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REVIEW OF ANALYSIS/MODEL REPORTS RELEVANT TO THE THERMAL EFFECTS ON FLOW KEY TECHNICAL ISSUE

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ABSTRACT

This report documents staff review of six Analysis/Model Reports (AMRs) relevant to the Thermal Effects on Flow Key Technical Issue. The AMRs reviewed in this report are (i) Thermal Tests Thermal-Hydrological AMR Revision 00 (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a), (ii) the Multiscale Thermohydrologic Model Revision 00 (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b), (iii) the Calibrated Properties Model Revision 00 (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c), (iv) Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux Revision 00 (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000d), (v) the Mountain-Scale Coupled Processes Models Revision 00 (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000e), and (vi) the Ventilation Model Revision 00 (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999a). A central theme of this review is evaluation of uncertainty in thermohydrologic variables and its potential effect on repository performance. This theme is followed from reviews of the Calibrated Properties Model through the Multiscale Thermohydrologic Model to the Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux. Lateral mass transport at the mountain-scale and effects of large-scale heterogeneities are incorporated in the Mountain-Scale Coupled Processes Models. In contrast, lateral flow is not represented by the Multiscale Thermohydrologic Model that actually provides thermohydrologic variables used in performance assessments, and neither model incorporates heterogeneities on smaller scales. Overall evaluation of uncertainty, including heterogeneities, is not adequately addressed in these AMRs. Lateral flow within and along drifts is also not incorporated in models used for computing thermohydrologic variables. This lateral flow may result in a cold-trap effect and water flux in drifts from condensation. Approaches to addressing these issues and alleviating concerns are suggested in a short summary at the end of each review and in the summary section. Finally, the Ventilation Model is discussed in terms of data needs and implementation in the thermohydrologic models.

References:

Civilian Radioactive Waste Management System Management and Operating Contractor. *Ventilation Model.* ANL–EBS–MD–000030. Revision 00. Las Vegas, NV: TRW Environmental Safety Systems, Inc. 1999.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Thermal Tests Thermal-Hydrological Analyses/Model Report.* ANL–NBS–TH–000001. Rev. 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000a.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Multiscale Thermohydrologic Model.* ANL–EBS–MD–000049. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000b.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Calibrated Properties Model.* ANL–NBS–HS–000003. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000c.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux.* ANL–EBS–HS–000003. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000d.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Mountain-Scale Coupled Processes (TH) Models.* MDL–NBS–HS–000007. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000e.

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QUALITY OF DATA AND CODE DEVELOPMENT

DATA: There are no original CNWRA data contained in this report. Quality assurance of the original documents should be referenced for all other data reviewed in this report.

CODE: No code was used in preparation of this report.

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1 INTRODUCTION

Six U.S. Department of Energy (DOE) Analysis/Model Reports (AMRs) were reviewed in support of analyses for the Thermal Effects on Flow (TEF) Key Technical Issue (KTI) and to seek staff-level resolution of TEF subissues. These AMRs are (i) Thermal Tests Thermal-Hydrological AMR (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a), (ii) Multiscale Thermohydrologic Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b), (iii) Calibrated Properties Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c), (iv) Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000d), (v) Mountain-Scale Coupled Processes Models (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000e), and (vi) Ventilation Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999a).

The TEF KTI subissues involve evaluating features, events, and processes (FEPs) influencing thermal effects on flow, technical bases used for screening FEPs to be included or excluded from performance assessments, and evaluating the data and models used for representing the thermohydrologic variables of temperature, saturation, relative humidity, and mass flux in Total System Performance Assessments (TSPA). The six AMRs were chosen for this review based on their relevance to the TEF KTI. These AMRs are all preliminary versions (Revision 00) and will likely soon be revised. The information contained in these AMRs, however, provides some indication of how DOE will incorporate thermohydrologic parameters and field variables into the TSPA. Thermohydrologic variables for TSPA were computed using the Multiscale Thermohydrologic Model (MSTHM) (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b). Hydrologic properties of the geologic media used in the MSTHM were obtained from the Calibrated Properties Model AMR (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c). Property sets developed in the Calibrated Properties Model AMR, however, are used for modeling many other aspects of the unsaturated zone (UZ) at Yucca Mountain and thus comments on the Calibrated Properties Model AMR in this review may have some relevance to other KTIs. The Thermal Tests Thermal-Hydrological AMR describes exercises of the TOUGH2 and NUFT codes attempting to verify or validate use of various property sets for modeling thermohydrologic processes at Yucca Mountain. The Thermal Tests Thermal-Hydrological AMR attempts to provide the technical justification for using isothermally developed property sets from the Calibrated Properties Model AMR to compute nonisothermal processes, but concludes by indicating that those properties are not unique in being valid for modeling thermohydrologic processes. The Ventilation AMR is relevant to TEF because ventilation is expected to significantly affect thermohydrologic conditions in the near-field and far-field environments, not only during the preclosure period, but also after repository closure because reduction of thermal loading by ventilation should result in an overall cooler repository. The Mountain-Scale Coupled Processes AMR appears to stand alone and it is not entirely clear to staff what role this AMR plays in repository characterization or performance assessments. It provides useful information regarding larger-scale 3D effects on thermal perturbations to flow and flux at the repository horizon but this information is not incorporated into the abstraction (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000d) for TSPA. The MSTHM AMR points to the Mountain-Scale Coupled Processes Model as an "alternative conceptual model" supporting the MSTHM results but the Mountain-Scale Coupled Processes Model is not so much an "alternative conceptual model" as a very similar conceptual model of a larger domain. Its purpose would be more clear if it were either incorporated with the MSTHM in the abstraction or were actually an "alternative conceptual model" used for building confidence in repository characterization.

The review of these AMRs follows a general format of (i) scope and purpose of the AMR, (ii) how the AMR is relevant to the TEF KTI, (iii) the DOE approach in the AMR, (iv) staff comments on the AMR, and (v) how the AMR helps in resolving the TEF subissues.

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2 THERMAL TESTS THERMAL-HYDROLOGICAL ANALYSIS/MODEL REPORT

2.1 SCOPE AND PURPOSE OF THE THERMAL TESTS THERMAL-HYDROLOGICAL ANALYSIS/MODEL REPORT

As stated on page 14 of the Thermal Tests Thermal-Hydrological AMR, "[t]he purpose of the Thermal Tests Thermal-hydrological (TH) Analysis/Model Report is to evaluate the drift scale thermal-hydrologic (DS) property set derived from the unsaturated zone (UZ) flow and transport analyses for use with thermally perturbed conditions. Also, the secondary purpose is to conduct sensitivity studies of other TH property sets, including the mountain scale thermal-hydrologic (MS) property set, and to investigate modifications that would result in adequate agreement between simulated and measured TH data" (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a).

The scope is further described on page 14. "As an analysis, this report used existing repository scale models to simulate smaller scale field tests, and compares the results to measured temperatures and saturations in the tests. As a model report, this document describes the formulation of the tests, including the conceptual models, properties, and boundary conditions; these formulations have been constructed for the purpose of this AMR" (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a).

2.2 HOW THE THERMAL TESTS THERMAL-HYDROLOGICAL ANALYSIS/MODEL REPORT RELATES TO THERMAL EFFECTS ON FLOW

The Thermal Tests Thermal-Hydrological AMR directly relates to the TEF KTI. This AMR evaluates and attempts to determine the most appropriate property set for models used to simulate thermohydrologic processes at the proposed Yucca Mountain repository.

2.3 U.S. DEPARTMENT OF ENERGY APPROACH

As stated on page 35 of the Thermal Tests Thermal-Hydrological AMR, "[t]his evaluation is carried out by comparing field measurements with numerical simulations of three field tests: SHT [Single Heater Test], DST [Drift scale Heater Test], and LBT [Large Block Test]. The simulations use alternative property sets to facilitate selection of a set for design and performance assessment" (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a).

