatures and relative humidity did not exceed 108 ^{o}C and 30 percent, respectively, for the storage period of 300 years with open ventilation (Figures 3-2 and 3-3). The temperatures and relative humidity in the air did not exceed 70 ^{o}C and 30 percent, respectively, for the same time period (Figures 3-4 and 3-5). The maximum temperature and relative humidity on the drift wall were kept below a maximum of 90 ^{o}C and 30 percent, respectively (Figures 3-6 and 3-7). The variation of the air-mass flow rate during the open ventilation operating mode shows a moderate decrease from the constant, forced value of 15.4 kg/s for 25 years to approximately 8 kg/s by the end of year 300 (Figure 3-8).

Subsequent to repository closure and backfilling of the access shafts and peripheral connecting tunnels with rubble, the air-mass flow rate shown on Figure 3-8 rapidly decreased to approximately 0.1 kg/s and remained approximately constant during the post-closure ventilation period of 4,700 years. This flow rate coincided in value with the lowest ventilation flow rate used in previous YM ventilation studies (TRW, 1996), which was restricted to the pre-closure time period, assuming open ventilation for 100 years.

Due to decreased cooling, the temperature experienced a second, higher surge than the first increase during pre-closure. Both the waste container surface and the air temperatures and relative humidity did not exceed 120 ^{o}C and 50 percent, respectively, for the post-closure ventilation period of 4,700 years (Figures 3-2 through 3-5). The maximum temperature and relative humidity on the drift wall were kept below the maximum of 125 ^{o}C and 55 percent, respectively (Figures 3-6 and 3-7).

It is interesting to note the rapid relative humidity decrease on Figure 3-3 through 3-5 starting at 300 years, in spite of a temperature increase due to the reduction in air flow rate in the drift. A temperature increase generally reduces relative humidity for a constant partial vapor pressure (p_v) because of the increase in saturated vapor pressure ($p_{sat}(t)$) with temperature (t) according to the defining equation relative humidity = $p_v/p_{sat}(t)$. The temperature effect, however, may be overridden by the stronger effect of an increasing partial vapor pressure driven by moisture flow from the rock due to higher temperatures. In the examples shown on Figures 3-2 through 3-8, the relative humidity, after reaching local peak values, decreased with time between 300 to 500 years, since the increase in $p_{sat}(t)$ with t is greater than the increase in p_v. A rapid temperature decrease after 2,000 years, however, increased the relative humidity again. These complexities suggest that a longer simulation time period will be needed to examine the long-term trends in the relative humidity variations in the emplacement drift.

It is also interesting to note how air flow quantity that varied with time, according to Figure 3-9 affected the variation of temperatures and relative humidity along the drift length. During the first 300 years, when ventilation air flow quantity was high, the longitudinal variation in both temperature and relative humidity was low. During post-closure, however, rapid changes were observed along the first few hundred meters of drift length both in temperature (i.e., an increase) and relative humidity (i.e., a decrease from a 30 percent intake value, followed by a cumulative increase).

Based on the observations of the spatial and temporal variations of temperature and especially the relative humidity, in the emplacement drift, it is apparent that the system has a complex, non-linear behavior. The resultant effects of competing influences can only be understood by examining the simulation results of the coupled hydrothermal processes, presented by the MF calculations.

The total buoyancy pressure driving force was different from the pressure loss due to air flow friction resistance during the mechanized, forced ventilation period of 25 years (Figure 3-8). The pressure difference between the curves in Figure 3-8 was provided by the fans. The total buoyancy pressure difference and air flow friction resistance curves are perfectly balanced during the natural ventilation period from year 25 to year 5,000 (Figure 3-8). The buoyancy pressure difference increased with time due to increasing temperature and resulting density difference between the intake and exhaust air. In addition, the density difference was increased further by the increasing water vapor content with time. The trend of the buoyancy pressure difference driving force indicated that natural, post-closure ventilation will most likely be maintained much longer than the time period used in this study.

3.5 Conclusions

- As a fully-coupled, hydrothermal-ventilation model and software, MF has proved efficient in solving the multiphase, non-equilibrium transport problem of heat, moisture, and ventilating air flows involving a large and geometrically complex geologic regime.

