OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

ERRATA

QA: QA

Page 1 of 3

1. TER No. TER-03-0012DC Tracking No. 34955

2. Product ID: ANL-EBS-MD-000030	Title: Ventilation Model Report	Revision: 02
3. Location	4. Clarification/Restriction	
page 29, Figure 6-1	Replace MULTIFLUX with DriftFlow in one instance, and with Analytical in another. See the attached Addendum 1 for the revised Figure 6-1.	
page 54, Table 6-6, note 1	Attachment VIII-11, flux based on the mean saturation of 0.76	
page 54, Table 6-6, note 2	Attachment VIII-14, flux based on the mean saturation plus ⁵ one standard deviation 0.91 <i>1-20-03</i>	
VIII-9, first sentence	The mean saturation from these 377 measurements is 0.76.	
page 60, last paragraph, first sentence	Moyné et al. 1990 (p. 116) attributes the weak dependence on temperature to the strong bond between vapor molecules and the solid.	
page 61, second paragraph, first sentence	Moyné et al. 1990 (Figure 6) also presents resistance factors for a lightweight concrete, and a C/SiC composite material as a function of the humidity ratio.	
page 70, Figure 6-21	Remove the reference to NUFT. See Addendum 2 for the revised Figure 6-21	
page 94, Section 7.1.3, first paragraph, first and second sentences	Conduction heat transfer dominates other heat transfer mechanisms (i.e. convection in fractures and lithophysae, and latent heat) in the host rock. This is based on results from the Multiscale Thermohydrologic Model (BSC 2001), and is also supported by data and modeling of the Drift Scale Test and earlier work by Sass (Sass et al. 1988).	
page 101, Section 9.5, last DTN	MO021MWDDFC02.005. DriftFlow Calculations in Support of the Ventilation Model Report (ANL-EBS-MD-000030 REV 02). Chipman, V. Las Vegas, Nevada.	
page I-3, columns 2, 3, and 4 of table (3) Decay of Linear and Volumetric Heat Load	Remove references (page II-3), (page II-3), and (page II-2)	
page VIII-2, first paragraph	Remove first paragraph that starts "Electronic files with their name and size are listed as follows:" The first paragraph of Attachment VIII-2 should begin with the paragraph that starts "Develop a steady state solution..."	
page VIII-4, Figure VIII-1	Remove Figure VIII-1	
page VIII-6 through VIII-13, and VIII-15 through VIII-22	The use of := is a MathCad operator which means "assign the right hand value or expression to the left hand variable"	
page VIII-18, first paragraph, second line	Remove the "rectangular" symbol after the greek letter psi	
5. QER Review: (Print Name) <i>Kenneth O. Gihlerson</i> (See Addendum 1)	Initials: <i>KG</i> (See Addendum 2)	Date: <i>1/20/2003</i> (See Addendum 3)
6. Responsible Manager: (Print Name) <i>Dan Thomas</i> (See Addendum 4)	Initials: <i>DT</i> (See Addendum 5)	Date: <i>1/20/03</i> (See Addendum 6)

Addendum 1

Figure 6-1. Conceptual Model for Heat and Mass Transfer Within and Around an Emplacement Drift

Addendum 2

Figure 6-21. Analytical and ANSYS Conduction-Only Transient Temperature Responses of a Homogeneous Porous Medium with Material and Thermal Properties of tsw-35 Rock (DTN MO0209MWDMOD30.003)

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT MODEL COVER SHEET

1. QA: QA
Page: 1 of: 102

Complete Only Applicable Items

2. Type of Mathematical Model

☒ Process Model ☐ Abstraction Model ☐ System Model

Describe Intended Use of Model:

Conceptual model for ventilation and its numerical applications and validation

Technical Contact/Department:
EBS

3. Title:
Ventilation Model Report

4. DI (including Rev. No. and Change No., if applicable):
ANL-EBS-MD-000030 REV 02

5. Total Attachments:
8

6. Attachment Numbers - No. of Pages in Each:
I-3, II-3, III-3, IV-2, V-2, VI-3, VIII-22

VII-2

	Printed Name	Signature	Date
7. Originator	Veraun Chipman*		12/20/02
8. CSO	Bruce Kirstein		12/20/02
9. Checker	Jim Kam		12/20/02
10. QER	Ken McFall		12/20/02
11. Responsible Manager/ Lead	Veraun Chipman		12/20/02
12. Responsible Manager	Dan Thomas		12/20/2002

13. Remarks:

*Other Originators: John Case

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

MODEL REVISION RECORD

1. Page: 2 of 102

2. Model Title:

Ventilation Model Report

3. DI (including Rev. No. and Change No., if applicable):

ANL-EBS-MD-000030 REV 02

4. Revision/Change No.	5. Description of Revision/Change
00	Initial issue
01	Complete Revision
01 ICN 01	<p>Issued for checking...for clarification purposes ICN 01 adds definitions for the ventilation heat removal efficiency (Section 6.1.3) and energy balance checks on the downstream use of the heat removal efficiencies to deliver the right amount of energy to the host rock (Section 6.6.2.1 through 6.6.2.3)</p>
02	<p>The use of Multiflux v.2.2 (STN 10485-2.2-10/29/02) software in ANL-EBS-MD-000030 REV 01 ICN 01, correctly characterized as an unqualified code was issued after the exemption for the interim use of unqualified software (Section 5.10) had expired in August, 2002. Work with the Multiflux v2.2 software had actually been performed in March 2002 when the exemption was in effect and full qualification/baselining of the code was in progress. However, a Project-level business decision was made to discontinue efforts to qualify the code. The significance of this decision with regard to the inclusion of the Multiflux work in the Report was not fully appreciated until the ANL-EBS-MD-000030 REV 01 ICN 01 was approved and issued on 10/29/02. A noncompliance was identified as Quality Observation BSC(B)-03-0-029 for the following reasons:</p> <ol style="list-style-type: none"> 1) The noncompliance is not a significant condition adverse to quality. Multiflux v2.2 was used in the corroboration of the ventilation model; 2) The noncompliance appears to be isolated and attributable to the unusual situation in which a business, not technical, decision resulted in abandoning software qualification activities; 3) The noncompliance requires only remedial action applicable to the ANL-EBS-MD-000030 REV 01 ICN 01; 4) The noncompliance has no impact or residual impact upon completion of the remedial action. Since Multiflux v2.2 was used for corroboration, software output will not be used as input/feeds to downstream analyses; 5) The noncompliance does not require a cause determination; the cause is known, and the uniqueness of the circumstances which led to the noncompliance suggest that specific actions to preclude are not needed. <p>ANL-EBS-MD-000030 REV 01 ICN 01 was revised to remove the discussion of the corroborative model using Multiflux v2.2, and other approaches were used to corroborate the ventilation model and assess the impacts of moisture on the ventilation efficiency.</p>

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1. PURPOSE

The purpose of the Ventilation Model is to simulate the heat transfer processes in and around waste emplacement drifts during periods of forced ventilation. The model evaluates the effects of emplacement drift ventilation on the thermal conditions in the emplacement drifts and surrounding rock mass, and calculates the heat removal by ventilation as a measure of the viability of ventilation to delay the onset of peak repository temperature and reduce its magnitude. The heat removal by ventilation is temporally and spatially dependent, and is expressed as the fraction of heat carried away by the ventilation air compared to the fraction of heat produced by radionuclide decay. One minus the heat removal is called the wall heat fraction, or the remaining amount of heat that is transferred via conduction to the surrounding rock mass. Downstream models, such as the *Multiscale Thermohydrologic Model* (BSC 2001), use the wall heat fractions as outputted from the Ventilation Model to initialize their post-closure analyses.

The Ventilation Model report was initially developed to analyze the effects of preclosure continuous ventilation in the Engineered Barrier System (EBS) emplacement drifts, and to provide heat removal data to support EBS design. Revision 00 of the Ventilation Model included documentation of the modeling results from the ANSYS-based heat transfer model. Revision 01 ICN 01 included the results of the unqualified software code MULTIFLUX to assess the influence of moisture on the ventilation efficiency. The purposes of Revision 02 of the Ventilation Model are:

1. To validate the conceptual model for preclosure ventilation of emplacement drifts and verify its numerical application in accordance with new procedural requirements as outlined in AP-SIII-10Q, *Models* (Section 7.0).
2. To satisfy technical issues posed in KTI agreement RDTME 3.14 (Reamer and Williams 2001a). Specifically to demonstrate, with respect to the ANSYS ventilation model, the adequacy of the discretization (Section 6.2.3.1), and the downstream applicability of the model results (i.e. wall heat fractions) to initialize post-closure thermal models (Section 6.6).
3. To satisfy the remainder of KTI agreement TEF 2.07 (Reamer and Williams 2001b). Specifically to provide the results of post-test ANSYS modeling of the Atlas Facility forced convection tests (Section 7.1.2). This portion of the model report also serves as a validation exercise per AP-SIII.10Q, *Models*, for the ANSYS ventilation model.
4. To assess the impacts of moisture on the ventilation efficiency.

The scope of developing, validating, and implementing the Ventilation Model is described in the *Technical Work Plan for Engineered Barrier System Department Modeling and Testing FY 02 Work Activities* (BSC 2002a). The work presented in this report is consistent with the EBS TWP with the following exception. The TWP specified that the Multiflux software be used to evaluate the effects of moisture removal during the ventilation period. At the time of this writing, a qualified version of Multiflux was not available, and could not be used in the ventilation analysis. The software program DRIFTFLOW V1.0 which is qualified as discussed in Section 3 was used for evaluation of the effects of moisture removal during the ventilation period.

The scope of the model documentation includes:

1. A description of the conceptual and numerical model for the heat transfer mechanisms in ventilated emplacement drifts and in the surrounding host rock.
2. A description of an alternative conceptual model and its applications, which assess the impacts of moisture, phase change, and mass transport on the ability of the ventilation system to remove heat from an emplacement drifts.
3. A discussion of the applicability of the wall heat fraction to initialize downstream post-closure thermal models.
4. Documentation of the model validation approach.

The primary limitation of this version Ventilation Model Report is that it does not attempt to predict repository performance during the preclosure period for the License Application. Rather, the intended purpose of the report is to validate a conceptual model for preclosure ventilation that may be exercised in subsequent and future analyses. Therefore, the use of the results presented herein is limited to the validation and verification processes of Sections 6 and 7. The DTNs of model output associated with this report should not be categorized as Technical Product Output for use in other models or analyses.

2. QUALITY ASSURANCE

The technical work and development of both a conceptual model and an alternative conceptual mode for preclosure ventilation heat transfer contained in this model report is a part of the EBS Modeling and Testing tasks listed in the EBS TWP (BSC 2002a), and classifies the activities to prepare, complete, and issue the Ventilation Model as Quality Affecting. Refer to the TWP for the work package numbers. Therefore, this document is subject to the requirements of the *Quality Assurance Requirements and Description* (QARD) document (DOE 2000). A Technical Change Request (T2001-0172) was approved in accordance with AP-3.4Q, *Level 3 Change Control*. The repository subsurface ventilation system has been classified as Conventional Quality from *Classification of the MGR Subsurface Ventilation System* (CRWMS M&O 1999a). The governing procedure for preparation of this model report is OCRWM procedure AP-SIII.10Q, *Models*.

Qualified and accepted input data and references have been identified. All electronic data used during the preparation of this Model Report were obtained from the Technical Data Management System as appropriate. Electronic data were controlled and managed in accordance with AP-SV.1Q, *Control of the Electronic Management of Information*. Computer software and model usage is discussed in Section 3 of this document.

3. USE OF SOFTWARE

Computer software was used in the preparation of this Model Report. Table 3-1 lists the software used as well as the software tracking numbers (where appropriate), CPU(s), operating systems, and physical location where the software was installed. All software listed in Table 3-1 was obtained from Software Configuration Management, was appropriate for the applications used, and was used within the range of validation in accordance with AP-SI.1Q, *Software Management*. Use of software has been documented in accordance with AP-SI.1Q.

Table 3-1. Software

Code	Software Tracking Number	CPU	Physical Location	Operating System
ANSYS V5.6.2	10145_5.6.2-00	SGI Octane, M&O #114441	Las Vegas, NV	IRIX 6.5
	10145_5.6.2-01	Sun Microsystems UltraSPARC, M&O #117683		Solaris 2.7
DriftFlow V.1.0	10722-1.0-00	Dell Pentium Workstation, M&O #151635	Las Vegas, NV	Windows 2000
Mathcad 2001 Professional	Exempt	Dell Pentium Workstation, M&O #151635	Las Vegas, NV	Windows 2000
Microsoft Excel 97	Exempt	Various YMP M&O Computers	Las Vegas, NV	Windows 95, Windows 2000

3.1 ANSYS V5.6.2

ANSYS v5.6.2 is a commercially available computer program and is classified as qualified software (per AP-SI.1Q, *Software Management*). ANSYS v5.6.2 is used to implement the ventilation conceptual model in one of two alternate numerical model calculations. ANSYS v5.6.2 is a general purpose finite element analysis (FEA) code, and is used in many disciplines of engineering that deal with topics including structural, geotechnical, mechanical, thermal, and fluids. ANSYS was used to numerically implement the ventilation conceptual model. Two ANSYS numerical models for ventilation are presented herein, ANSYS-Coarse and ANSYS-Refined.

3.2 DriftFlow V.1.0

DriftFlow v.1.0 is classified as qualified software (per AP-SI.1Q, *Software Management*). DriftFlow v.1.0 is used to implement the conceptual model similar to the ANSYS numerical models. DriftFlow v.1.0 was also used to implement parts of the alternative conceptual model.

3.3 Mathcad 2001 Professional

Mathcad 2001 Professional is a commercially available software package. The Mathcad software provides a technical computing environment centered on real mathematical expressions and notation. For this Model Report, the Mathcad software was used to solve an analytical expression as part of the host rock submodel validation exercises of Section 7. The Mathcad

software is an exempt software product in accordance with AP-SI.1Q. The formulas used, as well as their inputs and outputs, are documented in Attachments VI and VIII.

3.4 Microsoft Excel 97

Microsoft Excel 97 is a commercially available spreadsheet software package. Excel 97 is used in conjunction with the ANSYS v5.6.2 software to numerically implement the ventilation conceptual model. It is also used to make plots of data and perform computations using standard functions such as cell addition, subtraction, multiplication, and division. The Excel 97 software is an exempt software product in accordance with AP-SI.1Q. Only standard functions and formulas are used. They are documented in Attachments I, II, IV, V, and VI, and DTNs MO0210MWDTVE30.018, MO0210MWDTEM30.019, MO0209MWDANS30.017, MO0210MWDVEN30.005, and MO0212MWDDFC02.005. Sections 4 and 5 list the inputs to the formulas, and Section 6 and 7 present the output.

4. INPUTS

This section describes data, parameters, and criteria used to develop and validate the Ventilation Model. All data and parameters in this model report are used solely as inputs in the development of the numerical applications of either the ventilation conceptual model or the alternative conceptual model. As stated in Section 1, this version of the Ventilation Model Report does not attempt to predict repository performance during the preclosure period for the License Application. In addition, the DTNs produced by this report are not categorized as Technical Product Output for use in other models or analyses.

4.1 DATA AND PARAMETERS FOR THE VENTILATION MODELS

This section describes the data and parameters, and their sources, used to develop, numerically apply, and validate the ventilation conceptual and alternative conceptual models.

4.1.1 Emplacement Drift Location within the Repository Footprint

Northing 233760 and easting 170750 (CRWMS M&O 1999b) was chosen as a representative location within the repository footprint for the emplacement drift inlet of the ventilation model. This location is considered representative in terms of its distance from an edge of the footprint, geology and infiltration rate. It is from this location that the stratigraphic unit thicknesses and material and thermal properties were taken (Section 4.1.2).

4.1.2 Thickness, Density, Thermal Conductivity, and Specific Heat of the ANSYS Stratigraphic Units

The thicknesses of the ANSYS stratigraphic units (northing 233760, easting 170750), rock grain density, thermal conductivity, and specific heat used in the ANSYS model are listed in Table 4-1. These are average values at this location within the repository emplacement area (DTN: SN0003T0571897.013 and summarized by CRWMS 1999b). Note that DTN: SN0003T0571897.013 is unqualified and has been superseded by DTN: SN0011T0571897.014. Revision 00 of this report used DTN: SN0003T0571897.013 in an ANSYS based ventilation model. Because a primary purpose of this report is to compare various numerical models for corroboration and validation, subsequent models also used DTN: SN0003T0571897.013 to facilitate the comparisons without having to rerun the older case. Also note that there is no accounting in the ANSYS-based models for porosity. Therefore, the grain density shown in Table 4-1 represented the bulk density in the ANSYS-based models.

In order to determine the thickness of Tpcrv down to Tpcpv3, the following calculation is necessary. The average elevations of the surface and the top of Tpcpv2 are 1421.28 m and 1306.98 m (CRWMS M&O 1999b) respectively. Therefore, the thickness of the overburden above Tpcpv2 is 114.3 m (surface elevation - Tpcpv2 elevation).

In addition, the average elevation of the repository horizon (drift bottom) is 1072.3 m (DTN: SN0003T0571897.013). Therefore, the depth to the spring line of the emplacement drift is

calculated to be 346.23 m (surface elevation - repository horizon elevation - half the drift diameter).

The thickness of the units from Tpcpv2 (including Tpcpv2) down to Tacbt is 492.27 m as calculated from the unit thickness data of Table 4-1. Therefore, the total thickness for all the stratigraphic units shown in Table 4-1 is 606.57 m (overburden above Tpcpv2 + thickness of Tpcpv2 down to Tacbt). The thickness from the emplacement drift spring line to the bottom of the Tacbt unit is 260.34 m (total thickness - depth from the ground surface to the drift spring line).