2.4 STAFF COMMENTS

The objective of the Thermal Tests Thermal-Hydrological AMR was to assess property sets derived from UZ flow and transport analysis for use in modeling thermally perturbed conditions. However, this AMR ventured into evaluating the underlying conceptual and numerical models even though, as stated on page 14, "[h]eat and mass transfer models applicable to Yucca Mountain Site Characterization Project (YMP) have been developed and documented in other reports." Two TH simulators, TOUGH2 and NUFT, were used in the Thermal Tests Thermal-Hydrological AMR. The AMR further states "[t]he TOUGH2 software package implements a set of these conceptual heat and mass transfer models primarily in support of the Unsaturated Zone Flow and Transport Process Model Report. The NUFT software package implements another set of conceptual heat and mass transfer models (with a great deal of similarity to those implemented in TOUGH2) primarily in support of the Engineered Barrier System Degradation Process Model Report and the Total System Performance Assessment/Analyses (TSPA) thermal hydrological (TH) abstractions. Validation of these models (i.e., comparison with the actual behavior of the modeled system) is a key part of developing confidence in the DOE ability to meet regulatory requirements on repository performance with reasonable assurance. Application of the models to in situ thermal tests is one means of validation..." This discussion implies that the analyses of the DST were used to validate the two models, TOUGH2 and NUFT. If model validation is an objective of the Thermal Tests Thermal-Hydrological AMR, this should be stated and demonstrations of model validation should be clearly separated from evaluation of property sets.

The Thermal Tests Thermal-Hydrological AMR occasionally ventures beyond its stated objective of comparing property sets for use in modeling thermal perturbations in flow and delves into validation of conceptual models. For example, on page 35 the AMR states "[a]n analysis of SHT TH models and experimental measurements is performed for evaluating UZ drift scale hydrologic and thermal properties as well as calibration of the conceptual models." It is not clear what meaning of "calibration of conceptual models" is intended since the calibrated property sets were provided from the Calibrated Properties Model, and other sources, to be compared against the thermal tests in this AMR. Other quotes on pages 35–36 where the AMR states "[i]t has been found, in general, that the DKM [Dual Permeability Model] better represents the trends of the processes occurring in the host rock during a thermal perturbation than do the ECMs [Equivalent Continuum Model] using the same hydrological properties" and "In previous simulations of the SHT...the ECM model results are contrary to experimental measured results, and therefore it is not the appropriate flow model to use for the SHT analysis" suggest that "calibration of the conceptual models" is intended to mean conceptual model validation. If conceptual model validation is an objective of this AMR it should be stated and model validation versus property set comparisons tests clearly indicated.

Two methods were used to apply heat to the drift wall of the DST in the model simulations and were said to be "bounding studies" on page 41 of the AMR. One method implemented a thermal conductivity tangential to the drift wall several orders of magnitude higher that the rock thermal conductivity and the other method assigned the rock thermal conductivity values to both the orthogonal and tangential components of the drift wall. The first method produced uniform temperatures along the drift wall while the second produced significant temperature differences along the drift wall and between the middle and ends of the drift. Both of these methods, however, assume that 100 percent of the heat from the floor heaters is supplied to the drift wall and neglect convection in the drift through the bulkhead. Thus it is not obvious that these two methods bound the actual conditions in the heated drift.

The initial value assigned to the host rock matrix saturation of the DST has an important effect on the thermal-hydrological simulations as indicated by independent modeling studies conducted at the Center for Nuclear Waste Regulatory Analyses (Green et al., 2000). Additional documentation of the data supporting ambient rock matrix saturations used in DST modeling would assist in resolving concerns regarding uncertainties related to measurement bias and measurement error. Calibration by inversion to data having systematic bias, perhaps resulting from core dry out during drilling and handling, could result in biased property sets. Other data, such as *in situ* measurements from heat dissipation probes, could be used to enhance and support matrix saturation data from drilling cores. In addition, uncertainty from sources such as measurement

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scaling effects and spatial variability should be evaluated and propagated through the process-models to performance assessments.

On page 76 of the AMR is the statement, "[s]ince moisture redistribution in the fractures is fundamentally a function of water and vapor mobility, it is mainly governed by capillary pressure and relative permeability characteristic curves (both in the liquid and in the gas phase), which themselves are governed by the van Genuchten parameters." However, this is not necessarily true for water that drains by gravity down relatively large conduits. Or and Tuller (2000) and Or and Ghezzehei (2000) found that flow along a single face of a large aperture fracture is controlled by roughness of the fracture surface. Models that assume a porous continuum representation for flow in fracture networks, with moisture retention behavior characterized by van Genuchten parameters, implicitly assume that all flow in fractures bridges the fracture aperture. Potential effects of gravity driven flow along single fracture surfaces and film flow processes on seepage and reflux into emplacement drifts should be recognized and addressed. Note this comment pertains primarily to the deep percolation subissue of the Unsaturated and Saturated Flow Under Isothermal Conditions KTI and the DOE has committed to investigate film flow type processes in their investigations of seepage into drifts.[1]

Fate of thermally mobilized water in the DST is a significant source of uncertainty. Whether condensation zones develop above or below the Heated Drift (HD) may be important to repository performance and is key to determining if dryout of the rock is driven by buoyant advective flow. On page 77 and again on page 84, the AMR states in a discussion "ERT [Electrical Resistivity Tomography] data indicated that for the condensation zones around the HD , the rock was wetter below the heater horizon than above." There are no illustrations of electrical resistivity tomography (ERT) data presented in this section of the AMR. However, figures 53–56 of the section on NUFT simulations contain ERT illustrations at four simulation times. It is generally recognized that detecting condensation in fractures is difficult. So, to conclusively interpret these data as showing that the zone below the HD horizon is wetter than above may not be possible. Positive identification of condensation zones is hindered by uncertainties in measurement techniques and the accumulation of condensate in fractures may be reduced by losses through the bulkhead. Staff agree with concerns reflected on page 86 of the AMR, which identifies moisture loss out of the bulkhead as probably the most significant uncertainty in thermohydrologic modeling of the DST.

The purpose of the Thermal Tests Thermal-Hydrological AMR was to validate property sets for use in calculating thermal perturbations to UZ flow at Yucca Mountain. Two property sets (DS/AFM-UZ99 and DKM-TT99) were evaluated in the TOUGH2 analyses and four property sets (DS, MS, MSLK, and CON) were evaluated in the NUFT analyses. A root mean squared difference standard of 10 °C was arbitrarily selected to established whether or not a property set was acceptable for modeling thermal perturbations to UZ flow. That is, if the weighted mean squared difference between results of temperatures predicted by the model and temperatures measured in the DST was less than 10 °C, the property set was considered acceptable for modeling thermal perturbations in UZ flow. Weights were assigned based on the number of temperature data in given locations so that the results would not be biased by locations with more data. Of the six property sets evaluated, only model results for above-boiling regions obtained using the CON property set exceeded this criterion. The CON property set indicates that properties were defined for heat conduction

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[1] Unsaturated and Saturated Flow Under Isothermal Conditions U.S. Department of Energy and U.S. Nuclear Regulatory Commission Technical Exchange. Berkeley, CA: August 2000.

only with no coupling to hydrological processes. In summary, the TOUGH2 analyses did not discriminate between the property sets evaluated. The NUFT analyses rank the appropriateness among the different results for the various property sets. However, this difference was not large. The analyses concluded by noting that more work is needed and, hence, is planned. Given that temperature distributions appear to be controlled largely by heat conduction and the large degree of uncertainty inherent in detecting fracture saturations, it may be that additional modeling studies will not conclusively distinguish between property sets in determining the single most appropriate property set for calculating thermal perturbations to flow. Perhaps a more effective way of coping with this uncertainty would be to evaluate the variability in computations using all of the property sets, incorporate this variability into the model abstraction, and propagate the uncertainty through to performance assessments.

2.5 HOW THE THERMAL TESTS THERMAL-HYDROLOGICAL ANALYSIS/MODEL REPORT ADDRESSES ISSUE RESOLUTION

The objective of the Thermal Tests Thermal-Hydrological AMR was to compare the use of various property sets, determined from UZ flow, for modeling thermohydrologic processes. The bases of this comparison were temperature data from the DST. A maximum of 10 °C in the weighted root mean squared difference between model calculated temperatures and temperature data from the DST was selected as the criterion for determining if a property set was suitable for modeling thermohydrologic processes. Of the six property sets evaluated using the TOUGH2 and NUFT codes, five were found acceptable by this criterion. The only property set not found acceptable was for modeling heat transfer by conduction only, neglecting thermohydrologic processes entirely. These analyses point to the fact that it may be difficult to distinguish between various property sets on the bases of temperature data alone. Modeled temperatures were fairly similar for all property sets evaluated even though modeled saturations in fracture networks could be significantly different. Comparisons of property sets based on fracture saturations entail significant uncertainty in the measurement of fracture saturations, however. Fracture saturations measured by ERT, ground penetrating radar, and air permeability involve significant uncertainties and can be compared only qualitatively. In concluding, the AMR found most of the property sets compared to be valid for modeling thermohydrologic processes and also tried to lend weight toward favoring the Dual-Permeability Model (DKM) conceptual model rather than the Equivalent Continuum Model. Because thermal test data are not yet sufficient to determine which property sets are most suitable for modeling thermohydrologic processes, it may be necessary for the DOE to evaluate the uncertainty in thermohydrologic variables as computed by the various property sets and propagate this uncertainty through the abstraction to performance assessments.