- Natural ventilation was found to be efficient in keeping temperatures below boiling between years 25 and 300 in spite of the high-mass-load density of 85 MTU/acre. The air-mass flow rate decreased only moderately when the fans were removed in year 25 to approximately 11 kg/s, and was still approximately 8 kg/s at year 300.

- Subsequent to closure with loose backfill in the access shafts and tunnels (i.e., after year 300), the air flow rate rapidly decreased, but stabilized at a low level over the 4,700-year time period. The trend indicates that natural ventilation may continue for much longer time periods.

- The temperature reached a peak value around year 1,000, slightly exceeding the boiling temperature at the wall of the second half of the emplacement drift. A lower areal mass load density, or a longer pre-closure ventilation time period may alleviate this condition.

- The relative humidity was consistently lower than the intake humidity, and continuously decreased during the 300-year time period. This result provided more favorable conditions than those expected in some of the current corrosion and PA studies.

- The relative humidity continued to be lower than 50 percent until year 5,000. This result also provided more favorable conditions than those expected in some of the current corrosion and PA studies.

- The natural ventilation buoyancy driving pressure difference may be strong enough to drive air flow through the natural fractures, faults, and the lithophysal rock layers in the natural geologic system at YM. This phenomenon, not included in Task 2, may be beneficial in further reducing relative humidity around the waste packages for the entire thermally active time span of the repository. This spontaneous, natural process is part of the repository system; therefore, further studies are recommended.

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4.0 SENSITIVITY ANALYSIS OF VENTILATION PARAMETERS AND SITE INPUT PROPERTIES (TASK 3)

4.1 Introduction

It is difficult to determine the accuracy requirements of the main ventilation input parameters for calculations of temperature and humidity at YM based on judgment and experience, since 1) the heat load is relatively high when compared to that of deep, underground mines, and 2) decay heat characteristics are specific to nuclear waste. Lack of adequate analyses even for common mine climate simulations hampers the assessment of needed accuracy of input data. This problem is addressed in few publications; moreover, none have been related to a high-level nuclear waste storage arrangement.

One sensitivity study has been published by Danko et al. (1998), using a mine climate/heat flow simulation model. For a completely dry roadway and for short periods of time, the sensitivity of the dry bulb temperature to thermal conductivity was found to be slightly higher than the sensitivity to thermal diffusivity and to the heat transfer coefficient. It was found that for increasing periods of time after passing peak values, the impact of thermal diffusivity on dry-bulb temperatures remained constant, and the heat transfer coefficient decreased its influence, while the thermal conductivity became gradually more important. It was concluded that different accuracy requirements should be used for the thermophysical properties in different types of calculations; for example, construction/development and blast cooling calculations during potential retrieval or during continuous and long ventilation periods. For short periods of time in slightly wet roadways, the influence of the thermal conductivity on dry-bulb temperature increased, while that of the heat transfer coefficient strongly decreased.

Task 3 follows the method of numerical sensitivity analysis used in Danko et al. (1998). The selected input properties include rock heat conductivity (k), thermal diffusivity (α), and a heat transfer coefficient (h) on the drift surface. In addition, the ventilation air flow rate (AFR) , input air temperature, areal thermal heat load (ATL), and the average water percolation rate due to precipitation are also varied as input parameters.

The required MF input decks for the sensitivity analysis in Task 3 are presented in Appendix M. The results of this sensitivity study were previously published by Danko and Bahrami (2003b).

4.2 Work Description

The MF software used for the numerical sensitivity analysis was described in detail in Section 3.2. A base case was defined according to the ventilation AMR Rev. 01D, assuming 56 MTU/acre for the ATL and 15 m^3/s for the AFR (BSC, 2002). To be consistent with Task 2, a 600-m emplacement tunnel and 300-year ventilation period were assumed. The base case input values for k, α, and h were equal to the ventilation AMR Rev 01D values.