This information is used in constructing the ANSYS ventilation models of Section 6.

Table 4-1. Thermal Modeling Parameters by Stratigraphic Unit

T/M Unit	USGS Unit	ISM 3.0	Thickness	Grain Density	Thermal Conductivity		Specific Heat			
			(m)	(kg/m ³)	T<100°C (wet)	T>100°C (dry)	T<95°C	95°C<T<114°C	T>114°C	
					(W/m·K)		(J/kg·K)			
TCw	Tpcrv	No Data	No Data	2550	2.00	1.60	823	3879	823	
	Tpcrn	No Data	No Data	2550	2.00	1.60	823	3879	823	
	Tpcrl	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	
	Tpcpul	No Data	No Data	2520	1.67	1.23	882	4352	882	
	Tpcpmn	No Data	No Data	2510	1.94	1.53	837	4010	837	
	Tpcpll	No Data	No Data	2510	1.76	1.02	847	4019	847	
	Tpcpln	No Data	No Data	2510	1.88	1.28	837	4010	837	
	Tpcplnc	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	
PTn	Tpcpv	3	Tcpv3	0.0	2470	0.98	0.54	857	4570	857
		2	Tcpv2	5.49						
	Tpcpv1	Tcpv1	4.69	2380	1.07	0.50	1037	6048	1037	
	Tpbt4	Tcbt4	0.53	2340	0.5	0.35	1077	21976	1077	
	Tpy	Yucca	7.05	2400	0.97	0.44	849	16172	849	
	Tpbt3	Tcbt3_dc	4.58	2370	1.02	0.46	1016	20669	1016	
	Tpp	Pah	14.09	2260	0.82	0.35	1330	25560	1330	
	Tpbt2	Tpbt2	9.69	2370	0.67	0.23	1224	23878	1224	
	Tptrv3	Tptrv3	4.58	2510	1.00	0.37	834	5137	834	
	Tptrv2	Tptrv2	0.53							
TSw1	Tptrv1	Tptrv1	1.06	2550	1.62	1.06	866	5629	866	
	Tptrn	Tptrn	46.85							
	Tptrl	Tptrl	8.98							
	Tptpul	Tptpul	77.68							
TSw2	Tptpmn	Tptpmn	29.94	2530	2.33	1.56	948	4568	948	
	Tptpll	Tptpll	106.21	2540	2.02	1.20	900	4663	900	
	Tptpln	Tptpln	47.73	2560	1.84	1.42	865	4523	865	
TSw3	Tptpv3	Tptpv3	20.61	2360	2.08	1.69	984	1958	984	
CHn1	Tptpv2	Tptpv2	2.99							
	Tptpv1	Tptpv1	11.27							
	Tpbt1	Tpbt1	3.35	2310	1.31	0.7	1057	21076	1057	
	Tac5	Tac(v)	Calico	84.37	2240	1.17	0.58	1201	23863	1201
	Tac4									
	Tac3									
Tac2	Tac(z)	2350			1.2	0.61	1154	22086	1154	
Tac1										
CHn2	Tacbt					2440	1.35	0.73	1174	13561

DTN: SN0003T0571897.013

4.1.3 Atmospheric Pressure

At the average elevation of the repository horizon, 1072.3m (Section 4.1.2), the barometric pressure is 89,060 Pa (Hartman 1982). This input is used for all ANSYS calculations of Section 6 as well as the submodel verification exercises of Section 6.5.

4.1.4 Stefan-Boltzmann Constant

The Stefan-Boltzmann constant for radiative heat transfer calculations is $5.669 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$ (Icropera and DeWitt 1996). This input is used throughout for all radiative heat transfer calculations of Section 6 as well as the submodel verification exercises involving radiation of Section 6.5.

4.1.5 Waste Package Thermal Properties

The thermal properties for the waste package outer shell are listed in Table 4-2. These values are for Alloy 22 material based on *Thermal Calculation of the Waste Package with Backfill* (CRWMS M&O 1999c). This input is used for all ANSYS calculations of Section 6 as well as the submodel verification exercises of Section 6.5.

Table 4-2. Thermal Properties for Waste Package

Parameter	Value
Density (kg/m^3)	8690
Thermal Conductivity ($\text{W/m}\cdot\text{K}$)	12.52 ^a
Specific Heat ($\text{J/kg}\cdot\text{K}$)	435.25 ^b
Emissivity	0.87

Note: ^a Averaged value over the temperature range of 48 to 300°C.

^b Averaged value over the temperature range of 52 to 300°C.

4.1.6 Emplacement Drift Spacing

The emplacement drift spacing is 81 meters centerline to centerline from the *Emplacement Drift System Description Document* (CRWMS M&O 2000b). This information is used for establishing adiabatic boundary conditions for all ANSYS calculations of Section 6 as well as the submodel verification exercises of Section 6.5.

4.1.7 Waste Package Spacing

The waste packages are spaced 10 cm apart from the *Emplacement Drift System Description Document* (CRWMS M&O 2000b). This input is used for all ANSYS calculations of Section 6.

4.1.8 Emplacement Drift Diameter

The diameter of the waste emplacement drifts is 5.5 m from the *Emplacement Drift System Description Document* (CRWMS M&O 2000b). This input is used for all ANSYS calculations of Section 6 as well as the submodel verification exercises of Section 6.5.

4.1.9 Ventilation Air Properties

The properties of the ventilation air are listed in Table 4-3. The values of density, dynamic viscosity, thermal conductivity, and specific heat are based on an intake air temperature of 25°C (Section 5.6) and an atmospheric pressure of 89,060 Pa (Section 4.1.3). The other properties listed in Table 4-3 are derived using the following equations.

$$\nu = \frac{\mu}{\rho}$$

Eq. 4-3

$$\alpha = \frac{k}{\rho c_p}$$

Eq. 4-4

$$Pr = \frac{\nu}{\alpha}$$

Eq. 4.5

where

- ν = kinematic viscosity (m^2/s)
- μ = dynamic viscosity ($\text{kg}/\text{m}\cdot\text{s}$)
- ρ = density (kg/m^3)
- α = thermal diffusivity (m^2/s)
- k = thermal conductivity ($\text{W}/\text{m}\cdot\text{K}$)
- c_p = specific heat ($\text{J}/\text{kg}\cdot\text{K}$)
- Pr = Prandtl number (dimensionless)

The air properties and parameters in Table 4-3 are held constant throughout the length of the emplacement drifts during the entire ventilation period. This information is used for all ANSYS calculations of Section 6.

Table 4-3. Property Values for Ventilation Air

Parameter	Value	Source
Density, ρ (kg/m^3)	1.0561	CRWMS M&O 1998a
Dynamic Viscosity, ν ($\text{kg}/\text{m}\cdot\text{s}$)	1.8371×10^{-5}	Holman 1997, linear interpolation
Thermal Conductivity, k ($\text{W}/\text{m}\cdot\text{K}$)	0.0261	Holman 1997, linear interpolation
Specific Heat, c_p ($\text{J}/\text{kg}\cdot\text{K}$)	1005.7	Holman 1997, linear interpolation
Kinematic Viscosity, μ (m^2/s)	1.7395×10^{-5}	Eq. 4-3 (Daugherty et al. 1965)
Thermal Diffusivity, α (m^2/s)	2.4573×10^{-5}	Eq. 4-4 (Incropera and DeWitt 1996)
Prandtl Number, Pr (dimensionless)	0.7079	Eq. 4.5 (Incropera and DeWitt 1996)

4.1.10 Thermal Conductivity of Air at the Ground Surface Model Boundary

The thermal conductivity of air at 16°C (ground surface) is 0.0254 W/m·K (Holman 1997). This input is used in Section 6 to determine the thermal gradient from the ground surface to the water table for all the ventilation models.

4.1.11 Waste Package Lengths, Diameters, Quantities, Sequence, Spacings, and Initial Heat Generation Rates

The lengths, diameters, quantities, and initial heat generation rates for the waste packages are listed in Table 4-4, and are based on *Enhanced Design Alternative (EDA) II Repository Estimated Waste Package Types and Quantities* (CRWMS M&O 1999d). This information is used in Attachment I to compute a repository average heat decay curve for the ANSYS models of Section 6. The waste packages are placed end-to-end with a 0.1 m spacing in the following sequence (CRWMS M&O 2000b): The waste package segment shown below is mirrored down the entire length of the drift:

½ DHLW, 44 BWR, 21 PWR, DHLW, 21 PWR, 44 BWR, 21 PWR, ½ DSNF

where

DHLW = DOE high level waste package

BWR = boiling water reactor waste package

PWR = pressurized water reactor waste package

DSNF = defense spend nuclear fuel waste package

Table 4-4. Number and Initial Heat Generation Rates for Average CSNF and DHLW Waste Packages

Waste Package Type		Length of Waste Packages (m)	Diameter of Waste Packages (m)	Number of Waste Packages	Initial Heat Generation Rate (kW/package)
21-PWR	Absorber Plates	5.305	1.564	4,279	11.3337
	Control Rode	5.305	1.564	87	2.3709
12-PWR	Long	5.791	1.250	158	9.5402
44-BWR	Absorber Plates	5.275	1.594	2,889	7.1346
24-BWR	Thick Plates	5.245	1.238	6	0.4910
5-DHLW	Short	3.73	2.030	1,249	4.0580
5-DHLW	Long	5.357	2.030	414	5.8280 ^a
Navy (DSNF)	Combined	5.888	1.869	285	7.1350 ^b
DOE/Other		5.57	No Data	598	0.7930

Note: ^a Estimated value by assuming that the initial heat generation rates for 5-DHLWs, short and long, are linearly proportional to their lengths (4.058kW×5.357m/3.73m=5.828kW)

^b Averaged value equal to that of 44-BWR

4.1.12 Waste Package Thermal Decay

The decay characteristics of the commercial spent nuclear fuel (CSNF) waste packages are listed in Table 4-5 (CRWMS M&O 1999d). These values are used in Attachment I to calculate a repository average thermal decay curve that is used in all the numerical ventilation models of Section 6.

Table 4-5. Time-dependent Heat Generation Rates for Average CSNF Waste Packages

Time (years)	21-PWR Absorber Plates (kW/package)	21-PWR Control Rods (kW/package)	12-PWR Long (kW/package)	44-BWR Absorber Plates (kW/package)	24-BWR Thick Absorber Plates (kW/package)
0.01	11.3337	2.3709	9.5402	7.1346	0.4910
1	10.9954	2.3285	9.2722	6.9146	0.4829
5	9.9653	2.1785	8.4286	6.2682	0.4445
10	8.9956	2.0095	7.5901	5.6536	0.4030
15	8.1887	1.8547	6.8815	5.1467	0.3689
20	7.5138	1.7241	6.3149	4.7102	0.3341
25	6.9115	1.6038	5.8009	4.3098	0.3065
30	6.3792	1.4942	5.3407	3.9701	0.2806
40	5.4984	1.3106	4.5868	3.3915	0.2369
50	4.7912	1.1649	3.9792	2.9326	0.2033
60	4.2229	1.0443	3.5026	2.5621	0.1754
70	3.7685	0.9479	3.1031	2.2625	0.1536
80	3.3915	0.8698	2.7908	2.0227	0.1361
90	3.0866	0.8070	2.5304	1.8264	0.1222
100	2.8314	0.7545	2.3024	1.6685	0.1111
150	2.0790	0.5983	1.6766	1.1977	0.0799
200	1.7291	0.5244	1.3818	0.9878	0.0684
250	1.5128	0.4796	1.2029	0.8725	0.0622
300	1.3654	0.4452	1.0804	0.7889	0.0583

4.1.13 Physical and Thermal Properties for Simulated Waste Package

The physical and thermal properties used in the calculation for the simulated waste package and heating rod are listed in Table 4-6. These values are for carbon steel material. The values of density, thermal conductivity, and specific heat are the averages over a temperature range of 20°C to 50°C measured for the corresponding parameters (Stroe 2001). The emissivity value is obtained based on the *Heat Transfer* for sheet steel (Holman 1997).

According to the *Conceptual Arrangement Simulated Emplacement Ventilation Test* (CRWMS M&O 2000c), the designed diameter of the waste package pipe is 0.4064 m (16 in).

Table 4-6. Physical and Thermal Properties for Simulated Waste Package

Parameter	Value
Density (kg/m ³)	7840 ^a
Thermal Conductivity (W/m·K)	38.37 ^a
Specific Heat (J/kg·K)	410.98 ^a
Emissivity	0.8 ^b

Note:^a Stroe 2001, p.3. Averaged over a temperature range of 20 to 50°C.

^b Holman 1997, Table A-10, p. 651 for sheet steel.

4.1.14 Physical and Thermal Properties for Concrete Pipe

The physical and thermal properties for the concrete pipe used in the calculation are listed in Table 4-7. The values of density, thermal conductivity, and specific heat are the averages over a temperature range of 20°C to 50°C measured for the corresponding parameters (Stroe 2001).

The designed inner and outer diameters of the concrete pipe are 1.3716 m (54 in.) and 1.651 m (65 in.), respectively (CRWMS M&O 2000c).

Table 4-7. Physical and Thermal Properties for Concrete Pipe

Parameter	Value
Density (kg/m ³)	2280 ^a
Thermal Conductivity (W/m·K)	2.75 ^a
Specific Heat (J/kg·K)	1016.16 ^a
Emissivity	0.93 ^b

Note:^a Stroe 2001, p.3. Averaged over a temperature range of 20 to 50°C.

^b Incropera and DeWitt 1996, Table A.11.

4.1.15 Physical and Thermal Properties for Insulating Material

The physical and thermal properties for the insulating material (fiber glass) used in the calculation are listed in Table 4-8. The density and thermal conductivity are obtained from the *Standard Fiber Glass Duct Wrap* provided by the manufacturer (CertainTeed 1996). The other thermal property values are obtained based on the *Heat Transfer* (Holman 1997) and the *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996). The designed thickness of the insulation is 0.0508 m (2 in.) (CRWMS M&O 2000c).

Table 4-8. Physical and Thermal Properties for Insulating Material

Parameter	Value
Density (kg/m ³)	12 ^a
Thermal Conductivity (W/m·K)	0.04 ^a
Specific Heat (J/kg·K)	700 ^b
Emissivity	0.96 ^c

Note:^a CertainTeed 1996.

^b Holman 1997, Table A-3.

^c Incropera and DeWitt 1996, Table A.11, selected from a range of 0.93 to 0.96 for asbestos sheet.

4.1.16 Physical and Thermal Properties for Invert Material

The physical and thermal properties for the invert material (fine crushed tuff) used in the calculation are listed in Table 4-9. The density, thermal conductivity, and specific heat values based on the *Thermal and Physical Properties of Granular Materials* (CRWMS M&O 2000d). The emissivity is obtained based on the *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996).

Table 4-9. Physical and Thermal Properties for Invert Material

Parameter	Value
Density (kg/m ³)	2530 ^a
Thermal Conductivity (W/m·K)	0.14 ^b
Specific Heat (J/kg·K)	363 ^b
Emissivity	0.93 ^c

Note: ^a CRWMS M&O 2000d, Table 4, mean value for fine crushed tuff.

^b CRWMS M&O 2000d, Table 6, mean value for fine crushed tuff.

^c Incropera and DeWitt 1996, Table A.11, selected from a range of 0.93 to 0.96 for red brick.

4.1.17 Ventilation Test Flow Rates, Heat Loads, and Measured Data

The various cases of the Phase 1 Ventilation Test, and ventilation flow rates and heat loads used for the Post-Test ANSYS model are listed in Table 4-10 and were obtained from the *Development Plan for Ventilation Test* (CRWMS 2000g). The measured data from the test were used for input parameters and boundary conditions, as well for comparison to the ANSYS model results (Section 7.1.2)

Table 4-10. Ventilation Phase 1 Test Matrix

Test No.	Case No.	Nominal Flow (m ³ /s)	Nominal Power (kW/m)
1	4	1	0.18
2	5	0.5	0.18
3	1	1	0.36
4	5	2	0.36
5	3	0.5	0.36
6	6	3	0.36

4.2 CRITERIA

No design criteria were used in the model report. The model setup and inputs used in this report were numerical examples for model validation purposes only. No design analysis was performed in this document.

4.3 CODES AND STANDARDS

Not used.

5. ASSUMPTIONS

All assumptions in this model report are used solely as numerical examples for comparisons of outputs from models for model corroboration or validation purposes only. Each assumption treated as model input is appropriately used. No design analysis or parameters were generated based on the assumptions. Therefore, the assumptions listed in this section do not require confirmation.

5.1 REPRESENTATIVE REPOSITORY LOCATION

Northing 170,750 and easting 233,760 were chosen as a representative repository location in terms of distance from an edge, geology and infiltration rate. It is from this location that the thermal properties for the stratigraphic units (Section 4.1.2) are taken.

5.2 REPRESENTATIVE WASTE PACKAGE DIAMETER

For the purposes of this Model Report, it is assumed that all waste packages have the same diameter. The diameter used in all calculations is that of the 21-PWR waste packages, or 1.564 m (Table 4-4). This assumption is based on the waste stream, where the greatest quantity of waste packages is comprised of 21-PWRs. This information is used throughout Sections 6 and 7.