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3 MULTISCALE THERMOHYDROLOGIC MODEL ANALYSIS/MODEL REPORT

3.1 OBJECTIVE AND PURPOSE OF THE MULTISCALE THERMOHYDROLOGIC MODEL ANALYSIS/MODEL REPORT

As stated on page 16 of the AMR, "the purpose of the Multiscale Thermohydrologic Model (MSTHM) model is to describe thermohydrologic evolution of the near-field environment (NFE) and EBS throughout the high-level nuclear waste repository at Yucca Mountain for a particular engineering design." Furthermore, "the process-level model will provide TH information and data (such as in-drift temperature, relative humidity, liquid saturation, etc.) for use in other technical products."

3.2 HOW THE MULTISCALE THERMOHYDROLOGIC MODEL ANALYSIS/MODEL REPORT RELATES TO THERMAL EFFECTS ON FLOW

This AMR is central to the TEF review of the DOE safety case because it describes the modeling assumptions and the numerical models used to simulate thermohydrologic variables for TSPA. The output of the Multiscale Thermohydrologic Model (MSTHM) is a large number of data of thermohydrologic variables within the drift and in the near-field environment used in TSPA and in other AMRs, as needed, to account for the effects of thermal perturbations on unsaturated zone hydrology. Abstraction of the thermohydrologic variables calculated using the MSTHM is described in the Abstraction of the Near-Field Environment Drift Thermodynamic Environment and Percolation Flux AMR which is reviewed in section 5.0 of this report.

3.3 U.S. DEPARTMENT OF ENERGY APPROACH

The MSTHM consists of four submodels: (i) the Line-average-heat-source, Drift-scale, Thermohydrologic (LDTH) submodel; (ii) the Smeared-heat-source, Mountain-scale, Thermal-conduction (SMT) submodel; (iii) the Smeared-heat-source, Drift-scale, Thermal-conduction (SDT) submodel; and (iv) the Discrete-heat-source, Drift-scale, thermal-conduction (DDT) submodel. All four submodels are implemented using the NUFT code. The submodels are executed with boundary conditions and inputs simulating a range of conditions as shown on page 95 and the following pages of the AMR. The outputs are distributions of thermodynamic variables, such as temperature on the waste packages (page 96) and relative humidity in the invert (page 98). These distributions are to be used by TSPA abstractions as described in other AMRs for simulating the evolution of thermohydrologic variables in the engineered barrier system and in the near-field environment.

3.4 STAFF COMMENTS

3.4.1 General Comments

- Interactions of the different submodels are hard to follow. More complete descriptions of the relationships between submodels, as well as the parameters and field variable distributions exchanged between the submodels, would help with evaluating the methodology and would improve transparency of the approach.

- Some of the assumptions and techniques used, as discussed in the next section, may have the potential to reduce the representation of or the effect of natural heterogeneity of the modeled system. In particular, staff are concerned about the absence of accounting for water vapor and related advective heat flux parallel to the drifts and across the center lines between drifts.

3.4.2 Comments Regarding Modeling Assumptions

Boundary conditions and modeled domains of the MSTHM restrict lateral mass transport. Mass flux between drifts is not modeled in the MSTHM because the LDTH submodel "symmetry cells" end at the midplanes between drifts at no-flow boundaries and the other submodels represent heat transport by conduction only. Also, the MSTHM does not model mass flow in the direction parallel to the drifts because the LDTH submodel is a two-dimensional (2D) cross section of a drift. Thus, the MSTHM assumes that lateral flow in the unsaturated zone will not have an appreciable effect on moisture distribution at or below the repository horizon. Although this assumption is not explicitly stated, it is implicit in the construction of the MSTHM. Two conditions could exist where lateral flow in the unsaturated zone and repository-level interactions between moisture flow and thermal fluxes are important. First, mountain-scale heterogeneities, such as preexisting faults that intersect the Paintbrush nonwelded tuff (PTn), may create conditions that cause elevated moisture flux at the repository depth. This could result because these faults intercept lateral moisture flux in the PTn and redirect it vertically through the repository horizon (Ofoegbu et al., 1999).[1] Second, the proposed thermal loading pattern at Yucca Mountain may create mechanical conditions favoring development of laterally discontinuous zones characterized by increased horizontal permeability resulting from thermal-mechanical coupling (Ofoegbu, 2000). These laterally discontinuous zones may redirect moisture flow laterally resulting in elevated moisture flux crossing the repository horizon at the downstream end of the altered zones.[2] Consequently, faults that intersect the PTn, and development of thermal-mechanical altered zones at the repository horizon, may significantly effect temperature, humidity, saturation, and moisture flux at the repository horizon. Therefore, predictions of thermal effects on thermohydrologic variables should account for large-scale heterogeneities associated with faulting and potential thermal-mechanical altered zones. In addition, lateral migration of water vapor along a thermal gradient resulting from edge-cooling effects or variation in waste package heat output could result in condensation in cooler regions of the drifts. Limited domains of the MSTHM submodels and symmetric no-flow boundary conditions prevent evaluation of lateral mass transport effects on thermohydrologic variables computed for this AMR.

Heat removal through ventilation was represented in the MSTHM by reducing the waste-package heat source by 70 percent for the first 50 yr (preclosure period). This approach was used consistently in all the MSTHM submodels, and the same percentage of heat loss was applied everywhere irrespective of location along a drift. Representing ventilation as a spatially independent heat-loss percentage assumes that the effect of ventilation is independent of position along a drift length. However, the ventilation design specifies forced air entering the drifts at the east and west ends and exiting through a duct located midway between the ends, i.e., at about 600 m from the ends of a typical emplacement drift (Civilian Radioactive

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[1] Ofoegbu, G.I., S. Painter, R. Chen, R.W. Fedors, and D.A. Ferrill. Geomechanical and thermal effects on moisture flow at the proposed Yucca Mountain nuclear waste repository. *Nuclear Technology*. In review.

[2] Ibid.

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Waste Management System Management and Operating Contractor, 1999a). Air would enter the drifts at a relatively low temperature and exit relatively hotter. A consequence of this design may be that the drift-wall, drift-air, and waste-package temperatures would increase toward the middle of a drift from the east and west ends. This temperature gradient may cause a drift-parallel heat flux in addition to heat flux from repository edge-cooling effects. This ventilation-induced drift-parallel heat flux and its potential impact on temperature, humidity, saturation, or moisture flux should be investigated.

Radiative heat transfer in the drift of the LDTH and in some parts of the DDT was represented as conductive heat transfer by using an effective thermal conductivity defined as a function of time. Although this approach to modeling radiation is based on a standard concept, its implementation in these submodels was not standard. The approach used in these submodels was based on a linearization of the radiative heat transfer equation to obtain a heat-conduction equivalent thermal conductivity as a function of cavity geometry (radiation view factor) and boundary temperatures (cf. Kreith and Bohn, 1993, p. 23). Although radiation equivalent thermal conductivity is a nonlinear function of temperature, there may be specific situations where its dependence on temperature can be simplified by a linear approximation such as where the temperature does not vary widely. Because this linearized approximation of radiation may be subject to significant errors, these potential errors and their effects on thermohydrologic variables computed in the MSTHM should be evaluated and documented in the AMR.

Some discussions in this AMR are difficult to follow and would benefit from additional explanation. The following examples should be considered as requests for further clarification.

- The DKM modified with the active fracture concept is used for the LDTH simulations, according to a discussion in section 6.3 on page 78. This section describes how the DKM underestimates fracture-matrix interaction for steep gradients, but then says that this model is isothermal so there are no steep gradients. Because the LDTH is a nonisothermal submodel run for five different heat loads, it is not clear which model is being referenced. More complete documentation of conceptual models, as implemented in the codes used for the simulations, would help to avoid confusion.