Deviations from the base case in the sensitivity study were selected according to expected variations at Yucca Mountain and are summarized in Table 4-1. The lithophysal rock formation may decrease k; therefore, k was reduced from the base case of 2 to 1.6 and 1.2 W/m/K. In a similar manner, ρ was also reduced by 25 percent. The resultant values for thermal diffusivity can be determined from the formula $\alpha=k*(\rho\ c)$, where ρ is density and c is specific heat. Since MF applied NUFT as a module for simulating heat and moisture flows in the rock domain and did not require the explicit value of α as an input parameter, α was back-calculated. The AFR was varied to be lower than the base case of 15 to 5 and 1 m^3/s, while the ATL was varied from the base case of 56 MTU/acre to 5 MTU/acre, representing a cold design, and 85 MTU/acre, representing a hot design. The surface heat transfer coefficient varied between 1.89 to 4 $W/m^2/K$ based on the ventilation AMR Rev 01D input and the independent heat transport coefficient calculations, respectively (Danko and Bahrami, 2002).

Drift wall temperature, container surface temperature, drift wall relative humidity, and relative cumulative heat removal by ventilation were considered the most important output parameters for sensitivity calculations. The measure of sensitivity was calculated as the ratio of the relative change in the selected result (i.e., output) parameter to the relative variation of the selected input parameter, multiplied by 100 to convert it to a percentage.

4.3 Results and Discussions

An interesting and surprising preliminary finding was the negligible effect of ATL values on the output sensitivities. The same approximate sensitivity variation was obtained for different but fixed ATL values. The phenomenon may be explained by an approximately linear behavior of the heat and moisture transport processes in the study cases. Consequently, the ATL values were selected by convenience between 5 MTU/acre and 85 MTU/acre, in order to keep the output maximum wall temperature at the end of the emplacement drift below 200 ^{o}C in the various study cases. Since they were not used as independent input parameters, the ATL sensitivities were not processed on separate figure.

The drift and waste container wall temperature variations, wall relative humidity, and cumulative heat removal relative to the base case due to input parameter perturbations were calculated and are shown on Figures 4-1 through 4-12. Each figure has two curves for k, two for h, and one for ρ perturbations. The sensitivity results should be considered the percentage of change in the output as a response to a positive, 100-percent change in the input. The input, perturbed parameters of k, h, and ρ for the simulations are shown on the figure legends. The ventilation AMR Rev 0lD base case is represented as a horizonatal line at at zero percent in these figures.

Another interesting but not as surprising finding was the strong effect of ventilation rates on relative sensitivities, shown in sensitivity results for the high (Figures 4-1 through 4-4), medium (Figures 4-5 through 4-8), and low (Figures 4-9 through 4-12) ventilation flow rates. In general, sensitivities to density and thermal conductivity increased with decreasing ventilation rates, while the opposite was observed for heat transfer coefficients.

The sensitivities of the drift and waste container wall temperatures and especially the heat removal rate were found to be greatest to the input perturbations in thermal conductivity, exceeding 100 percent at a low ventilation rate. This finding underlines the importance of thermal conductivity in the thermal design of the repository.

High sensitivities were also obtained to the intake air temperature, underlining the importance of studying seasonal temperatures and possible future climate changes in the repository design (Figures 4-13 through 4-16). Finally the importance of the heat transport coefficient at high ventilation rates can be seen on Figures 4-1and 4-2, especially at longer ventilation time periods. Danko and Bahrami (2002) showed the importance of modeling heat transfer coefficient variations accurately, which is consistent with the new sensitivity results.

4.4 Conclusions

- Variations in ATL values showed a negligible effect on output sensitivities, which can be explained by the approximately linear behavior of the heat and moisture process in the study cases.

- Ventilation rates strongly affected the relative sensitivities of output parameters to input parameters. In general, sensitivities to density and thermal conductivity increased with decreasing ventilation rate and the opposite was found for sensitivities to heat transfer coefficients.

- Thermal conductivity is an important input parameter, especially with low ventilation rates, which will be naturally the case at YM after closure. This finding underlined the importance of evaluating lithophysal thermophysical properties at YM, since uncertainties in the bulk lithophysal thermal conductivity may be as high as 50 to 100 percent. These high uncertainities in thermal conductivity may translate into 50 to 100 percent error in the predicted temperature and heat removal rates at YM. A decrease in effective rock density due to lithophysae also increased temperatures, further aggravating the effect of uncertainities in thermal conductivity.

- High sensitivities were also obtained to the intake air temperature, underlining the importance of studying seasonal temperature and possible future climate changes in the repository design.

- Significant sensitivity to the surface heat transfer coefficient was found for strongly ventilated scenarios. This parameter was thought to be much less important in previous studies involving ordinary mine climate simulation applications for long periods of time.

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