5.3 CONCENTRIC WASTE PACKAGE EMPLACEMENT WITHIN THE DRIFT

To simplify the calculations, the waste packages are suspended in the center of the emplacement drift. Also, no invert or ground support systems are present to participate in the heat transfer processes. Ground support systems would tend to facilitate additional heat removal from the waste package, via conduction through the supports to the host rock. Although conservative in nature, the impact of this assumption on the output of the Ventilation Model (i.e. wall heat fractions) is considered minimal. This assumption is used throughout the document.

5.4 EMPLACEMENT DRIFT LENGTH

For the preclosure ventilation calculations, the drift length from the air inlet of emplacement drift to the central exhaust main is assumed to be 600 m. The basis for this assumption comes from *Subsurface Facility System Description Document* (CRWMS M&O 2000a) where the maximum emplacement drift split is specified to be 600 m, and any emplacement length in excess of 600 m will be assumed to be unusable space. This information is used throughout the document.

5.5 PRECLOSURE VENTILATION RATE

The preclosure ventilation calculations were performed using an airflow rate of 15 m³/s based on the assumption that at that rate, at least 70% of the heat generated by the waste packages can be removed. The 70% removal guidance comes from *Subsurface Ventilation System Description Document* (CRWMS M&O 2000e). This ventilation flow rate is used throughout the document.

5.6 AIRFLOW TEMPERATURE AT THE DRIFT ENTRANCE

The temperature of the intake airflow at the emplacement drift inlet is assumed to be 25°C based on *Repository Subsurface Waste Emplacement and Thermal Management Strategy* (CRWMS 1998a). This temperature is also assumed constant during the entire preclosure ventilation period. This assumption is used throughout the document.

5.7 ROCK PROPERTIES FOR OVERBURDEN ABOVE Tpcpv2 UNIT

As shown in Table 4-1, the rock properties for the overburden above the Tpcpv2 unit are incomplete. This is due to the lack of thickness data for individual units within the overburden. The rock properties for the each unit within the overburden are assumed to be the same as those of Tpcpv2 because of proximity.

5.8 HEAT OUTPUT FOR DHLW AND NAVY FUEL

The heat output data for the Naval and DHLW packages are not available. Therefore, the initial heat output of the Naval package is assumed to be the same as that of 44BWR, 7.1346 kW (Table 4-4). The heat decay curves for the Naval and DHLW packages are assumed to be the same as the CSNF. The rationale for this assumption is that the Naval and DHLW packages comprise a small portion of the total waste-stream such that uncertainties in this assumption will have no significant impact on the overall lineal heat load calculated in Attachment I.

5.9 HOST ROCK EMISSIVITY

An emissivity of 0.9 for the Tptpll unit where the majority of emplacement drifts will be located was used based on *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996).

5.10 WASTE PACKAGE INITIAL SURFACE TEMPERATURE

The initial temperature on the waste package surface at the time of emplacement is assumed to be 70°C. This assumption is based on the average of the initial temperatures of the waste package surfaces as calculated from *Multiple WP Emplacement Thermal Response -Suite 1* (CRWMS M&O 1998b).

6. MODEL DISCUSSION

During the preclosure period, the rate of heat generation by the waste package in the emplacement drifts is at its peak. Ventilation of the drifts can remove a portion of the thermal energy generated during the preclosure period by spent fuel as well as the moisture mobilized from the surrounding rock mass. The net effect of emplacement drift ventilation is to delay the onset of the peak waste package and drift wall temperatures as well as to decrease their magnitude.

The thermal energy removed by ventilation must be determined by analyzing, at the least, thermal radiation, thermal convection, and thermal conduction which occur simultaneously in the drift and the surrounding rock mass. The following sections provide:

1. An explanation of the conceptual model of the heat transfer mechanisms for ventilated emplacement drifts.
2. A discussion of the numerical application of the conceptual model using the ANSYS software code, and presentation of the results in terms of temperatures and ventilation heat removal rates.
3. A presentation of an alternative conceptual model which considers the effects of water phase change, mass transport, and heat transfer on the effectiveness of ventilation to remove heat from waste emplacement drifts.
4. A comparison of the numerical model results and energy balance closures that provide verification that these numerical techniques are applied properly to the conceptual model.
5. Further model verification using comparative submodels, and where applicable analytical solutions, which isolate the coupled heat transfer processes into individual phenomena.
6. A discussion of the applicability of the wall heat fraction (1 - heat removal) as computed by the numerical ventilation models to initialize downstream post-closure thermal-hydrologic models.

6.1 CONCEPTUAL MODEL FOR IN-DRIFT VENTILATION

When air is directed into an emplacement drift, thermal energy released from the waste packages is transferred to the in-drift and host rock surroundings. The heat transfer processes vary with time and with axial position (i.e. the distance down the length of the drift from the airflow entrance point).

6.1.1 Heat Transfer Processes

The heat transfer processes for ventilation of emplacement drifts are outlined below and shown in Figure 6-1. Figure 6-1 also includes other heat and mass transfer processes that will be outlined later in Section 6.3 when the alternate conceptual model for ventilation is presented.

1. Thermal radiation transfers heat from the surface of the waste package to the drift wall. The rate at which the heat is transferred can be calculated using the Stefan-Boltzmann Law for gray surface radiation exchange at any time during the preclosure period, using

the waste package surface and drift wall temperatures. This calculation also requires knowledge of the geometry and emissivities of the waste package and drift wall surfaces.

2. Convection transfers heat from the surface of the waste package to the airflow, due to the temperature differences between the surface and the moving air. The heat flow rate can be calculated using Newton's Cooling Law at any time during the preclosure period, using the bulk temperature of the airflow and the temperature of the waste package surface. This calculation also requires knowledge of the convective heat transfer coefficients that implicitly describe the effects of the airflow, the drift geometry, and surface properties on the heat transfer rates.
3. Convection transfers heat from the drift wall surface directly to the airflow, due to the temperature differences between the wall surface and the moving air, similar to process (2). The sum of the two convective heat transfer rates determines the rate of energy addition to the moving air, and can be used to calculate the axial rate of air temperature increase. This calculation also requires knowledge of the convective heat transfer coefficients that implicitly describe the effects of the airflow, the drift geometry, and surface properties on the heat transfer rates. Axially along the drift, the convection heat transfer (processes 2 and 3) can be combined with the air mass flow rate and its specific heat, to calculate the axial change of air temperature.
4. Conduction transfers heat within the rock mass due to changes in drift wall temperature. The heat flow rate into the rock can be determined using Fourier's Conduction Law at any time during the preclosure period, using the temperature gradient in the rock mass. This calculation requires knowledge of the thermal conductivity, saturation, density, and heat capacity of the rock (which may vary spatially).

The heat transfer rates for the processes described above can be related by considering the overall conservation of thermal energy except during the early transient response when the waste package temperature is rapidly changing. The following summarizes the coupled components of the thermal energy conservation during quasi-steady-state conditions when energy storage is relatively constant:

- The sum of the radiative heat transfer rate from the waste package to the drift wall (process 1 from above), and the convective heat transfer rate from the waste package into the airflow (process 2), must equal to the total rate of heat released from the waste package.
- The sum of the convective heat transfer rates from the waste package and drift wall into the airflow (processes 2 and 3), and the conductive heat transfer rate into the rock (process 4), must also be equal to the total rate of heat released from the waste package.
- The sum of the convective heat transfer rates from the drift wall into the airflow (process 3), and the conductive heat transfer rate into the rock (process 4), must be equal to the rate of radiant heat released from the waste.

Five additional processes have not been explicitly included in the conceptual model. The first includes the mass transport of water and water vapor and the coupled latent and sensible heat transfer associated with the phase change and movement of water. However, these latent heat effects and near-field host rock mass transport processes can be approximated using boiling point temperature dependent values for the thermal conductivity and specific heat of the rock. This can account for vaporization of pore water and dryout in an approximate sense, but cannot accurately track changes of saturation and evolution of properties. In most cases, the temperatures needed to change these properties are not reached during the preclosure period. These processes are presented in greater detail in Section 6.3.

Figure 6-1. Conceptual Model for Heat and Mass Transfer Within and Around an Emplacement Drift

The second process excluded from the conceptual model is the axial transport of heat and mass within the rock domain. This process is assumed to have negligible influence on the ventilation heat removal ratio during the duration of the ventilation period. This is due to the small thermal diffusivity of rock ($\sim 1 \times 10^{-7} \text{ m}^2/\text{s}$) and the large (hundreds of meters) scale of the repository footprint. The axial heat transport process is captured in the MSTH model that calculates preclosure and postclosure in-drift and rock temperatures and moisture contents for use in the TSPA. The MSTH model uses the ventilation heat removal ratio calculated by the Ventilation Model as input.

The third process not included in the ventilation conceptual model is the frictional heating of the air and engineered components due to the moving air. This process is assumed to be negligible (compared to the waste package heat source) due to the low flow velocities.

The fourth process not included in the ventilation conceptual model is episodic flow of liquid water into the drift air (due to heterogeneities in the host rock and episodic infiltration). It is assumed that the total heat added to the airflow by vaporizing such seeps is small compared to the heat from radionuclide decay. It should be noted that the conceptual model does account for vaporization of liquid water within the host rock and movement of the vapor into the drift, but that process adds only the sensible heat due to the temperature difference between the entering water vapor and the airflow.

Finally, the fifth process not included in the ventilation conceptual model is the participation of the drift gas in the radiation process. Water vapor is an effective absorber of infrared radiation, and the effect of its absorption and re-radiation of thermal energy is currently being evaluated.

6.1.2 Basis Heat Transfer Equations for the Ventilation Model

The following three equations represent energy balances for processes 1, 2 and 3 as outlined above in Section 6.1.1 and Figure 6-1:

$$Q_{wp} = \pi L \cdot [d_{wp} h_{rad} (T_{wp}^4 - T_{dw}^4) + d_{wp} h_{wp-air} (T_{wp} - T_{air-bulk})]$$

Eq. 6-1

$$Q_{dw} = \pi L \cdot [d_{wp} h_{rad} (T_{wp}^4 - T_{dw}^4) - d_{dw} h_{dw-air} (T_{dw} - T_{air-bulk})]$$

Eq. 6-2

$$(\dot{m} c_p)_{air} (T_{air-out} - T_{air-in}) = \pi L \cdot [d_{wp} h_{wp-air} (T_{wp} - T_{air-bulk}) + d_{dw} h_{dw-air} (T_{dw} - T_{air-bulk})]$$

Eq. 6-3

where

- Q_{wp} = heat generated by the waste package (W)
- Q_{dw} = heat conducted into the rock (W)
- T_{wp} = waste package surface temperature (K)
- T_{dw} = drift wall temperature (K)
- $T_{air-bulk} = (T_{air-in} + T_{air-out})/2$
- T_{air-in} = ventilation air temperature at the drift segment inlet (K)
- $T_{air-out}$ = ventilation air temperature at the drift segment outlet (K)
- h_{wp-air} = waste package surface convection heat transfer coefficient ($W/m^2 \cdot K$)
- h_{dw-air} = drift wall convection heat transfer coefficient ($W/m^2 \cdot K$)
- h_{rad} = radiation heat transfer coefficient ($W/m^2 \cdot K^4$)
- L = drift segment length (m)
- d_{wp} = waste package diameter (m)
- d_{dw} = drift diameter (m)
- $\dot{m}$ = ventilation mass flow rate (kg/s)
- c_p = specific heat of air ($J/kg \cdot K$)

For the purposes of this model report, the convection heat transfer coefficients are calculated using the Dittus-Boelter correlation for fully developed turbulent flow in smooth tubes (Incropera and DeWitt 1996, Hartman 1982). Other appropriate correlations may also be used. Separate heat transfer coefficients may be used for the convective heat transfer from the inner surface (i.e. waste package) to the air, and for the outer surface (i.e. drift wall) to the air. This model report uses the same convection heat transfer coefficient for both surfaces.

$$Nu = \frac{h_{DB} \cdot D}{k} = 0.023 \cdot Re^{0.8} \cdot Pr^{0.4} \quad \text{Eq. 6-4}$$

or

$$h_{DB} = 0.023 \cdot \left(\frac{k \cdot Re^{0.8} \cdot Pr^{0.4}}{d_{dw} - d_{wp}} \right) \quad \text{Eq. 6-5}$$

$$Re = \frac{\rho DV}{\mu} = \left(\frac{d_{dw} - d_{wp}}{A_{net}} \right) \cdot \left(\frac{\dot{m}}{\mu} \right) \quad \text{Eq. 6-6}$$

where

Nu = Nusselt Number (dimensionless)

D = length (m) = $d_{dw} - d_{wp}$

k = thermal conductivity (W/m·K)

h_{DB} = Dittus-Boelter convection heat transfer coefficient (W/m²·K) = $h_{wp-air} = h_{dw-air}$

Pr = Prandtl Number (dimensionless)

Re = Reynolds Number (dimensionless)

ρ = density (kg/m³)

V = ventilation airflow velocity (m/s) = Q/A_{net}

Q = volumetric ventilation airflow (m³/s) = $\dot{m} / \rho$

A_{net} = net cross-sectional available for airflow (m²)

μ = dynamic viscosity of air (kg/m·s)

The radiation heat transfer coefficient is calculated from an analytical solution for concentric cylinders (Incropera and DeWitt 1996):

$$h_{rad} \equiv \frac{\sigma A_{wp}}{\frac{1}{\varepsilon_{wp}} + \left(\frac{1 - \varepsilon_{dw}}{\varepsilon_{dw}} \right) \cdot \frac{d_{wp}}{d_{dw}}} \quad \text{Eq. 6-7}$$

where

σ = Stefan-Boltzmann constant ($\text{W/m}^2 \cdot \text{K}^4$)
 ε_{wp} = waste package surface emissivity
 ε_{dw} = drift wall surface emissivity

6.1.3 Basis Equations for Calculating the Ventilation Heat Removal

The amount of heat removed by ventilation is both a function of time and distance from the entrance of the drift. The instantaneous heat removal at some time, t , and some location from the drift entrance, x , is defined by:

$$\eta(t, x) \equiv \frac{Q_{air}(t, x)}{Q_{wp}(t)}$$

Eq. 6-8

where

$\eta(t, x)$ = instantaneous ventilation heat removal efficiency (dimensionless)
 Q_{air} = heat convected to the air from the waste package and drift wall surfaces (W/m)
 Q_{wp} = heat generated by the waste package (W/m)
 t = time since ventilation began
 x = distance from the drift entrance (m)

Past versions of the Ventilation Model have used a time-averaged method to calculate a single integrated value for the heat removal efficiency:

$$\eta_{time-ave} \equiv \frac{\int_0^t \int_0^x \frac{Q_{air}(t, x)}{Q_{wp}(t)} \cdot dx \cdot dt}{x \cdot t}$$

Eq. 6-9

where

$\eta_{time-ave}$ = time-averaged ventilation heat removal efficiency (dimensionless)

The use and consequence of the time-averaged method is described later in Section 6.6.2.2. An alternative approach for calculating a single integrated value for the heat removal by ventilation is:

$$\eta_{integrated} \equiv \frac{\int_0^x \int_0^t Q_{air}(t, x) \cdot dx \cdot dt}{x \cdot \int_0^t Q_{wp}(t) \cdot dt}$$

Eq. 6-10

where

$\eta_{integrated}$ = integrated instantaneous ventilation heat removal efficiency (dimensionless)

6.2 NUMERICAL APPLICATION OF THE CONCEPTUAL MODEL

Three numerical applications of the conceptual model described above for in-drift ventilation heat transfer are performed. Two of these applications use the ANSYS software code, and the third uses the DriftFlow software code. The results of each numerical application are compared later in Section 6.2.3. The first ANSYS based application, named ANSYS-Coarse, divided the drift into 6 equal segments of 100 meters. The second ANSYS based application, named ANSYS-Refined, divided the drift into 24 equal segments of 25 meters. The DriftFlow application, named DriftFlow-Coarse, is similar to the ANSYS-Coarse model, and was developed to benchmark the DriftFlow software against the ANSYS. DriftFlow is also used later to implement parts of the alternative conceptual model.

Table 6-1. Comparison of the ANSYS and DriftFlow Numerical Model Set-Ups and Input Parameters

Numerical model Setup/Inputs	ANSYS-Coarse	ANSYS-Refined	DriftFlow-Coarse
Boundary Conditions	$T_{\text{surface}} = 18.7^{\circ}\text{C}$ $T_{\text{water table}} = 32.4^{\circ}\text{C}$ $T_{\text{mid-pillar}} = \text{adiabatic}$		
Initial Heat Loading	1.5477 kW/m		
Decay Function	Average for all CSNF Waste packages		
Convective Heat Transfer Coefficient on both the WP and Drift Wall (Attachment II)	1.89 W/m ² ·K		
Ventilation Period	300 years		
Thermal Conductivity at the repository horizon (tsw-35)	Temperature Dependent: 2.02 W/m·K ($<100^{\circ}\text{C}$) 1.20 W/m·K ($\geq 100.1^{\circ}\text{C}$)		2.02 W/m·K
Specific Heat near the repository horizon (tsw-35)	Temperature Dependent: 900 J/kg·K ($<95^{\circ}\text{C}$ or $\geq 114.1^{\circ}\text{C}$) 4663 J/kg·K ($\geq 95.1^{\circ}\text{C}$ and $<114^{\circ}\text{C}$)		900 J/kg·K
Pillar Size	81-m (Drift Spacing)*		
Drift Diameter	5.5 m		
Waste Package Diameter	1.564 m		
Inlet Air Temperature	25°C		
Initial Drift Wall Temperature	25°C		
Initial WP Temperature	70°C		70°C
Emissivity	Gray Body to Gray Body: 0.87 for Waste package 0.90 for Drift Wall		
Axial Discretization	100 m	25 m	100 m

* The ANSYS numerical models spanned from mid-pillar to mid-pillar to eliminate small (~1%) errors in radiation view factors near reflecting boundaries.