- Temperature distributions, starting with figure 6-7 on page 143, represent results for a particular type of waste package. However, temperatures must vary as a result of variable heat loads in the DDT and LDTH submodels. None of this detail on temperatures (or other thermohydrologic variables) is provided in the AMR. More complete documentation, or access to output files from the simulations, would assist reviewers in evaluating variability in thermohydrologic variables as computed in the MSTHM.

- Grids for submodels shown in figures 6-1 through 6-6 represent only small portions of the modeled domains. Information for the entire modeled domains, including grids and boundaries, would help with evaluating the relationships between submodels and assessing limitations of particular submodels

- Scanning curves are apparently an important linkage between various submodels, but descriptions of these scanning curves in the AMR are brief and qualitative. More complete documentation on the implementation of the scanning curves would help understanding how the submodels fit together and how results from one submodel are used to modify results of another.

3.5 HOW THE MULTISCALE THERMOHYDROLOGIC MODEL ANALYSIS/MODEL REPORT ADDRESSES ISSUE RESOLUTION

A significant omission in the MSTHM may be its inability to evaluate the potential effects of lateral mass transport. Conditions where lateral mass transport may be important were identified in this review. Specifically these conditions are where large-scale faults transect the PTn unit, where laterally discontinuous zones of increased horizontal permeability result from thermal-mechanical coupling, and where edge-cooling effects of variable heat output from waste packages result in condensation from the cold-trap effect. Incorporation of heterogeneities at all scales of potential importance and incorporation of the potential cold-trap effect into the MSTHM would help to address concerns raised in this report. In addition, combining results from other models, such as the Mountain-Scale Coupled Processes Model, that include lateral flow and the effects of faults into the abstraction of thermohydrologic variables, along with results from the MSTHM, would assist in evaluating the potential effects of spatial variability and uncertainty.

Staff have been informed[3] that the potential effects of ventilation on thermal load and the repository environment remain a subject of experimental investigations. Results of these investigations will likely provide essential information regarding the use of a 70-percent reduction in thermal output to represent ventilation in the MSTHM submodels. These investigations may also provide important data regarding a potential drift-parallel heat flux caused by ventilation and its impact on temperature, humidity, saturation, and moisture flux in the near-field environment. Documentation of the results of these investigations, further explanations of model details such as the scanning curves, and actual model outputs provided or referenced in future revisions of this AMR would assist in resolving the concerns raised in this review.

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[3] Unsaturated and Saturated Flow Under Isothermal Conditions U.S. Department of Energy and U.S. Nuclear Regulatory Commission Technical Exchange. Berkeley, CA: August 2000.

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4 CALIBRATED PROPERTIES MODEL ANALYSIS/MODEL REPORT

The following section discusses staff review of the Calibrated Properties AMR (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c) as used in computing thermohydrologic variables with the MSTHM. These Calibrated Properties, however, are widely used in unsaturated zone flow and transport modeling at Yucca Mountain, and concerns discussed in this report may apply to models other than just the MSTHM.

4.1 SCOPE AND PURPOSE OF THE CALIBRATED PROPERTIES MODEL ANALYSIS/MODEL REPORT

The purpose of the Calibrated Properties Model AMR, as stated on page 11, is "to document the Calibrated Properties Model that provides calibrated parameters sets for unsaturated zone flow and transport process models for the YM Site Characterization Project." The DOE further defines the content and usage of the calibrated property sets on page 11. "The calibrated property sets include matrix and fracture parameters for the UZ Flow and Transport Model, drift seepage models, drift-scale and mountain-scale coupled-processes models, and Total System Performance Assessment models .... These process models provide the necessary framework to test conceptual hypotheses of flow and transport at different scales and predict flow and transport behavior under a variety of climatic and thermal-loading conditions."

4.2 HOW THE CALIBRATED PROPERTIES MODEL ANALYSIS/MODEL REPORT RELATES TO THERMAL EFFECTS ON FLOW

The property sets developed as described in the Calibrated Properties Model support several AMRs reviewed in this report. These include

- Thermal Tests Thermal-Hydrological AMR (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a)

- Multiscale Thermohydrologic Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b)

- Mountain-Scale Coupled Processes (TH) Models (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000e)

- Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000d).

The Calibrated Properties Model also supports several AMRs not reviewed in this report. Some of these AMRs include

- In-Drift Thermal-Hydrological-Chemical Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000f)

- Drift-Scale Coupled Processes (DST, THC Seepage) Models (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000g)

- Unsaturated Zone Flow and Transport Model Process Model Report (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000h)

- Seepage Model for PA Including Drift Collapse (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000i)

- UZ Flow Models and Submodels (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000j),

Note that this list is not complete. The property sets developed in the Calibrated Properties Model AMR are used throughout the modeling done for the Yucca Mountain Project, and results of these models are abstracted for TSPA.

4.3 U.S. DEPARTMENT OF ENERGY APPROACH

The DOE approach described in the Calibrated Properties Model AMR determined property sets for fracture and rock matrix continua comprising the hydrostratigraphic units and faults zones at Yucca Mountain. These fracture, rock matrix, and fault property sets were calibrated by inverse modeling with the ITOUGH2 computer code. The ITOUGH2 computer code is an implementation of a nonlinear, iterative weighted-least-squares minimization of model results relative to measured or observed data. The code implements Richards equation to perform the forward calculations required for the inverse method. Data used in the inversion were water potentials, saturations, and pneumatic pressure measured in the various hydrostratigraphic units and in the Ghost Dance fault. These data were used in the inversion to estimate permeabilities, van Genuchten parameters, and fracture-matrix interaction parameters for the various hydrostratigraphic units considered. Fracture porosity, matrix porosity, residual saturation, and satiated saturation were not estimated by the inverse procedure but were obtained by other methods. One hundred ninety-nine parameters were estimated by this inverse calibration procedure.

Fracture and matrix properties were determined from a one-dimensional inversion that assumed vertical flow within the unsaturated zone at Yucca Mountain. The approach further assumed that hydrostratigraphic units are homogeneous and that heterogeneity at Yucca Mountain results from differences in properties of various hydrostratigraphic units. Note that this assumption is valid only if the spatial variability across the hydrostratigraphic units is much larger than the variability within units.

Fault properties were determined using a 2D inversion from saturation, water potential, and pneumatic data in the single borehole USW UZ-7a that crosses the Ghost Dance fault. The observed data were interpolated onto the 2D mesh for use in the inversion.

Two spatial scales, the mountain scale and the drift scale, were considered in the inversion. Parameter sets for the mountain scale were determined first, followed by parameters at the drift scale. Pneumatic data used in the mountain-scale analysis were from barometric pressure signals monitored at depth. Where model properties are scale-dependent, some method of upscaling was a part of the calibration procedure. Note that procedures for upscaling hydrologic property data are not well-established and are an area of active research. From the mountain-scale parameter sets, the drift-scale parameter sets were estimated using a recalibration procedure that focused solely on parameters in the immediate vicinity of the drift. Pneumatic pressure data used in the drift-scale analysis were based on air permeability tests conducted in the hydrostratigraphic units surrounding alcoves and niches of the Exploratory Studies Facility (ESF). During the recalibration, parameters in close proximity to the drift were modified while parameters away from the drift were maintained at their mountain-scale values. This recalibration was intended to adjust properties to the scale of the drift.

The inverse calibration procedure involved three steps:

- Step 1. Perform the inversion for matrix properties using the water potential and saturation data. During this step, the fracture permeabilities for hydrostratigraphic units tcw11 through tsw37 were fixed at their prior estimated values.
- Step 2. Perform the inversion for fracture permeabilities for hydrostratigraphic units tcw11 through tsw37 using the pneumatic data. During this step, all other parameters were held constant.
- Step 3. Check the calibrated parameter set from the second step against the saturation and water potential data to determine if additional calibration is required. If further calibration is required, then repeat Step 1, and check the recalibrated parameter values against the pneumatic data.

This inverse procedure is based on several assumptions:

- Saturations computed from field data prior to inversion that were greater than one were assumed to be equal to one. Those measured saturations greater than one were assumed to be measurement error.
- It was assumed that values for the fracture–matrix interaction parameter, γ, may be estimated for common rock types.
- Because of data limitations and the way data were interpreted, estimates of uncertainty could not be directly calculated for some data. When uncertainty could not be estimated from data, a value was assumed based on uncertainties estimated from similar data.
- Properties calibrated based on the Ghost Dance fault were assumed to be representative of all faults in the region.

Other assumptions made for this modeling procedure included the assumption that liquid flow under ambient conditions is at steady state and flow of liquid and gas through fractures and matrix can be described by the dual-continuum approach. Additional assumptions were made for other components of the conceptual model. For example, the active fracture model of Lui et al. (1998) was incorporated into the DKM porous media continua model in an attempt to represent the effects of preferential (rivulet or fingering type) flow in fractures. Also it was assumed that heterogeneity of faults is a function of major hydrostratigraphic units. To accomplish the transition from dominant matrix flow to dominant fracture flow in the numerical model, the numerical method of down-stream weighting was used for downward matrix-to-matrix flow from the PTn to the TSw hydrostratigraphic units and from the vitric Calico Hills nonwelded tuff (CHn) to the zeolitic CHn hydrostratigraphic units.

4.4 STAFF COMMENTS

Geologic conditions that determine hydraulic properties vary enormously, and data on these properties are always sparse. The actual distribution of hydraulic properties and thus the flux and pressure variables determined from them using the physics of continuity and Darcy's law are highly uncertain (Gelhar, 1993). Fracture network permeabilites determined from air-injection tests conducted in Niches in the ESF varied at least five orders of magnitude within a single hydrostratigraphic unit (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999b), yet fracture permeabilities calibrated by the inverse method in the Calibrated Properties Model AMR typically varied within one or two orders of magnitude for comparable welded units. Accounting for variability and heterogeneity within both the welded and nonwelded units and transecting faults would undoubtedly increase the variability in computed thermohydrologic variables. Field data indicate that fault zones at Yucca Mountain are complex and show considerable variability in dimension and gouge material.[1] It appears to staff that this full range of variability and uncertainty has not been accounted for in the calibrated properties or in the model results computed using these calibrated properties. Uncertainty is acknowledged on page 58 of the AMR, which indicates that an uncertainty analysis could be performed using a Monte Carlo approach but that such an approach would not be performed because it is prohibitively time consuming given the number of parameters. However, uncertainty does need to be evaluated and ultimately accounted for in TSPA.

Nonlinear least-squares and maximum-likelihood inverse methods presume that the unknown parameters are deterministic, and randomness exists only in the measurement errors. Measurement errors, however, are in themselves usually insufficient to explain differences between observed and modeled variables. Thus, with this type of inverse method, the concept of measurement error should be extended to include other aspects of uncertainty such as modeling errors and scaling effects (McLaughlin and Townley, 1996). An example of a potential scaling effect is described on page 61. "Saturation, water potential, and pneumatic pressure data, which are inverted to obtain the calibrated parameter sets, are developed so that they can be compared to the numerical grid... ." Interpolating data from the sample scale onto the numerical grid at another scale may result in smoothing and loss of variability. Uncertainty also exists in the actual magnitude of measurement errors used in the inversion. For example, on page 24 "[i]t is assumed that reported saturation values greater than 1.0 are equal to 1.0" and that saturations greater than 1.0 result from measurement error. It is not obvious from the AMR how this assumption affected the measurement error used for the inversion. Also, in the same formulation of total error, an assumption was made that the standard error is 0.05, when only one sample was available. Where data were lacking or "[b]ecause of limitations and the way data were interpreted, estimates of uncertainty cannot be directly calculated for some of the data." In this case, "an appropriate uncertainty [of 1 to 2 orders of magnitude was] selected (assumed) based on the uncertainties of similar data."

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[1] Stamatakos, J.A., R. Chen, W.M. Dunne, D.A. Ferrill, M.B. Gray, P.C. La Femina, H.L. McKague, A.P Morris, D.W. Sims, and D.J. Waiting. *Input to Issue Resolution Status Report: Chapter 4, Technical Bases—Key Technical Issue: Structural Deformation and Seismicity.* San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

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Data used in the inversion may be representative only of localized conditions but were considered to represent larger areas or the entire mountain. For example, on page 17 "[s]aturation data measured on core from borehole USW UZ-7a are used for the 2D inversions. This borehole intersects the Ghost Dance Fault, and thus the saturation data from this borehole are representative of the faulted rock of Yucca Mountain." As previously mentioned, however, fault zones at Yucca Mountain are complex and show considerable variability. Also, on page 18 "[w]ater potential data measured in situ in boreholes USW NRG–6, USW NRG–7a, UE–25 UZ#4, and USW SD–12 are used in the 1-D inversions. These boreholes do not intersect known large faults, and thus the water potential data are representative of the rock mass at Yucca Mountain." In addition to representing localized conditions on a small sample scale, these data may be affected by errors that systematically bias the results. For example, in the discussion on measurement of *in situ* water potential on page 39, the AMR indicates that, prior to the installation of the *in situ* sensors, boreholes were open, and rock around the borehole may have dried out.

Along with measurement error, scale effects, sample bias, heterogeneity, and other sources of uncertainty in the data, uncertainty may also exist within the inverse modeling procedure. For example, rather than a simultaneous inversion on all data for all estimated parameters, an iterative approach was adopted. Matrix properties were calculated during the first step while fracture properties were kept constant. Next, matrix properties were kept constant while fracture properties were estimated. An evaluation of potential errors and uncertainties in this iterative approach would provide more confidence in final modeled results. On page 57, the AMR suggests that cross-correlated parameters may affect the calibrated properties. An evaluation of this potential effect and the uncertainty involved in neglecting parameter cross-correlations should be provided also.

The purpose of this discussion is not to criticize every minor detail and assumption of the inversion but to provide a few examples demonstrating that uncertainties in model calibration procedures are pervasive. Although the least-squares maximum likelihood inverse procedure used in the AMR is a generally accepted approach for calibrating numerical models, a thorough evaluation of uncertainty from all potential sources and effects on model results is necessary to provide confidence in the range of thermohydrologic variables provided to TSPA. One approach for evaluating uncertainty is to compare model results with alternative models. On page 30, the AMR indicates that alternative models have been considered. Traceable references to these alternative models and associated property sets may help resolve some concerns discussed in this report.

4.5 HOW THE CALIBRATED PROPERTIES MODEL ANALYSIS/MODEL REPORT ADDRESSES ISSUE RESOLUTION

The Calibrated Properties Model AMR is reviewed here primarily to evaluate uncertainties in the thermohydrologic variables computed from the MSTHM. Ultimately, uncertainty from all relevant sources should be included in the abstractions of thermohydrologic variables provided to TSPA so that the effect on performance can be addressed. As discussed in the staff comments of section 4.4, uncertainty comes from several sources, and only a few of those sources of uncertainty are adequately incorporated into TSPA. Faults at Yucca Mountain are a highly variable aspect of spatial heterogeneity and, as mentioned previously, there is no guarantee that properties of one fault are representative of all other faults. Results obtained from inverse methods are typically sensitive to the data used in the inversion. Uncertainty in these data affect estimates of properties. Results of inverse methods may also be affected by assumptions or techniques used in the inversion method. A thorough evaluation of uncertainty, including uncertainty in calibrated properties and thermohydrologic variables calculated from those properties, would greatly assist in resolving some concerns discussed in this report.

5 ABSTRACTION OF NEAR-FIELD ENVIRONMENT DRIFT THERMODYNAMIC ENVIRONMENT AND PERCOLATION FLUX ANALYSIS/MODEL REPORT

5.1 SCOPE AND PURPOSE OF THE ABSTRACTION OF NEAR-FIELD ENVIRONMENT DRIFT THERMODYNAMIC ENVIRONMENT AND PERCOLATION FLUX ANALYSIS/MODEL REPORT

As quoted from page 9 of the AMR, "The purpose of this analysis and model report (AMR) is to provide abstraction of the process-level thermal hydrology (TH) model that characterizes the in-drift thermodynamic environment. Specifically, this AMR details the abstraction of the multiscale TH model described in CRWMS M&O 2000[k] Sections 6.1 through 6.6."

Specifically, this AMR takes the output from the Multiscale Thermohydrologic Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b) and converts it into a form usable in TSPA. This conversion involves "development of appropriately averaged quantities of temperature, liquid saturation, relative humidity, evaporation rate, and percolation flux. In addition, the maximum and minimum temperature waste packages will be identified."