6.2.1 ANSYS Methodology

The ANSYS numerical model integrates the results of a heat transfer calculation using a two-dimensional cross-section through the drift with a one-dimensional calculation of the forced convection through an axial segment of the drift. This process assumes that the convective heat fluxes from the waste package and drift wall to the air are constant within the drift segment. This constant heat flux assumption is equivalent to assuming that the air temperature increases linearly within the segment, and that the drift wall and waste package temperatures also increase linearly at the same rate. Such an assumption is much closer to reality than an assumption of constant temperature within the segment and then a step change at the end. The departure from reality of the assumption of constant flux is slow along the drift, and is due to the increase of radiation heat transfer and conduction of heat into the host rock as the temperature increases. To test the validity of the assumption, the ANSYS numerical model was run with 100-m (ANSYS-Coarse) and 25-m (ANSYS-Refined) long segments.

Figures 6-2 and 6-3 illustrate the geometry and the main components of the ANSYS numerical models. In this method, a ventilated emplacement drift is treated as a series of finite drift segments. For each time step, a two-dimensional calculation of heat transfer between the waste package, drift wall, drift air, and the heat transfer into the host rock is done at the entrance to the

first drift segment using the inlet air temperature as a heat sink. The resulting convective heat fluxes (at the waste package and drift wall surfaces) are assumed to be constant along the segment, allowing a one-dimensional calculation of the air temperature increase within the segment, using the air flow rate. The air temperatures at the end of the drift segment, at both the beginning and end of the time step, are then used in the next two-dimensional calculation, which occurs at the beginning of the next drift segment. The process is repeated along the entire drift split (from the air entry at the perimeter drift to the air exit into the exhaust main at the mid-length point of the drift), alternating between two-dimensional ANSYS calculations and one-dimensional air heating calculations using Microsoft Excel. At each time and ANSYS location, the heat fluxes are also used to calculate the ventilation heat removal rate.

Figure 6-2. Flowchart Depicting the ANSYS Methodology for Calculating Heat Flow in and around a Ventilated Emplacement Drift

Figure 6-3. Schematic of the ANSYS Methodology for Calculating Heat Flow in and around a Ventilated Emplacement Drift

6.2.1.1 ANSYS Operational Details

The ANSYS process starts with defining a number of time-steps to represent the entire ventilation time period of interest. The total number of time intervals, and the length of each time-step can be selected according to the degree of calculational accuracy demanded and considerations of the expected computational time. The length of each timestep may be set differently to accommodate the variations of the thermal decay rate of the waste during different time periods. Generally, during the initial stages when the waste decays rapidly, short time steps can be arranged to provide detail during the more rapidly changing portion of the ventilation history. In the later stages of heat transfer, the thermal decay curves become relatively flat; thus longer time-steps can be used to reduce computational efforts.

In this approach, the entire drift is considered as a series of connected drift segments with some length. The total number of drift segments is related to segment length. It is desirable to choose a relatively short drift length for individual drift segments, to the extent practicable, so that the convective heat fluxes within a segment can be reasonably represented by a constant. The values of drift length may be set differently to accommodate the variations in rate of air temperature increase as the air flows through the drift.

Calculations are performed sequentially for each time-step through the ventilation period. At the entry to each drift segment two-dimensional thermal analysis is performed with ANSYS for the sequence of time steps. Each time step uses the waste package thermal power, initial rock and

waste package temperatures from the end of the previous time step, and the air temperature from the exit of the previous segment. The air temperature and waste thermal power are linearly interpolated in time during the time step, if ANSYS uses sub-time-steps to obtain numerical stability.

For each segment, applying the determined waste package and drift wall temperatures at the start and end of each time step, together with the air temperature at the same times, convective heat transfer rates at the segment entrance are calculated using Newton's Cooling Law. The obtained convective heat removal rate and the known airflow rate are used to determine the increase in internal thermal energy of the air, and the temperature of the airflow exiting the segment (at the start and end of each time step). The exit temperature history of the air is used in the ANSYS calculation at the entry of the next segment. This process is repeated to the end of the drift split, where a final ANSYS calculation determines the temperatures and ventilation heat removal ratio at that location.

6.2.2 DriftFlow Methodology

The DriftFlow numerical model implements the ventilation conceptual model using drift segment control volumes (similar to the ANSYS approach), where the heat transfer along the length of the control is considered to be constant. The thermal radiation of a drift segment control volume is approximated by linearizing the Stephan Boltzmann Law. DriftFlow contains two options for calculating an effective linearized radiation heat transfer coefficient which are documented in the *Software Definition Report for DriftFlow v.1.0* (BSC 2002b): (1) using an analytical solution for concentric cylinders described by equation 6-11 Below; or (2) by referencing a derived coefficient from an ANSYS calculation. The implementation of DriftFlow v.1.0 in this Model Report uses the former option for radiation heat transfer.

$$h_{rad} \equiv \frac{\sigma(T_{wp}^3 + T_{wp}^2 T_{dw} + T_{wp} T_{dw}^2 + T_{dw}^3)}{\frac{1}{\epsilon_{wp}} + \frac{d_{wp}}{d_{dw}} \cdot \left(\frac{1}{\epsilon_{dw}} - 1 \right)}$$

Eq. 6-11

The in-drift convection is calculated using Newton's Law of Cooling. The thermal conduction response in the host rock is calculated by Fourier's Law using a constant-flux temperature pulse-response method (BSC 2002b) and the principle of superposition. In theory, the transient temperature response of the host rock due to the time dependent waste package heat flux can be approximated by summing the temperature responses from individual constant waste package heat fluxes applied over short time intervals.

6.2.2.1 DriftFlow Thermal Pulse Calculation

A DriftFlow pulse for the transient thermal response of the host rock is developed by obtaining the composite of two analytical solutions for the temperature responses due to a constant heat

flux applied (1) at the wall of a region bounded internally by a cylinder (Carslaw and Jaeger, 1959), and (2) at the surface of a semi-infinite slab (Carslaw and Jaeger, 1959).

6.2.2.1.1 The Internally Bounded Cylinder

A calculation of the temperature response due to a constant flux for the region bounded internally by a cylinder can be used to generate the wall-temperature response for any values of cylinder radius (a), density (ρ), heat capacity (C), and thermal conductivity (K). The solution for the region bounded internally by a cylinder with constant flux Q at $r = a$ is obtained from *Conduction of Heat in Solids*, equation (17) on page 338 (Carslaw and Jaeger, 1959):

$$v = -\frac{2Q}{\pi K} \int_0^{\infty} (1 - e^{-\kappa u^2 t}) \frac{J_0(ur) Y_1(ua) - Y_0(ur) J_1(ua)}{u^2 [J_1^2(ua) + Y_1^2(ua)]} du \quad \text{Eq. 6-12}$$

where

u is the temporary integration, and
 v is the temperature.

κ is the thermal diffusivity written as:

$$\kappa \equiv \frac{K}{\rho C} \quad \text{Eq. 6-13}$$

Proceed by defining the dimensionless variable ξ as:

$$d\xi = a du \quad \text{Eq. 6-14}$$

$$\xi \equiv ua \quad \text{Eq. 6-15}$$

And eliminate u everywhere in equation 6-12 to obtain:

$$v = -\frac{2Q}{\pi K} \int_0^{\infty} (1 - e^{-\kappa(\xi/a)^2 t}) \frac{J_0\left(\xi \frac{r}{a}\right) Y_1(\xi) - Y_0\left(\xi \frac{r}{a}\right) J_1(\xi)}{\frac{\xi^2}{a^2} [J_1^2(\xi) + Y_1^2(\xi)]} \frac{d\xi}{a} \quad \text{Eq. 6-16}$$

Define a dimensionless time, τ , as:

$$\tau \equiv \frac{\kappa t}{a^2}$$

Eq. 6-17

Use this dimensionless time and set $r = a$ (which is the wall) in equation 6-16 to obtain:

$$v(r=a) = -\frac{2aQ}{\pi K} \int_0^\infty (1 - e^{-\xi^2 \tau}) \frac{J_0(\xi)Y_1(\xi) - Y_0(\xi)J_1(\xi)}{\xi^2 [J_1^2(\xi) + Y_1^2(\xi)]} d\xi$$

Eq. 6-18

And rearrange to obtain a dimensionless temperature at $r = a$ as:

$$\theta \equiv \frac{K v(r=a)}{Qa} = -\frac{2}{\pi} \int_0^\infty (1 - e^{-\xi^2 \tau}) \frac{J_0(\xi)Y_1(\xi) - Y_0(\xi)J_1(\xi)}{\xi^2 [J_1^2(\xi) + Y_1^2(\xi)]} d\xi$$

Eq. 6-19

Suppose that dimensionless temperatures have been generated as a function of dimensionless time (τ) for $\Delta\tau = 1/2$ up to some maximum $\tau_{\max}$. Now suppose that $v(r=a)$ is required at times of every year ($\Delta t = 1$); use equation 6-17 to write:

$$\tau_n = \left(\frac{\kappa}{a^2} \right) (n \Delta t), \text{ for } n = 1, 2, 3, \dots$$

Eq. 6-20

And to further illustrate, suppose that $\kappa = 26 \text{ m}^2/\text{yr}$ and $a = 2.75$ meters (for a 5.5-meter diameter drift) so that the above equation looks like:

$$\tau_n \approx 3.43(n \Delta t), \text{ for } n = 1, 2, 3, \dots$$

Eq. 6-21

To generate the temperature v at the desired value of time, the a priori calculated dimensionless temperature and dimensionless time response at discrete values of $1/2\tau$ can be interpolated accordingly.

Now consider how to generate a 1-year pulse temperature response from the general results of equation 6-19. From equation 6-17 calculate the dimensionless time for 1 year, i.e.:

$$\tau \equiv \frac{\kappa t}{a^2} = \frac{\kappa}{a^2}$$

Eq. 6-22

Obtain the dimensionless temperatures for the following values of dimensionless time:

$$\tau = \frac{\kappa}{a^2}, \frac{2\kappa}{a^2}, \frac{3\kappa}{a^2}, \dots, \frac{i\kappa}{a^2}$$

Eq. 6-23

where here i is the year (in years). From the dimensionless temperatures retrieved (calculated, interpolated, etc.) for each of the above, θ_i , calculate the temperature according to:

$$v_i = \frac{Q a \theta_i}{K}$$

Eq. 6-24

From the tabulated values of v_i for each year, shift these values of v_i by 1 year and subtract to obtain the 1-year pulse temperature response.

6.2.2.1.2 The Semi-Infinite Slab

The solution for one-dimensional heat flow due to a heat flux applied at the surface of a semi-infinite media is given by *Conduction of Heat in Solids*, page 75 (Carslaw and Jaeger, 1959):

$$v(t) = \frac{2 \cdot F_0}{K} \cdot \left[\left(\frac{\kappa \cdot t}{\pi} \right)^{\frac{1}{2}} \cdot e^{\frac{-x^2}{4\kappa \cdot t}} - \frac{x}{2} \cdot \operatorname{erfc} \left(\frac{x}{2\sqrt{\kappa \cdot t}} \right) \right]$$

Eq. 6-25

Where

$v(t)$ = Temperature change
 F_0 = Step Heat flux applied at $x = 0$
 K = Thermal conductivity
 κ = Thermal diffusivity
 x = x coordinate
 t = Time

Now consider the convolution integral. The convolution integral is given by (Sokolnikoff and Redheffer, 1966, p. 224):

$$v(x, t) = \int_0^t f(\tau) \bullet w_\tau(x, t - \tau) d\tau$$

Eq. 6-26

Where

$F(\tau)$ = Arbitrary function for the flux rate

$w_\tau(x, \tau)$ = Time derivative of the constant heat flux function for a unit loading.

Evaluate the function at $x = 0$.

$$v(t) = \frac{2 \cdot F_0}{K} \cdot \sqrt{\frac{\kappa \cdot t}{\pi}}$$

Eq. 6-27

For the convolution integral, the derivative is required due to a unit load ($F_0 = 1 \text{ w/m}^2$)

$$\frac{dv}{dt} = \frac{1}{K \cdot \sqrt{\frac{\kappa \cdot t}{\pi}}} \cdot \frac{\kappa}{\pi}$$

Eq. 6-28

Form the convolution integral. Evaluate the convolution integral for times less than one year (Sokolnikoff and Redheffer, 1966, p. 224):

$$v(t) = \int_0^t f(\tau) \bullet w_\tau(t - \tau) \cdot d\tau$$

Eq. 6-29

Substituting in the functions

$$v(t) = \int_0^t F_0 \bullet \frac{1}{\left(K \cdot \sqrt{\frac{\kappa \cdot (t - \tau)}{\pi}} \right)} \bullet \frac{\kappa}{\pi}$$

Eq. 6-30

yields

$$v(t) = \frac{2 \cdot F_0}{K} \cdot \sqrt{\frac{\kappa \cdot t}{\pi}}$$

Eq. 6-31

This is the same result as presented above.

For times greater than one year, we evaluate the following integrals. Note that the solution to the PDE is actually the temperature response to a step function of constant value applied at time $t = 0$. Define $t' = t - 1$, and apply a step function of equal and opposite sign at $t' = 0$. The

superposition of these two loadings results in the pulse solution of duration one year. Applying equation 6-29

$$v(t) = \int_0^t f(\tau) \cdot \frac{1}{\left(K \cdot \sqrt{\frac{\kappa \cdot (t - \tau)}{\pi}} \right)} d\tau + \int_0^{t'} -f(\tau) \cdot \frac{1}{\left(K \cdot \sqrt{\frac{\kappa \cdot (t' - \tau)}{\pi}} \right)} d\tau$$

Eq. 6-32

$$v(t) = \int_0^t F_0 \cdot \frac{1}{\left(K \cdot \sqrt{\frac{\kappa \cdot (t - \tau)}{\pi}} \right)} d\tau + \int_0^{t'} -F_0 \cdot \frac{1}{\left(K \cdot \sqrt{\frac{\kappa \cdot (t' - \tau)}{\pi}} \right)} d\tau$$

Eq. 6-33

The temperature is given by

$$v(t) = 2 \cdot \sqrt{\frac{\kappa \cdot t}{\pi}} \cdot \frac{F_0}{K} - 2 \cdot \sqrt{\frac{\kappa \cdot t'}{\pi}} \cdot \frac{F_0}{K}$$

Eq. 6-34

Factoring the expression, and substituting in the $t' = t-1$

$$v(t) = 2 \cdot \frac{F_0}{K} \cdot \left(\sqrt{\frac{\kappa \cdot t}{\pi}} - \sqrt{\frac{\kappa \cdot (t-1)}{\pi}} \right)$$

Eq. 6-35

6.2.2.1.3 Implementation of the Internally Bounded Cylinder and Semi-Infinite Slab Pulses to Build the Composite Pulse

The implementation of the theoretical equations for the pulses for the DriftFlow-Coarse ventilation model is shown in Figure 6-4.

Figure 6-4. Thermal Pulse and DriftFlow Methodologies Used for the DriftFlow-Coarse Ventilation Model

The implementation involves developing the dimensionless cylinder pulse response in MathCAD (**Dimensionless Pulse.mcd**) from equation 6-18. The results of this calculation are pasted into an Excel workbook (**DriftFlow-Coarse Composite Pulse.xls, worksheet Dimensionless Cylinder Pulse**). The results of this calculation (**DriftFlow-Coarse Composite Pulse.xls, worksheet C&J Fig 44 p. 338**) are in agreement with that of Figure 44 on page 338 of Carslaw and Jaeger (Carslaw and Jaeger, 1959).

Using the results of the internally bounded cylinder dimensionless pulse response applied to the set of thermal properties for Tsw-35 (Section 4.1.2) and drift diameter and spacing (Section 4.1.8 and 4.1.6 respectively), a non-dimensional pulse response is calculated by:

- Calculating the dimensionless time as $\alpha \cdot t/a^2$ where α is the thermal diffusivity (m^2/yr), t is time (yrs) and a is the tunnel radius(m).

- Calculating over a period of 300 years the dimensional temperature response from the dimensionless pulse relationship by linear interpolation. At this point in the process, the temperature response to an initial step unit heat loading at time zero has been calculated (**DriftFlow-Coarse Composite Pulse.xls**, *worksheet Cylinder Pulse*).
- Superimposing the initial unit heat loading at time zero with an unit heat unloading after one year to determine the actual incremental heat response due to the one year pulse and out to 300 years (**DriftFlow-Coarse Composite Pulse.xls**, *worksheet Cylinder Pulse*).

The temperature pulse response of the semi-infinite slab to a 1 W/m heat load is calculated by determining the unit heat loading F_0 . Using the drift diameter and spacing, F_0 is calculated to be:

$$F_0 = \frac{\pi R}{D_s} = \frac{\pi \cdot 2.75m}{81m} \cdot \frac{1 \cdot W}{m} = 0.106655 \cdot \frac{W}{m}$$

Eq. 6-36

The cumulative response at one year is:

$$2 \cdot \frac{F_0}{K} \cdot \left(\sqrt{\frac{\alpha \cdot t}{\pi}} \right) = 2 \cdot \frac{0.106655}{2.02} \sqrt{\frac{27.88554331}{\pi}} = 0.31462^\circ C$$

Eq. 6-37

The cumulative response at two years is:

$$2 \cdot \frac{F_0}{K} \cdot \left(\sqrt{\frac{\alpha \cdot t}{\pi}} \right) = 2 \cdot \frac{0.106655}{2.02} \sqrt{\frac{27.88554331 \cdot 2}{\pi}} = 0.44494^\circ C$$

Eq. 6-38

The temperature response due to a pulse of duration one year is:

$$2 \cdot \frac{F_0}{K} \cdot \left(\sqrt{\frac{\kappa \cdot t}{\pi}} - \sqrt{\frac{\kappa \cdot (t-1)}{\pi}} \right) = 0.13032^\circ C$$

Eq. 6-39

This calculation is continued for 300 years in 1 year increments (**DriftFlow-Coarse Composite Pulse.xls**, *worksheet Slab Pulse*).