5.2 HOW THE ABSTRACTION OF NEAR-FIELD ENVIRONMENT DRIFT THERMODYNAMIC ENVIRONMENT AND PERCOLATION FLUX ANALYSIS/MODEL REPORT RELATES TO THERMAL EFFECTS ON FLOW

The abstraction of thermohydrological variables described in this AMR provides TSPA with conditions in the near-field environment (i.e., temperature, relative humidity, saturation, and flux). The abstraction described in this AMR forms the link between process-level models of the MSTHM and the performance assessment models of TSPA.

5.3 U.S. DEPARTMENT OF ENERGY APPROACH

Results of the MSTHM were obtained by combining output from various submodels to develop a representation of thermohydrologic conditions in the near- and far-field environments resulting from the heat emitted during decay of radioactive waste. The MSTHM used property sets for high, low, and median infiltration rates developed in the Calibrated Properties Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c). Output files from the MSTHM were subsequently binned, averaged, and the extreme values extracted during the abstraction process for use in TSPA. Rather than binning results according to repository subdivisions, as was done for the Viability Assessment (TRW Environmental Safety Systems, Inc., 1998), this AMR binned process-level thermohydrologic results according to infiltration rate during the glacial period. The MSTHM gave output results for 623 repository locations. These results were placed in bins of 0–3, 3–10, 10–20, 20–60, and 60+ mm/yr based on net infiltration at the 623 locations for the simulation time interval 2,000–1,000,000 yr. Note that even though high, low, and median infiltration maps were used in determining the calibrated property sets, the same bins for glacial infiltration rate were used in the abstraction. Thus, for the low infiltration map, only the two lowest infiltration rate bins contained thermohydrologic values and for the high infiltration map, the lowest infiltration rate bin was empty.

Each of the 623 repository locations supplied by the MSTHM represents thermohydrologic conditions expected for a waste package at that physical location. The sum of the areas for a particular glacial infiltration rate bin corresponds to the area of the repository associated with those particular infiltration conditions. Thus, each infiltration rate bin has an associated area weighting factor that accounts for the area of the repository represented by that bin. Average values were calculated for each bin, and the minimum and maximum values were retained. In addition, the number of points in time for thermohydrologic variables was reduced from those supplied by the MSTHM to decrease TSPA runtimes. A section of this AMR attempts to demonstrate that reducing the number of points in time does not diminish temporal resolution of the thermohydrologic variables.

Thermohydrologic variables required by TSPA are averaged values weighted according to the area represented by a given infiltration bin. Averaged quantities are used in the transport and in-drift geochemical models. Raw data directly taken from the MSTHM, however, were binned only with no averaging for use by the waste package corrosion model. In addition to the thermohydrologic variables of temperature, relative humidity, saturation, and flux at various locations within and near the drift, flux from a location 5 m above the drift crown was taken from the MSTHM model and input to the TSPA seepage model.

5.4 STAFF COMMENTS

This AMR describes the reformatting of the MSTHM output into a form suitable for use by TSPA. Thus, concerns identified regarding the MSTHM process-level models and the Calibrated Properties Model used by the MSTHM propagate through this abstraction and into TSPA. These concerns identified in the MSTHM process-level models and Calibrated Properties Model are discussed in other sections of this report. Representation of the thermohydrologic variables used in TSPA from this abstraction are dependent entirely on results from process-level models and property sets.

The greatest difficulty encountered in reviewing this AMR was in following exactly how thermohydrologic variables are actually used in TSPA. Use of these variables is only alluded to, as in the statement on page 18 that "the TSPA model requires infiltration bin averaged quantities for the transport model and the in-drift geochemical models" and the statement on page 36 that "TSPA raw files, a total of 623 location dependent results ..., are used in the waste package corrosion model... ." It is difficult to ascertain from this discussion but perhaps utilizing bin averaged results for some models, such as the in-drift geochemical models, could result in under-representation of variability and uncertainty in the model results.

Most of the concerns regarding this AMR, however, occur in the process-level models and associated property sets that are propagated through this abstraction. For example, the statement, "results of this AMR provide an indication of the variability and uncertainty in the TH parameters that are used to describe the geological system during the thermal perturbation," is true only insomuch as variability and uncertainty are adequately characterized in the MSTHM and calibrated property sets. Host rock variability was accounted for in the MSTHM and calibrated property sets only in relatively smaller changes in the mean parameters representing hydrostratigraphic units, while variability of spatial heterogeneity over several orders of magnitude within hydrostratigraphic units was neglected.

One issue specific to the abstraction of thermohydrologic variables is the use of flux at 5 m above the drift crown as input to the isothermal seepage model to represent liquid water contacting waste packages during the thermal period of the repository. This approach is apparently based on an assumption that thermohydrologic models are wrong regarding fluxes at the drift wall and within the drift and need to be corrected in the abstraction for TSPA. The approach taken of using flux from the MSTHM at 5 m above the drift crown as input to the isothermal seepage model is not entirely physically plausible, however. A more physically based process-level modeling approach where subvertical, high-permeability fractures are included directly in the MSTHM as a submodel could result in a physically based defensible approach to dealing with the potential for liquid water contacting waste packages during the thermal period. Care must be taken with such an approach, however, so that small-scale processes such as preferential fingering flow through above-boiling fractures are not masked by volume-averaging on a mesh size too coarse to resolve the small-scale processes.

5.5 HOW THE ABSTRACTION OF NEAR-FIELD ENVIRONMENT DRIFT THERMODYNAMIC ENVIRONMENT AND PERCOLATION FLUX ANALYSIS/MODEL REPORT ADDRESSES ISSUE RESOLUTION

Thermohydrologic variables calculated using the MSTHM as described in the Multiscale Thermohydrologic Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b) were based on a repository design that includes backfill in the emplacement drifts. Both the MSTHM and the abstraction described in this AMR should represent the final repository design.

As mentioned previously, lateral mass transport involving larger-scale heterogeneities and thermal gradients along the drifts were not accounted for in the MSTHM and the abstracted thermohydrologic variables. Effects of lateral mass transport, such as the potential cold-trap effect, could result in thermohydrologic conditions within the near-field environment and perhaps condensation on the engineered barrier system. Lateral mass transport resulting from thermal gradients and larger scale heterogeneties should be accounted for in the MSTHM, the abstraction, and the TSPA.

A thorough analysis of uncertainty accounting for measurement error and bias, scale dependance, modeling error, spatial heterogeneity at all relevant scales, and variability, as seen in various property sets determined to be valid for modeling thermohydrologic processes, would likely result in more variability in abstracted thermohydrologic variables than is reflected in Revision 00 of the Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux AMR. Uncertainty in thermohydrologic variables from all sources should be included to evaluate potential effects on TSPA.

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6 MOUNTAIN-SCALE COUPLED PROCESSES MODELS ANALYSIS/MODEL REPORT

6.1 OBJECTIVE AND PURPOSE OF THE MOUNTAIN-SCALE COUPLED PROCESSES MODELS ANALYSIS/MODEL REPORT

As stated on page 13 of this AMR, the purpose is to "evaluate the effects of coupled TH processes on mountain-scale conditions at Yucca Mountain, Nevada, with particular attention to the impact of thermal loading on percolation at and near the repository horizon."

6.2 HOW THE MOUNTAIN-SCALE COUPLED PROCESSES MODELS ANALYSIS/MODEL REPORT RELATES TO THERMAL EFFECTS ON FLOW

The AMR documents the only 2- and three-dimensional (3D) thermohydrologic models from DOE that include a scale large enough to explore the effects of large-scale, structural-geologic features (such as faults and dipping stratigraphic interfaces) on ambient and thermally induced moisture flow at Yucca Mountain. Although DOE uses the MSTHM (reviewed in chapter 3 of this report) to develop histories of thermohydrologic field variables abstracted for use in TSPA, the only submodel within the MSTHM group that includes explicit representation of thermohydrologic processes is the drift-scale LDTH submodel, which has restrictive lateral-flow boundary conditions. Consequently, the MSTHM is unable to model lateral mass transport or investigate the effects of large-scale heterogeneities on lateral mass and energy transport. In this respect, the Mountain-Scale Coupled Processes Models AMR has the potential to provide information that may help to evaluate DOE's abstractions of thermohydrologic processes.

6.3 U.S. DEPARTMENT OF ENERGY APPROACH

As described in table 5 on page 43 of the AMR, the Mountain-Scale Coupled Processes Models consist of two 3D models and four 2D models based on two approximately north-south vertical sections through the repository area (also refer to figure 1, page 30, of the AMR). Each of the models extends vertically from the ground surface to a depth of 1,000 m below the water table, except for one 3D model that extends from the ground surface to the water table. Hence, the approach used to represent processes below the water table would benefit from further explanation. The repository is represented as a continuous slab (i.e., individual drifts and pillars are not represented) in the 3D models and one 2D model and as an array of individual drifts separated by pillars in three 2D models. The models were used to develop predictions of temperature, liquid saturation, and flux and to develop estimates of 3D effects on the predictions of these variables. The analyses were performed using TOUGH2 Version 1.4 as stated on page 28 of the AMR.

6.4 STAFF COMMENTS

An important aspect of this AMR that makes it useful for comparisons with the MSTHM is the size of the modeled domain and model dimensionality that permit investigating potential effects of large-scale heterogeneities and lateral flow. Some results presented in this AMR, however, appear to contradict earlier findings. For example, on page 50 of this AMR, the ambient percolation-flux distribution at the repository horizon was found to be almost the same as the surface-infiltration distribution because lateral flow in the PTn hydrostratigraphic unit was not significant except at low infiltration areas. This conclusion is contrary to an earlier conclusion by the same modeling group (Wu et al., 1999) that flow is diverted laterally 500 m or more to the east between the ground surface and the repository horizon. The Wu et al. (1999) conclusion is in agreement with conclusions from other work (Ofoegbu et al., 1999)[1] that also indicates significant lateral flow in the PTn intercepted by faults and causing localized high-flux areas at the repository horizon. This difference between these results and the Wu et al. (1999) results, both obtained by the same modeling group, warrants further explanation.

Assumptions regarding thermal-mechanical effects on permeability of fracture systems are not yet validated (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000l). All models used for calculating thermal effects on flow, including the models described in this AMR, make assumptions that the effects of thermal-mechanical and thermohydrologic-chemical processes on hydrologic properties can be ignored because such effects may be important only at or near drifts during the first few years of the thermal-loading period (page 25 of the AMR). These assumptions need to be validated and the supporting technical bases provided or these effects need to be accounted for in the process-level models and TSPA.

6.5 HOW THE MOUNTAIN-SCALE COUPLED PROCESSES MODELS ANALYSIS/MODEL REPORT ADDRESSES ISSUE RESOLUTION

FEPs of thermal-mechanical and thermohydrologic-chemical effects on fracture permeability that may potentially affect thermohydrologic variables are excluded from this AMR and other AMRs without sufficient technical bases supporting the screening arguments. The assumptions made for excluding these FEPs remain to be validated.

Confidence in the completeness of the thermohydrologic variables abstracted for TSPA would be enhanced by including results of larger-scale, 2D and 3D coupled process models, such as those described in this AMR, in the abstractions. Also, more thorough comparisons of the results of these models against results computed using the MSTHM would assist in understanding the effects of lateral mass transport and large-scale heterogeneities. A more thorough comparison and evaluation of the effects of lateral flow would lead toward resolution of the concerns discussed in this report.

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[1] Ofoegbu, G.I., S. Painter, R. Chen, R.W. Fedors, and D.A. Ferrill. Geomechanical and thermal effects on moisture flow at the proposed Yucca Mountain nuclear waste repository. *Nuclear Technology*. In review.

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7 VENTILATION MODEL ANALYSIS/MODEL REPORT

7.1 OBJECTIVE AND PURPOSE OF THE VENTILATION MODEL ANALYSIS/MODEL REPORT

The purpose of the Ventilation Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999a), as stated on page 9 of the AMR, "is to analyze the effects of pre-closure continuous ventilation in the Engineered Barrier System (EBS) emplacement drifts and provide heat removal data to support EBS design. It will also provide input data (initial conditions, and time varying boundary conditions) for the EBS postclosure performance assessment and the EBS Water Distribution and Removal Process Model."

7.2 HOW THE VENTILATION MODEL ANALYSIS/MODEL REPORT RELATES TO THERMAL EFFECTS ON FLOW

Thermal Effects on Flow KTI is concerned with evolution of the thermohydrologic field variables saturation, flux, temperature, and relative humidity in the near- and far-field environments resulting from the heat generated by decay of nuclear waste. Ventilation during the repository preclosure period will strongly influence these thermohydrologic variables. In fact, the design objective of maintaining between-drift pillar temperatures below boiling to allow drainage of thermally mobilized condensate to depths below the repository horizon is dependent on the efficacy of the preclosure ventilation system.

7.3 U.S. DEPARTMENT OF ENERGY APPROACH

The Ventilation Model as described in the Ventilation Model AMR (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999a) was based on heat conduction only using the commercially available computer program ANSYS Version 5.2. Moisture removal by ventilation and potential water movement in the rock mass were not included in the model. Heat removal by ventilation was based on airflow rates of 10 and 15 m^3/s. The approach used with the program ANSYS was developed to obtain only an approximate solution to the complete problem of heat transfer by conduction, advection, radiation, and interaction with the thermally perturbed rock mass. The ventilated drift was treated as a series of finite drift segments. Thermal analysis with the program ANSYS was performed for each drift section sequentially from the beginning at the air-inlet to the end at the air-exhaust. Heat transfer processes for the entire drift were evaluated by assembly and comparison of the results from individual segments. The entire drift was considered as a series of connected drift segments, and calculations were performed sequentially for each time step to predict rock temperature distributions in the vicinity of the drift segment. Using the average wall temperature of the drift segment together with the mean airflow temperature, the convective heat transfer rate in each segment was calculated from Newton's cooling law. Increase in internal thermal energy of the air and mean air temperature of air flow exiting the drift segment were then used as input for the next drift segment. This process was performed repetitively until the calculation reached the last drift segment at the end of the drift. When calculations for all drift segments were completed for a time step, the results were then used as input to the next time step. Heat removal calculated by this method showed 68 percent of the heat generated after 50 yr was removed by an air flow rate of 10 m^3/s, and 74 percent of the heat generated after 50 yr was removed by an air flow rate of 15 m^3/s.

7.4 STAFF COMMENTS

The Ventilation Model used in this analysis considered only sensible heat transfer. The actual situation occurring during ventilation of a potential repository drift would be much more complex than the simplified model considered in this AMR. Convective heat transfer from waste package to air flow, thermal radiation between waste package and drift wall, convective heat transfer between drift wall and air flow, and conduction heat transfer within the rock mass are all time-dependent and coupled throughout the ventilation process. Presumably, because the air temperature leaving the exhaust was higher than air temperature at the inlet, waste packages and the drift environment would also be hotter near the exhaust. This situation could result in gradational heat removal where most of the heat is removed near the inlet at early time while heat is removed closer to the exhaust later in time as the entire drift cools. This situation could result in different distributions of thermohydrologic variables than computed from the MSTHM, where heat loss representing ventilation was removed uniformly from the entire drift length. Considering nonuniform heat removal along with thermohydrologic interactions may have consequences to model results.

Staff believe it is difficult to ascertain from this simplified approximate calculation whether or not the Ventilation Model results are adequate or if the uniform heat loss distribution assumption in the MSTHM is adequate. Conclusions drawn from simplified models incorporating unsubstantiated assumptions do not have an adequate supporting technical basis. At a minimum, the Ventilation Model needs to be supported by experimental results. In addition, monitoring the rock mass and checking repository conditions within drifts against the model predictions during the ventilated preclosure period would help increase confidence in the adequacy of the Ventilation Model.

7.5 HOW THE VENTILATION MODEL ANALYSIS/MODEL REPORT ADDRESSES ISSUE RESOLUTION

The Ventilation Model should be supported by results from experimental investigations. Once the Ventilation Model is supported and validated by comparisons to experimental data, staff will review and evaluate incorporation of the effects of ventilation in thermohyrologic models and on thermohydrologic conditions calculated and abstracted for TSPA.

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8 SUMMARY

8.1 SYSTEM DESCRIPTION AND MODEL INTEGRATION

An apparent inadequacy in the present MSTHM approach is omission of potential lateral mass transport and the cold-trap effect. Mass movement along the length of drifts from thermal gradients may result in condensation in the cooler regions. The SMT submodel of the MSTHM shows the repository edge to be cooler than the central regions. This temperature gradient could cause vapor flow, condensation, and moisture deposition on engineered components in cooler regions of the repository.