The composite temperature pulse response is the maximum temperature pulse response for each time step from either the internally bounded cylinder or the semi-infinite slab pulses (**DriftFlow-Coarse Composite Pulse.xls**, *worksheet Composite Pulse*). All three temperature pulses are presented graphically in Figure 6-5.

Figure 6-5. Temperature Responses for the Internally Bounded Cylinder, Semi-Infinite Slab, and Composite Pulses Due to a 1 W/m Heat, Applied for 1 Year (DTN: MO0212MWDDFC02.005).

6.2.3 Results

The results for the ANSYS-Coarse, ANSYS-Refined, and DriftFlow-Coarse models are presented in terms of temporally and spatially varying temperatures and heat removal rates. In addition, energy balances are presented for each numerical model. A comparison between the ANSYS-Coarse and ANSYS-Refined models quantifies the impact of the axial discretization along the drift length and serves as a model verification exercise. A comparison between the ANSYS-Coarse and DriftFlow-Coarse models benchmarks the DriftFlow code in preparation for further use herein.

6.2.3.1 The Effects of Axial Discretization

The general trends of waste package, drift wall, and drift air temperatures as a function of time and axial drift length for the ANSYS-Refined numerical model are shown in Figure 6-6. The waste package and drift wall temperatures are perimeter-averaged results, while the in-drift air temperatures are bulk averaged. The following general observations with respect to waste package, drift wall, and drift air temperatures for each of the ANSYS numerical models can be made:

- With respect to time, temperatures peak early (between 2 to 5 years) and afterwards decline in an exponential fashion similar to the heat input decay curves
- With respect to location along the length of the drift, temperatures increase linearly, with the maximum temperatures occurring at the end of the 600-m long drift

Figures 6-7 and 6-8 not only reinforce these two general observations about temperatures, but also quantify the temperature differences between the ANSYS-Coarse and ANSYS-Refined numerical models. Table 6-2 summarizes the temperature results.

Figure 6-6. Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Time and Drift Length for the ANSYS-Refined Ventilation Numerical Models (DTN MO0210MWDTVE30.018)

Figure 6-7. Plots of Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Time at 0, 300, and 600 Meters from the Drift Entrance for the ANSYS-Coarse and ANSYS-Refined Ventilation Numerical Models (DTNs MO0210MWDTVE30.018 and MO0210MWDTTEM30.019)

Figure 6-8. Plots of Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Drift Length at 5, 50, and 300 Years from the Time of Waste Emplacement for the ANSYS-Coarse and ANSYS-Refined Ventilation Numerical Models (DTNs MO0210MWDTVE30.018 and MO0210MWDTEM30.019)

Table 6-2. Summary of Waste Package, Drift Wall, and Drift Air Temperatures for the ANSYS-Coarse and ANSYS-Refined Numerical Models

		Drift Entrance (0 m)			Drift Middle (300 m)			Drift Exit (600 m)		
		Temperature (°C)								
		Waste Package	Drift Wall	Drift Air	Waste Package	Drift Wall	Drift Air	Waste Package	Drift Wall	Drift Air
ANSYS-Coarse	5 years	73.4	48.2	25.0	90.5	67.9	47.0	106.1	85.6	66.8
ANSYS-Refined		73.4	48.2	25.0	90.2	67.7	46.7	105.7	85.2	66.3
ANSYS-Coarse	50 years	50.2	36.6	25.0	60.2	47.5	36.4	69.7	57.7	47.2
ANSYS-Refined		50.2	36.6	25.0	60.1	47.4	36.3	69.5	57.6	47.0
ANSYS-Coarse	300 years	32.5	28.4	25.0	35.8	31.8	28.4	39.1	35.2	31.8
ANSYS-Refined		32.5	28.4	25.0	35.8	31.8	28.4	39.1	35.2	31.8

The ANSYS-Coarse peak waste package, drift wall, and drift air temperatures occur at about 2 years and are, respectively 108.2, 84.7, and 67.0°C at 600 meters from the drift entrance. The ANSYS-Refined peak temperatures at the same time and drift location are 107.8, 84.2, and 66.4°C or about 0.4 to 0.6°C lower than the ANSYS-Coarse results. This trend for the two ANSYS numerical models is persistent throughout the entire set of temperature results as functions of both time and drift location.

Table 6-3 compares the sum of the heat fluxes from the waste package and drift wall to the air, within one 100-m segment, from direct calculation in ANSYS-Refined and interpolated between end members of the ANSYS-Coarse segment. The segment and time shown in the table have heat fluxes near the maximum.

Table 6-3. Linearity of Heat Flux into the Air (W/m) within one ANSYS-Coarse Segment (Between 100 and 200 m, at 5 years After Emplacement)

Numerical Model	100 m	125 m	150 m	175 m	200 m
ANSYS-Refined	1166.6	1156.7	1146.8	1137.1	1127.7
ANSYS-Coarse – end members	1166.0	-	-	-	1126.7
ANSYS-Coarse – interpolated values	-	1156.2	1146.3	1136.5	-
(Refined – Interpolated) / Refined	0.05%	0.05%	0.04%	0.05%	0.09%

The flux variation along the segment is about 3%. This small variation leads to changes in the heat fluxes that are about two orders of magnitude smaller. The fractional difference between the interpolated and calculated values is as small as the differences between the models at the common points (100 m and 200 m). These results, and temperature results presented earlier, support the assumption of nearly constant heat flux within the segment. These results also reinforce the hypothesis that the methodology of these ANSYS numerical models is generally insensitive to the number and length of sub-sections in the axial direction.

6.2.3.2 Temperature Comparisons for the ANSYS-Coarse and DriftFlow-Coarse Models

The same general trends of temperature variation with time and distance from the drift entrance, as noted in Section 6.2.3.1 for the ANSYS numerical models, is observed for the DriftFlow-Coarse numerical model. Figure 6-9 shows the DriftFlow-Coarse and ANSYS-Refined temperature results as a function of time for locations near the drift entrance (100 m) and drift exit (600 m). Figure 6-10 shows results as function of distance from the drift entrance for times around the maximum and minimum temperatures. Table 6-4 summarizes the temperature results.

Figure 6-9. Plots of Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Time at 50 and 550 meters from the Drift Entrance for the ANSYS-Refined and DriftFlow-Coarse Ventilation Numerical Models (DTNs MO0210MWDTVE30.018 and MO0212MWDDFC02.005)

Figure 6-10. Plots of Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Drift Length at 5 and 300 Years from the Time of Waste Emplacement for the ANSYS-Refined and DriftFlow-Coarse Ventilation Numerical Models (DTNs MO0210MWDTVE30.018 and MO0212MWDDFC02.005)

Table 6-4. Summary of Waste Package, Drift Wall, and Drift Air Temperatures for the ANSYS-Refined and DriftFlow-Coarse Numerical Models

		Near Drift Entrance (50 m)			Drift Exit (550 m)		
		Temperature (°C)					
		Waste Package	Drift Wall	Drift Air	Waste Package	Drift Wall	Drift Air
ANSYS-Refined DriftFlow-Coarse	5 years	76.3	51.6	30.6	103.2	82.4	63.2
		81.2	56.3	32.6	108.4	87.5	68.2
ANSYS-Refined DriftFlow-Coarse	50 years	51.9	38.5	27.9	68.0	55.9	45.3
		53.9	40.4	28.7	70.0	57.9	47.3
ANSYS-Refined DriftFlow-Coarse	300 years	33.1	29.0	25.9	38.6	34.6	31.2
		33.6	29.4	26.1	38.9	34.9	31.6

The temperature distributions for the waste package and drift wall for the two numerical models are within 3°C at all locations and times. The DriftFlow-Coarse temperatures at all three components are generally higher than the corresponding ANSYS values. The DriftFlow-Coarse air temperature air exhibit the largest differences to the ANSYS drift-air. This is due to the fact that DriftFlow alters the thermal properties of the air based on temperature, whereas ANSYS uses constant thermal properties based on a temperature of 25°C.

6.2.3.4 Heat Removal Comparisons for the ANSYS and DriftFlow-Coarse Models

The overall efficiency for the ANSYS and DriftFlow based numerical models is shown in Table 6-5. The overall efficiency is calculated using equation 6-10. Sections 6.6.2.1 through 6.6.2.3 discuss the use of the efficiency.

Table 6-5. Overall Ventilation Heat Removal Efficiencies for the 600-m Drift Split (for 50 and 300 yr Ventilation Durations)

	50 yr Ventilation Duration	300 yr Ventilation Duration
Numerical Model	$\eta_{\text{integrated}}$ (Eq. 6-10)	$\eta_{\text{integrated}}$ (Eq. 6-10)
ANSYS-Coarse	84.0%	91.0%
ANSYS-Refined	84.0%	91.0%
DriftFlow-Coarse	82.5%	90.3%

6.3 ALTERNATIVE CONCEPTUAL MODEL FOR IN-DRIFT VENTILATION

The alternative conceptual model for in-drift ventilation includes the addition of water and water vapor transport in the host rock, across the drift wall, and into the ventilation airstream. Water and water vapor mass transport is directly coupled to the heat transfer processes described in the conceptual model for in-drift ventilation. The impacts of the mass transport, in terms of latent heat transfer, temperature, heat removal rates, and near-field host rock dryout are evaluated using analytical approaches coupled with the DriftFlow v.1.0 software code.

6.3.1 Alternative Conceptual Model Heat and Mass Transfer Processes

The coupled heat and mass transfer processes for the alternative conceptual model for in-drift ventilation are the same as those for the conceptual model described in Section 6.1.1 and Figure 6-1 with the addition of two other processes:

5. Water phase change (evaporation and condensation) occurs within the host rock as the temperature and vapor pressure change which causes the host rock saturation to decline, thus lowering the thermal conductivity of the rock.
6. Water (liquid and vapor phases) mass transfer occurs within the host rock and the in-drift air. Water vapor may move within the host rock via diffusion to cooler regions where it condenses, as described in process 5. It also may enter the in-drift airflow at the drift wall, causing a change in relative humidity, and can potentially condense in cooler regions of the ventilation system, such as the exhaust main drift and exhaust shafts.

The heat transfer rates for processes 5 and 6 can be related to processes 1 through 4 by again considering the overall conservation of thermal energy except during the early transient response when the waste package temperature is rapidly changing. The following is an addition to the thermal energy conservation described in Section 6.1.1:

- The sum of the convective heat transfer rates from the waste package and the drift wall into the airflow (processes 2 and 3), and the heat of the water vapor transported back across the drift wall (process 6) equal the total heat added to the ventilation air.

Additionally, the mass transfer rates for processes 1 through 6 can be related by considering the overall conservation of mass during the ventilation period. The following summarizes the coupled components of the mass balance:

- The sum of the mass of the ventilation air into the drift and the water vapor that moves across the drift wall from the surrounding host rock, equals the mass of the air exiting the drift.

Vapor diffusion or enhanced vapor diffusion have the potential of locally increasing the heat flux rate for saturations that are intermediate to full matrix-fracture saturation, in the dry condition in which water vapor is absent. Vapor diffusion is defined as the movement of water vapor under Fick's Law. Enhanced vapor diffusion is the movement of water vapor to areas where water is retained, condensed and then evaporated.

The alternative conceptual model considers how the ventilation efficiency changes when water phase change and mass transfer occurs across the drift wall and within the host rock. Consider the situation where water in the rock evaporates, and the water vapor moves down the thermal gradient and condenses. When this occurs, the apparent thermal conductivity of the rock decreases in the region of evaporation, and increases in the region of condensation. When the thermal conductivity of the rock increases, more energy would be transferred to the rock, thus

decreasing the ventilation efficiency. Conversely when the thermal conductivity of the rock decreases, the in-drift environment becomes more insulated, and the ventilation efficiency increases.

When water in the rock evaporates, the water vapor may also move back up the thermal gradient through the rock and exit into the ventilation air stream. When this occurs, the latent heat (energy) of the phase change must be supplied by the source, and this latent heat (energy) must be put into the rock. The exiting of the water vapor from the rock into the air involves no energetics. More energy must be put into the rock to attain the same temperature when there is no evaporation. In this situation, again, the ventilation efficiency must decrease because more energy is put into the rock.

6.4 APPLICATION OF THE ALTERNATIVE CONCEPTUAL MODEL

To assess the impact on the ventilation efficiency to the alternative conceptual model processes, the following analyses were performed:

- An analytical calculation which bounds the latent heat contribution to the in-drift ventilation air stream.
- A ventilation analysis using the DriftFlow v.1.0 software (named DriftFlow- k_{th}) and the methodology for calculating the thermal pulse (outlined in Section 6.2.2.1) for host rock at different levels of saturation (and therefore different values of thermal conductivity).
- An analysis of experimental data for vapor diffusion and enhanced vapor diffusion.

6.4.1 Latent Heat Contribution to the In-Drift Ventilation Air Stream

An analytical calculation was performed which bounds the latent heat contribution to the in-drift ventilation air stream over the 600 m drift length and 300 year ventilation period. Analytical equations for steady state unsaturated flow in porous media to a specified moisture potential boundary condition at the drift wall were developed with the help of *Soil Physics* (Jury et al. 1991) and *Contaminant Hydrogeology* (Fetter 1993). Using an assumption of 30% relative humidity in the drift, the moisture potential at the drift wall was calculated to be -1.691×10^6 cm (Attachment VIII-7). The moisture potential in the surrounding host rock at some distance from the drift wall was calculated using the mean of 377 measurements, from several boreholes, of matrix saturation in the tsw35 geologic unit (Attachment VIII-8). Based on the mean and the mean plus one standard deviation of the measurements, bounding steady state moisture fluxes to the drift wall from the surrounding host rock were calculated to be 0.484 mm/yr and 2.259 mm/yr respectively (Attachment VIII-11 and VIII-14). Assuming that all the moisture which fluxes to the drift wall over the entire length of the emplacement drift is evaporated at an assumed constant temperature, the total latent heat contribution to the in-drift air over the 300-year preclosure period can be calculated. The latent heat contribution was then divided by the total heat output by the waste packages over the same 300-year period and 600 meter long drift. The results are presented in Table 6-6.

Table 6-6. Latent Heat Contribution Expressed as a Percentage of the Total Waste Package Heat Over 300 Years and 600 Meters of Drift

Model	Latent Heat Contribution
Analytical model with a moisture flux = 0.484 mm/yr ¹	0.15%
Analytical model with a moisture flux = 2.259 mm/yr ²	0.70%

¹ Attachment VIII-11, mean² Attachment VIII-14, mean plus one standard deviation

The analytical calculation indicates that:

- The contribution of heat by vaporization of moisture is rate limited by the hydrogeologic properties of the host rock
- The contribution of heat by vaporization of moisture is a very small percentage of the total heat input

6.4.2 Ventilation Analysis for Host Rock at Varying Degrees of Saturation

Two DriftFlow analyses, DriftFlow-Wet and DriftFlow-Dry, assessed the impact of varying degrees of host rock saturation on the ventilation efficiency. A summary of the input used in the analysis is shown in Table 6-7. The analysis first uses the methodology described in Figure 6-4 and developed in Section 6.2.2.1.3 for the analytical calculation of the thermal response to a unit pulse for saturated and unsaturated rock. These thermal responses are then used in the DriftFlow ventilation model, whose inputs are shown in Table 6-8, to assess the ventilation efficiency at various times and locations in the emplacement drift.

Table 6-7. Thermal Properties the Near the Repository Horizon for the DriftFlow-Wet and DriftFlow-Dry Analysis¹

USGS Unit	Hydrological Unit	Rock Grain Density (kg/m ³)	Rock Grain Specific Heat (J/kg·K)	Dry Conductivity (W/m·K)	Wet Conductivity (W/m·K)
Tptpmn	Tsw34	2530	948	1.56	2.33
Tptpll	Tsw35	2540	900	1.2	2.02
Tptpln	Tsw36	2560	865	1.42	1.84

¹See Section 4.2.4 Table 4-1 (DTN: LB990861233129.001)

Table 6-8. Summary of DriftFlow-Wet and DriftFlow-Dry Input Parameters

Parameter	Value	Units	Reference
Atmospheric Pressure	89,060	Pa	Section 4.1.3
Stefan Boltzman Constant	5.669×10^{-8}	$W/m^2 \cdot K^4$	Section 4.1.4
Emplacement Drift Spacing	81	m	Section 4.1.6
Emplacement Drift Diameter	5.5	m	Section 4.1.8
Waste Package Emissivity	0.87	dimensionless	Section 4.1.5
Drift Wall Emissivity	0.90	dimensionless	Section 5.9
Flow Area	21.83	m^2	Calculated ¹
Waste Package Initial Power and Decay	1.5477	kW/m	Attachment I
Initial Air Temperature	25	$^{\circ}C$	Section 5.6
Initial Rock Temperature	25	$^{\circ}C$	Calculated ²

¹ $(p/4) \cdot (d_{dw}^2 - d_{wp}^2)$

² Thermal gradient from ground surface to the water table as calculated by the ANSYS model

6.4.2.1 Temperature Comparisons for the DriftFlow-Wet and DriftFlow-Dry Models

The waste package, drift wall, and drift air temperature results for the DriftFlow-Wet and DriftFlow-Dry ventilation analyses are shown in Figures 6-11 and 6-12. The DriftFlow-Dry case clearly shows an increase in temperature for all components due the lower value of host rock thermal conductivity. The impact on the integrated ventilation efficiency is presented later in Section 6.4.4.