8.2 DATA AND MODEL JUSTIFICATION

Heat removal by ventilation was represented in the thermohydrologic models as a 70 percent heat reduction for the 50 yr preclosure period. However, ventilation air would enter the drifts at a relatively low temperature and exit at a higher temperature, potentially creating a temperature gradient in drifts in addition to gradients resulting from repository edge-cooling effects. These drift-parallel gradients and resulting lateral mass transport are not incorporated in the thermohydrologic models. Experimental investigations of ventilation are needed to provide data on the effects of ventilation and support for implementation of ventilation in thermohydrologic models.

8.3 DATA UNCERTAINTY

Regarding uncertainties in the calibrated property sets used in the MSTHM, the Calibrated Properties Model (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c) states, "[q]uantifiable uncertainties are difficult if not impossible to establish for the estimated parameter sets." However, the range of uncertainties in the property sets, and thus the variables calculated from them, may be significantly under-represented. Measurement error, bias, and scale dependence in the saturation, water potential, and pneumatic pressure data used in the inversion are not adequately represented in the calibrated properties or in the variables calculated using the MSTHM. The nonlinear least-squares maximum likelihood inverse method used in the Calibrated Properties Model is essentially deterministic in that the only source of randomness or uncertainty is in the measurement error. Thus, the measurement error must be generalized to include such things as scale-dependence and modeling errors because there is no other way to account for uncertainty in the least-squares inverse approach (McLaughlin and Townley, 1996).

A discussion of the calibrated property sets (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c) states, "[h]eterogeneity of hydrologic properties is predominantly a function of geological layering." In the calibrated properties, each geological layer in the model is homogeneous and the difference in permeabilities between comparable welded layers is usually within about one order of magnitude. A statistical analysis of air-injection data collected from the niches in the ESF, however, found fracture permeabilities varying by about five orders of magnitude (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b).

The Thermal Tests Thermal-Hydrological AMR compared several different property sets and found that, of "the numerous combinations of property sets and thermal tests considered in the analyses, no one property set is distinctly superior in simulating thermal response" and that, based on comparisons of measured with modeled temperatures, all the models and property sets "considered were sufficiently valid for the purposes of these analyses" (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a). Comparison of model results for variables such as fracture saturations and fluxes, however, shows significant differences in results computed using the different property sets.

A thorough evaluation of uncertainty in data should include (i) measurement error, bias, and scale-dependence in the saturation, water potential, and pneumatic pressure data used for model parameter calibration; (ii) heterogeneity and spatial variability in thermohydrologic properties; and (iii) variability in model results using the various property sets found to be valid for thermohydrologic modeling.

8.4 MODEL UNCERTAINTY

Uncertainty in thermohydrologic process models is a combination of parameter uncertainty and conceptual model uncertainty. Uncertainty in fracture fluxes and losses through the bulkhead of the DST create uncertainty in validating conceptual thermohydrologic models. Uncertainty inherent in conceptual models, however, may be evaluated from the range of results predicted by alternative conceptual models. Incorporating results from various models in the abstraction of thermohydrologic variables for performance assessments would allow evaluation of the effects of model uncertainty.

Use of flux at 5 m above the drift crown as input into the isothermal seepage model to represent liquid water contacting waste packages during the thermal period of the repository seems to imply that thermohydrologic model predictions of fluxes at the drift wall are incorrect. Physically based process-level models incorporating small-scale heterogeneities, such as subvertical, high-permeability fractures and preferential flow, may be necessary to appropriately account for potential near-field fluxes during the thermal period.

8.5 MODEL SUPPORT

Confidence in the evaluation of thermohydrologic variables and associated uncertainty would be enhanced by including results of larger-scale 2D and 3D coupled process models, such as those described in the Mountain-Scale Coupled Processes Model. More thorough evaluation of the effects of lateral mass transport and heterogeneities on all important scales is also needed and would help with alleviating concerns discussed in this report.

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9 REFERENCES

Civilian Radioactive Waste Management System Management and Operating Contractor. *Ventilation Model.* ANL–EBS–MD–000030. Revision 00. Las Vegas, NV: TRW Environmental Safety Systems, Inc. 1999a.

Civilian Radioactive Waste Management System Management and Operating Contractor. *In Situ Field Testing of Processes.* ANL–NBS–HS–000005. Revision 00. Las Vegas, NV: TRW Environmental Safety Systems, Inc. 1999b.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Thermal Tests, Thermal-Hydrological Analyses/Model Report.* ANL–NBS–TH–000001. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000a.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Multiscale Thermohydrologic Model.* ANL–EBS–MD–000049. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000b.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Calibrated Properties Model.* ANL–NBS–HS–000003. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000c.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Abstraction of Near-Field Environment Drift Thermodynamic Environment and Percolation Flux.* ANL–EBS–HS–000003. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000d.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Mountain-Scale Coupled Processes (TH) Models.* MDL–NBS–HS–000007. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000e.

Civilian Radioactive Waste Management System Management and Operating Contractor. *In-Drift Thermal-Hydrological-Chemical Model.* Revision 00. ANL–EBS–MD–000026. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000f.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Drift Scale Coupled Processes (DST, THC Seepage) Models.* Revision 00. MDL–NBS–HS–000001. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000g.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Unsaturated Zone Flow and Transport Process Model Report.* Revision 00. Preliminary Draft. TDR–NBS–HS–000002. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000h.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Seepage Model for PA Including Drift Collapse*. MDL–NBS–HS–000002. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000i.

Civilian Radioactive Waste Management System Management and Operating Contractor. *UZ Flow Models and Submodels*. MDL–NBS–HS–000006. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000j.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Input Transmittal to Performance Assessment for Multiscale Thermohydrologic Model*. ANL–EBS–MD–000049. 00176T. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000k.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Features, Events, and Processes in Thermal Hydrology and Coupled Processes*. ANL–NBS–MD–000004. Revision 00. North Las Vegas, NV: Civilian Radioactive Waste Management System, Management and Operating Contractor. 2000l.

Civilian Radioactive Waste Management System, Management and Operating Contractor. *Development Plan for the Ventilation Test*. TWP–EBS–MD–000001. Revision 00. North Las Vegas, NV. Civilian Radioactive Waste Management System, Management and Operating Contractor. 2000m.

Gelhar, Lynn. *Stochastic Subsurface Hydrology*. Englewood Cliffs, NJ: Prentice Hall. 1993.

Green, R.T., D.L. Hughson, S.L. Painter, and M.E. Hill. *Evaluation of the Drift-Scale Heater Test Thermal-Hydrological Conceptual Model, Data, and U.S. Department of Energy Thermal Test Results–Status Report*. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

Kreith, F., and M.S. Bohn. *Principles of Heat Transfer*. 5th Edition. New York: West Publishing Company. 1993.

Liu, H.H., C. Doughty, and G.S. Bodvarsson. An Active fracture model for unsaturated flow and transport in fractured rocks. *Water Resources Research* 34(10): 2,633–2,646. 1998.

McLaughlin, D., and L.R. Townley. A reassessment of the groundwater inverse problem. *Water Resources Research* 32(5): 1,131–1,161. 1996.

Ofoegbu, G.I. *Thermal-Mechanical Effects on Long-Term Hydrological Properties at the Proposed Yucca Mountain Nuclear Waste Repository*. CNWRA 2000-03. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

Ofoegbu, G.I., A.C. Bagtzoglou, R.T. Green, and M.A. Muller. Effects of perched water on thermally driven moisture flow at the proposed Yucca Mountain repository for high-level nuclear waste. *Nuclear Technology* 125: 235–253. 1999.

Or, D., and T.A. Ghezzehei. Dripping into subterranean cavities from unsaturated fractures under evaporative conditions. *Water Resources Research* 36(2): 381–393. 2000.

Or. D., and M. Tuller. Flow in unsaturated fractured porous media: Hydraulic conductivity of rough surfaces. *Water Resources Research* 36(5): 1,165–1,177. 2000.

TRW Environmental Safety Systems, Inc. *Total System Performance Assessment—Viability Assessment Analyses—Technical Basis Document.* B00000000–01717–4301–00001. Revision 01. Las Vegas, NV: TRW Environmental Safety Systems, Inc. 1998.

Wu, Y-S., C. Haukwa, and G.S. Bodvarsson. A site-scale model for fluid and heat flow in the unsaturated zone of Yucca Mountain, Nevada. *Journal of Contaminant Hydrology* 38: 185–215. 1999.