Figure 6-11. Plots of Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Time at 50 and 550 meters from the Drift Entrance for the DriftFlow-Wet and DriftFlow-Wet Ventilation Analyses (DTN: MO0212MWDDFC02.005)

Figure 6-12. Plots of Waste Package, Drift Wall, and Drift Air Temperatures as a Function of Drift Length at 5 and 300 Years from the Time of Waste Emplacement for the DriftFlow-Wet and DriftFlow-Dry Analyses (DTN: MO0212MWDDFC02.005)

6.4.3 Evaluation of Vapor Diffusion and Enhanced Vapor Diffusion on the Host Rock Thermal Conductivity and Thus Ventilation Efficiency

In addition to the conduction of heat under a temperature gradient, it is possible to have vapor phase diffusion (Jury et al. 1991) within the rock mass. In addition, enhanced vapor phase diffusion may occur (Jury et al. 1991). These related phenomena are not included in the ventilation analysis presented above nor in the ANSYS calculations that applies to stagnant fluid components. Vapor diffusion and/or enhanced vapor diffusion (due to evaporation and condensation in the pores) tend to increase the apparent thermal conductivity from that for stagnant fluid components.

The following discussion presents information regarding vapor diffusion and enhanced vapor diffusion by Jury et al., 1991. Experimental results obtained by Moyne et al., are then discussed to illustrate vapor and enhanced vapor diffusion effects. Experimental results obtained from laboratory measurements on core samples and the results from the large scale Drift Scale Test are then presented.

6.4.3.1 Vapor Diffusion by Jury et al. 1991

Jury et al. 1991 provides a general discussion of vapor diffusion. Laboratory tests have shown that when temperature gradients were placed across soil samples, the measured vapor flux were 10 times larger than that predicted by Fick's Law. It was found that two mechanisms could increase the potential for vapor diffusion. The first mechanism is that water vapor that is fluxing towards moisture that is retained in the pore space may condense on one side and evaporate on the other side (Jury et al. 1991).

The second enhancement mechanism relates to the thermal gradients across the liquid phase contained within the pore space. The thermal conductivity of the solid phase is several times larger than the thermal conductivity of water. Since the thermal gradients within the pore space

are more likely to be influenced by liquid water, the effective thermal gradients for a uniform heat flux would be higher. Theoretical considerations suggest that the thermal gradients might be a factor of two to three higher.

6.4.3.2 Vapor Diffusion by Moyne et al. 1990

Moyne et al. 1990 presented experimental measurements of these phenomena for various materials as a function of a term that he defined as the humidity ratio. These included lightweight porous concrete, glass spheres, and compacted clay. For intermediate saturations, their analysis and experimental data showed the potential for increased thermal conductivity due to enhanced vapor phase diffusion with increasing saturation for the lightweight concrete but not for compacted clay.

Moyne et al. 1990 provides an alternate method for evaluating the combined effects of tortuosity, and enhanced vapor diffusion. Figure 6-13 presents a series of gas tortuosity factors as a function of air content for comparison. Moyne et al. 1990 deduced the experimental resistance factor to gaseous diffusion from the experimental results. It should be noted that while Moyne et al. refers to a high resistance factor, a high factor is associated with increased apparent thermal conductivity, and a low resistance to heat flow.

Figure 6-13. Comparison of the Experimental Resistance Factor with Other Factors (Jury 1991 Moyne et al. 1990)

Figures 6-14 and 6-15 present the experimental resistance factor and the apparent thermal conductivity for glass beads. The results show that as humidity ratio increases reflecting a decrease in air content, there is a decrease in the experimental resistance factor. This is in contrast to the factored tortuosity relationships presented above. Apparently, the experimental resistance factor for glass spheres at high air content reflects the absence of water vapor condensation/evaporation that results a high resistance factor.

Figure 6-14. Apparent Thermal Conductivity for Glass Spheres (Moyne et al. 1990).

Figure 6-15. Experimental Resistance Factor for Glass Spheres (Moyne et al. 1990).

The apparent thermal conductivity for the glass spheres is a function of both the humidity ratio, and temperature. The results show that at the extreme of complete saturation, the voids are filled with water, and are unavailable for the diffusion of vapor. The apparent thermal conductivity equals the saturated thermal conductivity for stagnant water. At the other extreme the porous media is devoid of water, and the apparent thermal conductivity equals the dry thermal conductivity for stagnant air. At low humidity ratios (0 to 10) and at higher temperature, the experimental results show that very high apparent thermal conductivities can occur. For the glass spheres, the measured results show apparent thermal conductivity of 2 W/m·K that is 66% higher than the saturated thermal conductivity.

Figure 6-16 presents the apparent thermal conductivity for compacted clay. Moyne et al. 1990 describes this material as “a very highly compacted clay (calcite smectite compacted over 2000 bars.” It would be expected that this material would be highly consolidated, and the nature of the clay while exhibiting porosity might not exhibit an interconnected porosity. The experimental results show a sharp contrast to the results presented for glass spheres. The results do not show any evidence of vapor diffusion or enhanced vapor diffusion.

Figure 6-16. Experimental Resistance Factor for Glass Spheres (Moyne et al. 1990).

Moyne et al. (1990, p. 116) attributes the weak dependence on temperature to the strong bond between vapor molecules and the solid. However, it is also true that if the material had tortuous paths for the movement of water vapor that the effect of this resistance would reduce vapor movement and the apparent increase in apparent thermal conductivity. It would be expected that

a material exhibiting a high interconnected porosity such as glass spheres would be subject to vapor diffusion effects while a material such as a highly compacted clay with a smaller interconnected porosity would show no apparent increase in thermal conductivity.

Moyne et al (1990 Figure 6) also presents resistance factors for a lightweight concrete, and a C/SiC composite material as a function of the humidity ratio. These results show high factors for low humidity ratios. The maximum factor for light concrete ($f_{exp}=0.90$) is similar to the maximum ratio for glass beads. However, the maximum value is higher for C/SiC composite ($f_{exp}=0.90$).

6.4.3.3 Measured Results for the Tptpmn Unit

The following presents a discussion of the relationship of apparent thermal conductivity to saturation on core measurements and as can be inferred from the large-scale drift scale test.

SNL conducted a laboratory investigation in which thermal conductivity as a function of saturation state for welded and nonwelded tuff specimens. Rock core samples were recovered from the proposed repository site at Yucca Mountain, Nevada to determine the relationship between thermal conductivity and saturation state for both welded and nonwelded tuffs. Welded tuff was taken from Alcove 5 of the Exploratory Studies Facility at Yucca Mountain. All thermal conductivity tests were conducted at 30 °C and at intermediate moisture conditions.

The results of the laboratory investigations below a saturation of 90 percent are presented in Figure 6-17 (DTN: SNL22100196001.006). The measured values are compared to the measurements for enhanced vapor diffusion from Moyne et al. 1990.

Figure 6-17. Rock Matrix Thermal Conductivity as a Function of Saturation (DTN: SNL22100196001.006).

The measured results at a temperature of 30 °C on the densely welded tuff recovered from core are in general agreement with the measured results for a highly compacted clay from Moyne et al. 1990. It should be emphasized that at a low temperature of 30 °C, the vapor pressure of water is not very high, and the general theory presented by Moyne et al. 1990 would not predict a very large increase in apparent thermal conductivity. Nevertheless, there is no indication of vapor diffusion or enhanced vapor diffusion when the potential uncertainty of the results is considered.

Wildenschild and Roberts (1999) performed an investigation of thermally driven water vapor diffusion in the middle nonlithophysal zone of the Topopah Spring Tuff (Tptpmn) using a transient-state thermal conductivity measurement. Thermal conductivity was measured for a single sample of welded tuff indirectly as a function of total pore pressure, temperature and water content. Enhancement of vapor diffusion in welded tuff was not observed at any of the combinations of saturation, temperature and imposed pressures. At a temperature of approximately 50 °C, the apparent rock matrix thermal conductivity increased modestly with the degree of saturation from about 1.1 W/(m•K) at a saturation of 0.1 to about 1.3 W/(m•K) at a saturation of 0.78 (Wildenschild and Roberts 1999, Figure 5). From a saturation of 0.1 to a saturation of 0.35, the thermal conductivity was approximately constant. The results showed a stronger dependence on temperature than on saturation. The guarded heat flow results are corroborative with the experimental results for a single sample of welded tuff presented by Wildenschild and Roberts (1999).

The Drift Scale Test (DST) provides the insitu temperature response over a broader range of temperatures. The DST is the third and largest of several planned and conducted insitu thermal tests to investigate coupled processes in the local rock-mass surrounding the potential repository. These coupled processes are thermally driven by heat released from electrical heaters that simulate heat from emplaced nuclear waste. A block of rock, approximately 60 m wide, 50 m deep and 50 m high includes 9 floor/canister heaters in a 5 m diameter drift and 50 wing heaters installed in the horizontal boreholes drilled perpendicular to the drift into the rock. Numerous sensors located in the DST block measure the thermal-hydrological- mechanical-chemical behavior.

For the first 820 days of the test, the power was reasonably constant dropping from an initial value of about 188 kW to about 178 kW. On March 3, 2000 the first of five intentional interim power reductions was implemented to maintain drift wall temperature near 200 °C. The fourth interim reduction in power occurred on May 5, 2001. A fifth interim power reduction occurred on August 22, 2001. After these five interim reductions, the total power was approximately 140 kW, or approximately 70% of its initial level. On January 14, 2002, all heaters to the drift scale test were reduced to zero power.

Temperature profiles at various times for Borehole 158 located in the roof and Borehole 162 located in the floor are illustrated in Figures 6-18 and 6-19. Note that these boreholes are located away from the DST sidewalls, and reflect heating from the driftwall. The results show that temperature is inversely related to radius from the driftwall, and follows an approximate logarithmic relationship as would be predicted on the basis of heat conduction. Initially the steep temperature gradients would reflect transient heat conduction into the rock. At later times, the temperature rise at a location would be more gradual reflecting a quasi steady state condition. At early times the theory of heat conduction through solids would predict higher temperature gradients. At later times, the enhanced vapor diffusion theory for moist porous media would predict an increase in apparent thermal conductivity as temperatures rise. Vapor diffusion or enhanced vapor diffusion would be small at lower temperatures (5 to 50 °C), and much higher at higher temperatures (50 °C to 85 °C) if vapor diffusion or enhanced vapor diffusion were present. For conditions in which the heat flux rates are nearly constant, the application of Fourier's Law would predict a decrease in thermal gradient to offset the increase in apparent thermal conductivity.

Figure 6-18. Temperature Profile Along DST Borehole 158 into the Rock (DTN: Mo0208RESTRDST.002)

Figure 6-19. Temperature Profile Along DST Borehole 162 into the Floor (DTN: Mo0208RESTRDST.002)

The temperature measurements presented for Borehole 158 and Borehole 162 do not show a reduction in temperature gradients in the temperature range of 50 °C to 85 °C that would be necessary to offset the increase apparent thermal conductivity due to vapor diffusion or enhanced vapor diffusion. Of the four materials that were tested by Moyne et al. 1990, a compacted clay would reflect the DST temperature measurements made in the densely welded tuff.

6.4.4 Effect of Host Rock Thermal Conductivity and Apparent Thermal Conductivity on the Ventilation Efficiency

A series of DriftFlow ventilation runs were made at 100 (DriftFlow-Wet), 80, 60, 40, 20, and 0% (DriftFlow-Dry) saturation for stagnant fluids (i.e. no vapor or enhanced vapor diffusion). Another series of DriftFlow ventilation runs were made at these same saturation levels using apparent thermal conductivity values generated by enhanced vapor diffusion. Table 6-9 presents the results in terms of the integrated ventilation efficiency over the entire 600 meters of drift length and 300 year ventilation period. Figure 6-20 presents the same results graphically. The results show very little enhanced vapor diffusion and effect on the ventilation efficiency. This demonstrates that the ventilation efficiency in a conduction-dominated system during the preclosure period would range from 90 to 93 % depending on the extent of dryout in the absence of vapor diffusion. To provide a bounding calculation, the enhanced vapor diffusion occurs at a temperature of 95 °C.

Table 6-9. Summary of the Effects of Thermal Conductivity on the Ventilation Efficiency (DTN: MO0212MWDDFC02.005)

Saturation	Thermal Conductivity	Ventilation Integrated Efficiency
100%	2.02	90.33%
80%	1.86	90.76%
60%	1.69	91.21%
40%	1.53	91.69%
20%	1.36	92.19%
0%	1.20	92.73%

Attachment VI

Figure 6-20. Relationship of the Ventilation Efficiency and Host Rock Thermal Conductivity to Saturation (DTN: MO0212MWDDFC02.005)

6.5 VERIFICATION OF THE NUMERICAL MODELS

Sections 6.2.3 and 6.4.2 present a verification process where the results of the ANSYS-Coarse and ANSYS-Refined models are compared to each other. Besides these comparisons, various other model verification approaches were taken to assure that the ANSYS numerical application of the ventilation conceptual model conserved both energy and mass. These verification approaches are outlined in Table 6-10, in addition to those presented in earlier sections. The approaches that use submodel comparisons are intended to separate the coupled heat transfer mechanisms into individual components in which a single heat transfer phenomenon can be investigated. The results of these submodels are compared to analytical or text book solutions.

Table 6-10. Verification Methods

Numerical Application Requiring Verification	Description	Section
In-drift radiation heat transfer	Two-dimensional steady-state radiation heat transfer between concentric horizontal cylinders	6.5.1.1
In-drift convection heat transfer	Two-dimensional steady-state forced convection heat transfer between concentric horizontal cylinders	6.5.1.2
Host rock conduction	Two-dimensional (cylindrical) temperature dependent thermal conductivity heat conduction,	6.5.2.1

6.5.1 In-Drift Domain

Verification exercises involving in-drift radiation and convection heat transfer were investigated. The first group of submodels focuses on the two-dimensional (or radial) radiation heat transfer between the in-drift waste package and the drift wall. The second set of submodels is a duplication of the first, but uses forced convection heat transfer instead of radiation.

6.5.1.1 Submodel for Two Dimensional Radiation Heat Transfer between the Waste Package and Drift Wall

The submodel used to validate two-dimensional radiation heat transfer between the waste package and drift wall use a modified ANSYS simulation compared to an evaluation of an analytical solution. The ANSYS submodel was run to steady state (using a constant heat source and constant drift wall temperature), at which time the waste package temperatures were compared.

The ANSYS submodel used the same cylindrical mesh geometry and inputs as those used in the ventilation numerical models documented in Section 4 and 6.2, with the exception that a constant heat source of 1 kW/m was applied to the waste package rather than the exponential heat decay for repository models. The temperature of the drift wall was held constant at 25°C, and there was no forced ventilation. These problem specifications eliminate both heat transfer by conduction into the rock, and convection into the air, to isolate the radiation heat transfer mechanism.

The steady state waste package temperature was also evaluated analytically using equation 6-7 for radiation heat transfer between concentric cylinders. The equation for gray to black body radiation heat transfer for the same case of infinite concentric cylinders is as follows (Incropera and DeWitt 1996):

$$q_{12} = \varepsilon_{eff} \sigma A_1 (T_1^4 - T_2^4)$$

Eq. 6-40

where

q_{12} = radiative heat transfer from the inner cylinder (1) to the outer (2) (W)

ε_{eff} = effective emissivity of the gray body (subscript 1) when radiating to another gray body that is represented by a black body in the equation

σ = Stefan-Boltzmann constant $5.670 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$

A_1 = surface area of the inner cylinder (m^2)

T_1 = surface temperature of the inner cylinder (K)

T_2 = surface temperature of the outer cylinder (K)

Table 6-11 summarizes the results. The difference between the ANSYS and analytical solution was due to numerical error associated with the time stepping.

Table 6-11. Waste package Temperatures for the Two Dimensional Radiation-Only Submodel

Method	T _{waste package at Steady State} (°C)	T _{model} – T _{analytical} (°C)
In-Drift Radiation Only Model (1 kW/m heat load, 0.847 effective emissivity)		
Analytical	58.8	Na
ANSYS	57.7	-1.1

6.5.1.2 Submodel for Two Dimensional Forced Convection for the In-Drift Air Space

This submodel calculates two-dimensional forced convection heat transfer between concentrically located cylinders. The geometry and air flow rate are the same as those used in the ANSYS numerical models presented in Section 6.2 and 6.5.1.1. The submodel includes a constant 1 kW/m waste package and a constant drift wall temperature of 25°C. The submodel simulated a two-dimensional cross-section at the entrance of the drift where the in-drift air temperature was fixed at 25°C. Radiation was inactivated. The ANSYS submodel used a convective heat transfer coefficient of $1.89 \text{ W/m}^2 \cdot \text{K}$.

Newton's Law of Cooling for convection as applied to horizontal concentric cylinders is (Incropera and DeWitt, 1996):

$$q_{12} = hA_1(T_1 - T_2) \quad \text{Eq. 6-41}$$

where:

q_{12} = convection heat transfer from the inner cylinder (1) to the outer (2) (W)

h = convective heat transfer coefficient ($\text{W/m}^2 \cdot \text{K}$)

A_1 = surface area of the inner cylinder (m^2)

T_1 = surface temperature of the inner cylinder (K)

T_2 = surface temperature of the outer cylinder (K)

The submodel steady state waste package temperature was compared to the result of the analytical solution, and is reported in Table 6-12. Agreement between the analytical and ANSYS model results is around 3%.

Table 6-12. Waste Package Temperatures for the Two-Dimensional Convection-Only Submodel

Method	T _{waste package at Steady State} (°C)	T _{model} – T _{analytical} (°C)
In-Drift Convection Only Model (1 kW/m heat load, 1.89 W/m² K convective heat transfer coefficient)		
Analytical	113.2	NA
ANSYS	113.0	-0.2

6.5.2 Host Rock Domain

The conduction-only submodel investigated the temperature response of the near-field host rock using a concentric cylinder arrangement similar to that used in the ventilation models.

6.5.2.1 Two Dimensional Conduction in the Host Rock Region Bounded Internally by a Cylindrical Drift

This submodel calculates two-dimensional conduction in the host rock using a heat flux boundary condition at the drift wall. This submodel used ANSYS and compared the results to an analytical solution by Carslaw and Jaeger to compute the host rock temperature evolution at a location some distance from the drift wall.

The ANSYS simulation again used the geometries and meshes discussed for the previous submodels. Above and below the repository horizon, the elements representing the lithostratigraphic units were modified to represent a homogeneous media with thermal properties of tsw-35. This facilitated the comparison to the analytical solution. The temperature was fixed for the top and bottom boundaries to represent the atmosphere and the water table. Also, adiabatic (no heat flow) and no-mass-flow boundaries were implemented at the lateral edges of the domain (40.5 m from the cylinder axis). Because conduction was the only method of heat transfer being investigated for this submodel, the elements representing the waste package and open drift were modified to act as a single heat source. A constant heat source of 0.2 kW/m was distributed among these elements resulting in a constant heat flux into the host rock. This value of heat flux was chosen to produce repository-like drift wall temperatures. The thermal conductivity of the rock was held constant at the value representing 100% liquid saturation.

MATHECAD was used to evaluate an analytical solution for conduction (Carslaw and Jaeger 1956) for the transient temperature response as a function of location from a constant heat source applied to the surface of an infinite domain bounded internally by a circular cylinder. Because the analytical solution represents an infinite domain, it is only suitable for comparison to the ANSYS simulation at early times, before the simulation is influenced by the finite boundaries.

The results are shown in Table 6-13 and Figure 6-21. The plot shows the transient temperature response at a point 6 meters horizontally from the center of the drift (3.25 meters from the 5.5-m-diameter drift wall). For very early times (less than 1 year), the drift wall temperature change is small, and the grids may be too coarse to capture the detailed temperature fields. For times between 5 and 10 years, the agreement between the ANSYS model and the analytic solution is

within 1°C. At 30 and 50 years, the ANSYS simulation becomes progressively warmer than the analytic solution. Due to the small rock thermal diffusivity ($\sim 1 \times 10^{-7} \text{ m}^2/\text{s}$), and the large size of the rock pillars (40.5 m to the mid-pillar), the numerical solutions are expected to be progressively warmer than the analytic solution after several decades. After that time, the insulating effect of the adiabatic lateral boundaries affects the numerical solution, while the analytic solution does not include these boundaries.

Table 6-13. Host Rock Conduction Verification

Host Rock Conduction Only Model (0.2 kW/m heat flux at the drift wall, homogenous with tsw-35 properties, $T_0 = 27.3^\circ\text{C}$, $k = 0$ to preclude mass transport)					
Method	$T_{\text{DW}} (^\circ\text{C})$				
	1 yr	5 yr	10 yr	30 yr	50 yr
Analytical	34.8	44.6	50.0	57.7	61.6
ANSYS	35.6	45.6	50.5	59.4	65.0
$T_{\text{DW}(\text{model})} - T_{\text{DW}(\text{analytical})} (^\circ\text{C})$					
ANSYS	0.8	1.0	0.5	1.7	3.4
$(T_{\text{DW}(\text{model})} - T_{\text{DW}(\text{analytical})}) / (T_{\text{DW}(\text{analytical})} - T_{0(\text{model})})$					
ANSYS	11%	5.8%	2.2%	5.6%	9.9%

Figure 6-21. Analytical and ANSYS Conduction-Only Transient Temperature Responses of a Homogeneous Porous Medium with Material and Thermal Properties of tsw-35 Rock (DTN MO0209MWDMOD30.003)

6.6 APPLICABILITY OF WALL HEAT FRACTION TO DOWNSTREAM MODELS

The wall heat fraction is defined as one minus the ratio of heat removed by the ventilation to the heat generated by the waste package. The wall heat fraction can be expressed as a single value by integrating over both the duration of the pre-closure period and the length of the drift (equation 6-9). It may also be applied as a function of time and drift length (equation 6-7). Downstream models that do not explicitly model the ventilation period may implement the wall heat fraction in one of two ways during their preclosure runs to initialize their postclosure runs.

The first way is to introduce the heat flux adjusted by the wall heat fraction directly to the drift wall. Typically, a downstream model that uses the wall heat fraction in this manner does not model the in-drift components. Since the definition of the wall heat fraction is the amount of waste package heat delivered to the drift wall during the ventilation period, this method is the most straightforward. In this case, the only heat transfer mechanism being simulated is the conduction from the drift wall out to the host rock. Because the solution of the heat conduction equation is linear in nature with constant temperature heat sinks at the upper and lower boundaries of the domain, a unique solution for the temperature of the drift wall exists. Therefore, this method will result in both the same heat flux at the drift wall and the same drift wall temperature history as that predicted by the ventilation model from which the wall heat fraction was derived.

The second way the wall heat fraction may be used involves downstream models that include the in-drift components in their domains. These models typically reduce the waste package heat generation rate by the wall heat fraction and apply this new heat flux directly to the waste package rather than the drift wall. This type of application relies on both radiation and conduction heat transfer to deliver the right amount of heat to the drift wall, and replicate the drift wall temperature history as predicted by the upstream ventilation model. This approach is less straightforward than the first and requires further discussion as to its feasibility.

6.6.1 Theoretical Use of the Wall Heat Fraction at the Waste Package

Consider the case where the waste package heat output reduced the wall heat fraction, as calculated by a ventilation model, is used as a substitute for the preclosure convection to represent the preclosure heat removal by ventilation. An energy balance for the ventilation model is:

$$Q_{wp} = Q_{conv-wp} + Q_{rad}$$

Eq. 6-42

where

$$Q_{conv-wp} = A \cdot (T_{wp} - T_{air})$$

Eq. 6-43

$$Q_{rad} = C \cdot (T_{wp}^4 - T_{dw}^4)$$

Eq. 6-44

The fraction of heat removed by the ventilation (i.e. by convection) is:

$$\eta = \frac{Q_{conv-wp} + Q_{conv-dw}}{Q_{wp}}$$

Eq. 6-45

where

$$Q_{conv-dw} = B \cdot (T_{dw} - T_{air})$$

Eq. 6-46

The constants A , B , and C are defined as:

$$A = d_{wp} \cdot h_{wp-air}$$

Eq. 6-47

$$B = d_{dw} \cdot h_{dw-air}$$

Eq. 6-48

$$C = d_{wp} \cdot h_{rad}$$

Eq. 6-49

Substituting equations 6-43 and 6-44 into 6-42 yields:

$$Q_{wp} = A \cdot (T_{wp} - T_{air}) + C(T_{wp}^4 - T_{dw}^4)$$

Eq. 6-50

Substituting equations 6-43, 6-44, and 6-46 into 6-45 yields:

$$\eta = \frac{\left[A \cdot (T_{wp} - T_{air}) + B \cdot (T_{dw} - T_{air}) \right]}{\left[A \cdot (T_{wp} - T_{air}) + C \cdot (T_{wp}^4 - T_{dw}^4) \right]}$$

Eq. 6-51

For the downstream model, the waste package heat output is multiplied by the wall heat fraction to account for the heat removed during the preclosure ventilation period. Equation 6-52 represents the fraction of heat delivered to the drift wall:

$$Q'_{dw} \equiv Q_{wp} \cdot (1 - \eta)$$

Eq. 6-52

Substituting equations 6-50 and 6-51 into 6-52 yields:

$$Q'_{dw} = [A \cdot (T_{wp} - T_{air}) + C \cdot (T_{wp}^4 - T_{dw}^4)] \cdot \left[1 - \frac{[A \cdot (T_{wp} - T_{air}) + B \cdot (T_{dw} - T_{air})]}{[A \cdot (T_{wp} - T_{air}) + C \cdot (T_{wp}^4 - T_{dw}^4)]} \right]$$

Eq. 6-53

An energy balance for the downstream model considered in this case (i.e. where the wall heat fraction is used as substitute for the heat transfer via convection) is:

$$Q'_{dw} = Q'_{rad}$$

Eq. 6-54

where

$$Q'_{rad} = C \cdot (T'^4_{wp} - T'^4_{dw})$$

Eq. 6-55

where

T'_{wp} = waste package temperature of the downstream model (K)

T'_{dw} = drift wall temperature of the downstream model (K)

Substituting equations 6-53 and 6-55 into 6-54 and simplifying yields:

$$(T'^4_{wp} - T'^4_{dw}) = (T_{wp}^4 - T_{dw}^4) - \frac{B}{C} \cdot (T_{dw} - T_{air})$$

Eq. 6-56

If $T'_{wp} = T_{wp}$ and $T'_{dw} = T_{dw}$ are to be true, then the term $\frac{B}{C} \cdot (T_{dw} - T_{air})$ must be zero. For this to be true either the coefficient B must be zero, and/or the terms T_{dw} and T_{air} must be equal. The implication for either of these conditions is that there is no convective heat transfer between the drift wall and the drift air, which of course is not true. Therefore, a downstream application in which the wall heat fraction is used as a substitute for the convective heat transfer to simulate the preclosure heat removal by ventilation cannot accurately represent both the preclosure waste package and drift wall temperatures as calculated by the ventilation model.

However, if the use of the wall heat fraction in the downstream is model is to simply initialize the drift wall temperature such that $T'_{dw} = T_{dw}$, then T'_{wp} can be numerically forced to be:

$$T'_{wp} = \sqrt[4]{(T_{wp}^4 - T_{dw}^4) - \frac{B}{C} \cdot (T_{dw} - T_{air})} + T_{dw}^{'4}$$

Eq. 6-57

6.6.2 Numerical Example Using the Wall Heat Fraction

Two numerical examples that apply the theoretical use of the wall heat fraction as described in Section 6.6.1 are presented below in Sections 6.6.2.4 through 6.6.2.5. Beforehand, total energy balances are presented using the results of the ANSYS-Refined model and equation 6-8 for calculating the instantaneous heat removal efficiency as a function of time and drift length, equation 6-9 for calculating a time-averaged heat removal efficiency, and equation 6-10 for calculating an integrated heat removal efficiency.

6.6.2.1 Using Equation 6-8 to Calculate the Heat Removal Efficiency as a Function of Time and Drift Length

Using the results of the ANSYS-Refined model and equation 6-8 to calculate the heat removal efficiency as a function of both time and drift length, the total energy delivered to the host rock over the 300-year preclosure period and 600 meter long drift becomes:

$$Energy_{rock-total} = \int_0^{600m} \int_0^{300yr} Q_{wp}(t) \cdot (1 - \eta(t, x)) \cdot dt \cdot dx$$

Eq. 6-58

where

$Energy_{rock-total}$ = total energy to the host rock (J)

Q_{wp} = waste package lineal heat decay (W/m)

$\eta(t, x)$ = instantaneous ventilation heat removal efficiency at some time, t, and some distance from the drift entrance, x, (dimensionless)

Using the lineal waste package heat decay calculated for the ANSYS-Refined ventilation model in Attachment I, and the heat removal efficiencies calculated as a function of time and drift length for the ANSYS-Refined model, the total energy delivered to the host rock over 300 years and 600 meters is 2.12×10^{14} J.

6.6.2.2 Using Equation 6-9 to Calculate a Time-Averaged Ventilation Heat Removal Efficiency

Using the results of the ANSYS-Refined model and equation 6-9 to calculate a time-averaged ventilation heat removal efficiency, the total energy delivered to the host rock over the 300-year preclosure period and 600 meter long drift becomes:

$$Energy_{rock-total} = 600m \cdot \int_0^{300yr} Q_{wp}(t) \cdot (1 - \eta_{time-ave}) \cdot dt$$

Eq. 6-59

where

$\eta_{time-ave}$ = time-averaged ventilation heat removal efficiency given by equation 6-8 (dimensionless)

Using the lineal heat decay calculated for the ANSYS-Refined ventilation model in Attachment I, and the time-averaged heat removal of 94.6% reported in Table 6-6 for the ANSYS-Refined model, the total energy to the system over 300 years and 600 meters is 1.26×10^{14} J, or approximately 60% less energy than was calculated using equation 6-58.

6.6.2.3 Using Equation 6-10 to Calculate an Integrated Ventilation Heat Removal Efficiency

Finally, using the results of the ANSYS-Refined model and equation 6-10 to calculate an integrated ventilation heat removal efficiency, the total energy to the system over the 300-year preclosure period and 600 meter long drift becomes:

$$Energy_{total} = 600m \cdot \int_0^{300yr} Q_{wp}(t) \cdot (1 - \eta_{integrated}) \cdot dt$$

Eq. 6-60

where

$\eta_{integrated}$ = integrated ventilation heat removal efficiency given by equation 6-8 (dimensionless)

Using the lineal heat decay calculated for the ANSYS-Refined ventilation model in Attachment I, and the time-averaged heat removal of 91.0% reported in Table 6-5 for the ANSYS-Refined model, the total energy to the system over 300 years and 600 meters is 2.12×10^{14} J. This result balances with the energy calculated in Section 6.6.2.1 using equation 6-58.

6.6.2.4 Numerical Example of Using the Wall Heat Fraction as Function of Time and Drift Length

A numerical example of the theoretical use of the wall heat fraction as described above in Section 6.6.1 is presented below. The example uses the wall heat fraction as function of time and drift length, as calculated by the ANSYS-Refined ventilation model, to reduce the waste package heat generation rate in a radiation and conduction only based ANSYS model. The results are depicted in Figures 6-22.

This examples illustrates the conclusion reached in Section 6.6.1 that it is numerically impossible to use the wall heat fraction as substitute for the heat removed by convection and predict the same waste package and drift wall temperatures as those from which the wall heat fraction came. This example also illustrates the numerical difficulty in solving the non-linear radiation heat transfer. Because the radiation involves the difference in temperatures to the fourth power, a unique solution depends upon the energy balance between the other heat transfer mechanisms. However, the constant temperatures imposed at the ground surface and the water table are far enough away from the repository horizon that they act as semi-infinite boundaries, leaving the numerical solution somewhat unbounded. The results of this example clearly illustrates this, as the temperatures of the waste package and drift wall for the model that used the wall heat fraction are different than the original temperatures.

6.6.2.5 Numerical Example of Using T'_{wp} as Function of Time and Drift Length Calculated From Equation 6-57

This example used equation 6-57 to constrain the waste package temperature over time and drift length. The derivation of equation 6-57 takes into account the reduction of the waste package power by the wall heat fraction (equation 6-52), however in this case a temperature boundary condition is assigned to the waste package surface rather than inputting the adjusted heat flux. The energy radiated to the drift wall is the same as in the example presented in Section 6.6.2.4. However for this application, the numerical solver is able to calculate the right temperature history of the drift wall as shown in Figure 6-23.

Figure 6-22. Application of the Wall Heat Fraction as a Function of Time and Drift Length to Reduce the Waste Package Heat Decay, Adjusted Heat Load Applied at the Waste Package Surface with Temperature Results Shown for the Drift Entrance and Exit (DTN: MO0210MWDVEN30.005)

Figure 6-23. Application of the Wall Heat Fraction as a Function of Time and Drift Length to Reduce the Waste Package Heat Decay, Adjusted Waste Package Temperature Calculated from Equation 6-57 and Applied at the Waste Package Surface with Temperature Results Shown for the Drift Entrance and Exit (DTN: MO0210MWDVEN30.005)

7. MODEL VALIDATION

This section presents the results of model validation exercises. The EBS Technical Work Plan determined the level of validation to be low for the Ventilation Model based on the following:

1. It is not extrapolated over large distances, spaces, or time frames
2. It has nominal uncertainties in pertinent input parameters such as surface emissivities, convection heat and mass transfer coefficients, and rock mass thermal conductivity.
3. It is not used to demonstrate compliance or licensing positions
4. It's output will not have significant impacts on TSPA dose calculations results

The approach for validating the conceptual model for preclosure ventilation involves an inspection of the processes 1 through 4 as outlined in Section 6.1.1 in terms of their applicability to adequately simulate the heat transfer in and around a ventilated emplacement drift. These processes and the methods to validate them are outlined in Table 7-1.

Table 7-1. Validation Methods

Conceptual Model Process	Validation Method	Pertinent Input Parameter	Criteria used to Determine Validation	Section
Thermal radiation heat transfer between the surfaces of the waste package and the drift wall using the Stefan-Boltzmann Law	Corroboration with published literature	Surface Emissivity	Engineering Judgement	7.1.1
Convection heat transfer to the ventilation airstream off the waste package and drift wall surfaces by use of convection heat transfer coefficients	Corroboration of post-test analyses with acquired testing results from the quarter-scale ventilation tests conducted at the Atlas Facility	Heat Transfer Coefficient	Match the model results to the test data within $\pm 5^{\circ}\text{C}$ using a reasonable range of heat transfer coefficients	7.1.2
Conduction dominated heat transfer within the rock mass surrounding the emplacement drift using Fourier's Law	Corroboration with published results from the Drift Scale Heater Test	Rock Thermal Conductivity	Engineering Judgement	7.1.3

If these processes can be validated for a range of pertinent input parameters (i.e. surface emissivities, convection coefficients, and host rock thermal conductivities), then any numerical application of the conceptual model that uses the input parameters appropriately need only satisfy the conservation of energy and mass to be of use.

7.1 VALIDATION OF THE HEAT TRANSFER PROCESSES OF THE VENTILATION CONCEPTUAL MODEL

The following sections provide the validation exercises for the heat transfer processes outlined above in Table 7-1.

7.1.1 Validation of the Radiation Heat Transfer Model

The use of the Stefan-Boltzmann Law to calculate the radiative heat transfer between two surfaces is an accepted approach within the scientific and engineering community. The valid use of the Stefan-Boltzmann Law to calculate the radiative heat transfer between the surface of an eccentrically located waste package and the drift wall requires the following:

1. An assumption that the in-drift air does not participate in the radiation heat transfer by absorbing significant amounts of energy that would have been otherwise transferred to the drift wall
2. Appropriate values for the emissivities of the waste package and drift wall surfaces

7.1.1.1 Thermal Radiation to a Participating Gas

For enclosures such as an emplacement drift, a medium such as air that separates the radiating surfaces is said to be nonparticipating if it neither absorbs nor scatters the radiation, and it emits no radiation itself. Incropera and DeWitt (Incropera and DeWitt 1996) state that:

The foregoing conditions and the related equations [summarized in Section 6.1.2 Of this Model Report] may often be used to obtain reliable first estimates and, in most cases, highly accurate results for radiation heat transfer in an enclosure...For *nonpolar* gases, such as O₂ or N₂, such neglect [of participating gaseous radiation] is justified, since the gases do not emit radiation and are essentially transparent to the incident thermal radiation. However, the same may not be said for polar molecules, such as CO₂, H₂O (vapor), NH₃, and hydrocarbon gases, which emit and absorb over a wide temperature range.

The design of the preclosure ventilation system draws air from the outside environment to the intake shafts and then to the emplacement drifts. The initial composition of the ventilation airstream will resemble that of the outside air, or approximately 78% N₂ and 22% O₂ with some small fraction of water vapor. The composition of the ventilation airstream may change as it proceeds through the emplacement drift and acquires additional water vapor and CO₂ from the host rock. However, the range of relative humidities observed in the ESF, 20 to 40% (Section 5.10), shows that the ventilation airstream does not acquire enough water vapor to make any significant impact on the thermal radiation heat transfer.

7.1.1.2 Validation Criteria Met for the Radiation Heat Transfer Model

Engineering judgement dictates the use of the Stefan-Boltzmann Law to model radiation heat transfer within waste emplacement drifts. This is corroborated by its use in the engineering

community outside of the Yucca Mountain Project. Further bounding calculations, and where available analysis of exhaust air from the ESF, may be needed to further validate the argument that the in-drift air does not offer any significant participation in the radiation heat transfer between the waste package and drift wall during the ventilation period. However, for the level of confidence required for the Ventilation Model, this validation criteria is met.

7.1.2 Validation of the Convection Heat Transfer Model

The validation of the convection heat transfer model used in the Ventilation Conceptual Model hinges upon the appropriate use of convective heat transfer coefficients. Phases 1 and 2 of the one-quarter scale ventilation tests performed at the North Las Vegas Atlas Facility during 2001 and 2002 provide valuable data for determining a range of valid convection heat transfer coefficients. A detailed description of the ventilation tests is provided in the *Development Plan for EBS Ventilation Test* (CRWMS M&O 2000g) and an interoffice correspondence *Guidance for the Ventilation Test* (Kramer 2001). The primary difference between phases 1 and 2 is that the ventilation air in Phase 2 was conditioned to better control its inlet temperature and relative humidity. The Phase 1 test brought in ambient air from outside the test train that exhibited diurnal temperature changes of around 4 °C. The same ventilation air flow rates and linear heat loads were used for both phases. Considering these aspects, and that the ANSYS methodology for simulating ventilation does not account for the relative humidity of the in-drift air, the Phase 1 test data is sufficient to provide the level of validation required for the ANSYS model. Therefore, the use of the ventilation test data for post-test ANSYS modeling and validation for this revision of the Ventilation Model Report is confined to the Phase 1 cases. It is not anticipated that post-test modeling of the Phase 2 ventilation test cases will provide any higher level of confidence in the validation process. Table 7-2 lists the Phase 1 ventilation tests and cases for which ANSYS post-test modeling was performed.

Table 7-2. Ventilation Phase 1 Test Matrix

Test No.	Case No.	Nominal Flow (m ³ /s)	Nominal Power (kW/m)
1	4	1	0.18
2	5	0.5	0.18
3	1	1	0.36
4	5	2	0.36
5	3	0.5	0.36

7.1.2.1 Post-Test ANSYS Model

Figure 7-1 shows the saddle-like temperature trends for the waste package of Test 1, Case 4 of Ventilation Test Phase 1. The same trend is observed in all the other cases. The temperature peaks that occur around Station 3 are due to heat losses at the inlet and outlet of the test train. However, the ANSYS methodology outlined in Section 6.2.1 is not capable of modeling the profile of axial temperature exhibited by the test data. An underlying assumption of the ANSYS methodology is that temperatures of the in-drift components, drift wall, and ventilation air are always increasing as the calculation proceeds down the length of the drift. This limitation forced the development of a two-dimensional ANSYS-based ventilation model. In other words, only a

two-dimensional cross-section at Station 3 was modeled using ANSYS rather than the ANSYS/Excel methodology described in Section 6.2.1 for a pseudo-three-dimensional analysis from Station 1 to Station 5.

Figure 7-1. Ventilation Phase 1, Test 1, Case 4 Waste Package Temperatures Versus Axial Distance Down the Test Train for Data Recorded 10/15/00 (DTN: SN0107F3409100.004)

7.1.2.2 Mesh

Figure 7-2 shows a detailed drawing through a cross-section of the test train. It also includes the relative locations of the instrumentation. Figure 7-3 shows the discretization of the test domain or the computational mesh used for the ANSYS post-test modeling. The meshes for the post and pre-test modeling are the same with the exception that additional groupings of elements have been created for the application of post-test boundary conditions. The pallet that supports the simulated waste package is not continuous in the test configuration. Rather, it supports the ends of the package. The contribution of heat transfer via conduction from the package through the pallet, and into the invert is considered to be negligible in comparison to the amount of heat transferred by radiation. For this reason, the pallet was not modeled.

Figure 7-2. Cross-sectional View of the Ventilation Test Train (MOL.20001219.0107 and DTN: SN0107F3409100.004)

Figure 7-3. ANSYS Mesh

7.1.2.3 Inputs

Table 7-3 summarizes the material and thermal properties used in the ANSYS post-test modeling (Section 4.13 through 4.16).

Table 7-3. Material and Thermal Properties for the Ventilation Test Components

Parameter	Simulated Waste Package	Concrete Pipe	Insulation	Invert
Density (kg/m ³)	7840	2280	12	2530
Thermal Conductivity (W/m·K)	38.37	2.75	0.04	0.14
Specific Heat (J/kg·K)	410.98	1016.16	700	919
Emissivity	0.8	0.93	0.96	0.93

7.1.2.4 Boundary Conditions

The recorded temperatures on the outer insulation at Station 3 of the test train were used as the outer boundary conditions for the ANSYS post-test models. Each test case had a different set of recorded temperatures over its life span. Due the difficulty in maintaining constant ambient conditions in the high-bay of the facility, a data fit for each case was performed on the outer insulation temperature histories to aid in the implementation of this boundary condition. Figure 7-4 shows the outer insulation temperature histories and the data fits for the cases modeled.

The ANSYS methodology requires that an inlet ventilation air stream temperature be specified. Therefore, the temperatures of the ventilation air stream recorded at Station 3 were used as input to the ANSYS post-test models. Each test case had a different set of air stream temperature histories. Again, a data fit for each case was performed on the recorded temperature data to simplify its implementation into the models. Figure 7-5 shows the ventilation air stream temperature histories and the data fits for the cases modeled.

The simulated waste packages were hollow rolled steel tubes, with heater rods suspended concentrically inside. Due to the nature of the experimental set-up, natural convection cells developed within the placid annulus of the waste packages. This caused a non-uniform heat flux, and hence temperature distribution, around the circumference of the waste package. No temperature measurements were recorded inside the waste package (i.e. the annulus air or the rod-heater). Rather than model the complexity of the natural convection inside of the waste package, the ANSYS model supplied a heat flux at the waste package wall. The heat flux was partitioned around the waste package circumference using the recorded steady-state temperature distributions as a basis. Table 7-4 summarizes the distributions for the test cases listed in Table 7-2. The validity of this partitioning methodology is confirmed by the consistency of the calculated distributions from case to case.

Figure 7-4. Outer Insulation Boundary Temperatures for the ANSYS Post-Test Ventilation Model (DTN MO0209MWDANS30.017)

Figure 7-5. Measured Air Temperature Histories at Station 3 used as the Inlet Air for the ANSYS Post-Test Ventilation Model (DTN MO0209MWDANS30.017)

Table 7-4. Distribution of Total Power to the Top, Sides, and Bottom Quarters of the Waste Package Based on Temperature Measurements

Test No.	Case No.	Nominal Power (kW/m)	WP Top Quarter	WP Side Quarter	WP Bottom Quarter
1	4	0.18	32%	24%	20%
2	5	0.18	32%	24%	20%
3	1	0.36	32%	24%	20%
4	5	0.36	32%	24%	20%
5	3	0.36	31%	24%	21%

7.1.2.5 Correlating the Model Results to the Test Data Using Heat Transfer Coefficients

Having determined appropriate distributions of power around the circumference of the waste package, ANSYS models were run iteratively using different values for the heat transfer coefficients until the model results reasonably matched the test data.

7.1.2.6 Results

Table 7-5 shows the heat transfer coefficient values which resulted in reasonable comparisons to the measured temperature data. The temperature results from the ANSYS models are compared to the recorded test data in Figures 7-6 through 7-10. Table 7-6 compares the average heat transfer coefficient calculated for each test case from Table 7-5 to heat transfer coefficients calculated using the Dittus-Boelter correlation.

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Figure 7-6. ANSYS Post-Test Ventilation Model versus Measured Results for Ventilation Test Phase 1, Test 1, Case 4 (DTN MO0209MWDANS30.017)

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Figure 7-7. ANSYS Post-Test Ventilation Model versus Measured Results for Ventilation Test Phase 1, Test 2, Case 5 (DTN MO0209MWDANS30.017)

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Figure 7-8. ANSYS Post-Test Ventilation Model versus Measured Results for Ventilation Test Phase 1, Test 3, Case 1 (DTN MO0209MWDANS30.017)

Ventilation Model Report

Figure 7-9. ANSYS Post-Test Ventilation Model versus Measured Results for Ventilation Test Phase 1, Test 4, Case 5 (DTN MO0209MWDANS30.017)

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Figure 7-10. ANSYS Post-Test Ventilation Model versus Measured Results for Ventilation Test Phase 1, Test 5, Case 3 (DTN MO0209MWDANS30.017)

Table 7-5. Developed Heat Transfer Coefficients from the ANSYS Post-Test Modeling of Phase 1 of the Ventilation Test

Test No.	Case No.	Heat Transfer Coefficient (W/m ² ·K)					
		WP Top Quarter	WP Side Quarter	WP Bottom Quarter	Upper Concrete	Lower Concrete	Invert
1	4	0.5	7.5	7.0	5.0	9.0	9.0
2	5	0.0	7.0	7.0	5.0	15.0	9.0
3	1	2.0	8.0	8.0	7.0	11.0	6.0
4	5	3.5	9.5	10.5	13.0	15.0	2.0
5	3	1.0	7.5	8.5	9.5	16	5.0

Table 7-6. Comparison of Heat Transfer Coefficients using Data-Fitting and the Dittus-Boelter Correlation

Test No.	Case No.	Flow Rate (m ³ /s)	Heat Transfer Coefficient (W/m ² ·K)	
			ANSYS Fitted Average	Dittus-Boelter
1	4	1.0	6.3	2.7
2	5	0.5	7.2	1.5
3	1	1.0	7.0	2.7
4	5	2	8.9	4.6
5	3	0.5	7.9	1.5

The average of the heat transfer coefficients range from approximately two to five times larger than heat transfer coefficients calculated using the Dittus-Boelter correlation. Two reasons would tend to account for the differences. First, the Dittus-Boelter equation is a forced convection correlation. Analyses of the ventilation test data indicate a mixed (i.e. natural and forced) convection regime inside the concrete pipe annuls. Second, the Dittus-Boelter correlation for calculating a forced convection heat transfer coefficient was developed for hollow tube geometries. The correlation can be extended to a cylinder within a tube (i.e. waste package inside a drift) by using the hydraulic diameter instead of the geometric diameter. However, a cylinder within a tube, eccentrically located, is a very different geometry which would tend to invalidate the Dittus-Boelter correlation within the range of air flow velocities being considered herein. Add an invert, and the geometry of the problem lies even farther beyond the range of the Dittus-Boelter correlation. The values presented in Table 7-6 for the ANSYS fitted heat transfer coefficients argue that both natural and forced convection are important heat removal mechanisms for the experimental set-up of the Ventilation Test. Although scaling the quarter scale test results to a full scale drift is beyond the scope of this model report, it stands to reason that a convection coefficient correlation which considers both natural and forced convection is more appropriate for use than the simple Dittus-Boelter equation (for the current drift design, heat load range, and ventilation flow rate).

Table 7-7 summarizes the ventilation heat removal rates for the 5 cases as modeled by ANSYS.

Table 7-7. Heat Removal Ratios for the ANSYS Post-Test Ventilation Models

Test No.	Case No.	Heat Removal Ratio
1	4	0.87
2	5	0.83
3	1	0.78
4	5	0.93
5	3	0.81

7.1.2.7 Validation Criteria Met for the Convection Heat Transfer Model

The ANSYS numerical model matched the Phase I Ventilation Test results within the validation criteria of $\pm 5^{\circ}\text{C}$ using a reasonable range of heat transfer coefficients. The range of heat transfer coefficients required to match the test results indicates a mixed convection regime inside the test train. The Dittus-Boelter correlation for calculating forced convection heat transfer coefficients is therefore, at best, only a conservative approach. The impact of using such a correlation, as was done for the ventilation models presented in this model report, is a lower or more conservative rate of heat removal by ventilation. A more realistic correlation would be one that accounts for both natural and forced convection to remove heat from the drift. Even so, the use of heat transfer coefficients calculated using only a forced convection correlation would produce reasonable results. Therefore, the validation criteria for the convection heat transfer model is considered to be met with respect to the level of confidence required in the model. Additional sensitivity runs using a range of heat transfer coefficients may be required to determine the effects on the heat removal rates and peak postclosure temperatures.

7.1.3 Validation of the Host Rock Conduction Heat Transfer Model

It is assumed that conduction heat transfer dominates other heat transfer mechanisms (i.e. convection in fractures and lithophysae, and latent heat) in the host rock. This assumption is a conclusion reached by the Multiscale Thermohydrologic Model (BSC 2001) and is supported by preliminary and unpublished numerical modeling of the Drift Scale Test and earlier work documented by Sass (Sass et al. 1988). Additional effort may be needed to confirm this assumption. However, for the level of confidence required for the Ventilation Model, the assumption that conduction dominates the heat transfer in the host rock does not compromise the validity of the conceptual model.

8. CONCLUSIONS

This model report presents a conceptual model for the thermal energy processes in ventilated emplacement drifts. As described in Section 6.1, these processes include:

1. Thermal radiation between the waste package and drift wall.
2. Thermal convection from the waste package to the ventilation air stream.
3. Thermal convection from the drift wall to the ventilation air stream.
4. Thermal conduction in the surrounding host rock.

An alternative conceptual model is also presented which includes, in addition to the thermal processes described above, the following mass transfer processes:

5. Phase change of near-field host rock pore water.
6. Movement of mobilized water vapor and liquid water in the rock and into the ventilation air stream.

The implementation of the conceptual model using the ANSYS code confirmed that ventilation is a viable option for not only delaying the onset of peak waste package and drift wall temperatures, but also reducing their respective magnitudes. In addition, the implementation of the alternative conceptual model showed that water and water vapor mass transport is limited by the properties of the rock, and had little effect on the ability of ventilation to remove heat generated by the waste packages. Therefore, the mass transfer processes and their associated effects on the overall heat transfer need not be included at this time in the conceptual model for ventilation of waste emplacement drifts.

8.1 SUMMARY ACCOMPLISHMENT OF THE VENTILATION MODEL PURPOSES

The purposes of the Ventilation Model Report were numerated in Section 1. A brief summary of their accomplishment is outlined below:

1. The heat transfer mechanisms, which describe the conceptual model for preclosure ventilation of emplacement drifts, were successfully validated in Section 7. Additionally, the numerical application of these processes using ANSYS and DriftFlow were verified by comparing the results of each model, along with comparisons from other submodels.
2. With respect to KTI agreement RDTME 3.14, a comparison between the two ANSYS ventilation models in Section 6.2.3.1 showed the adequacy of the coarse discretization of the drift along its axis. Also with respect to KTI agreement RDTME 3.14, the applicability of the wall heat fraction to initialize postclosure thermal models was shown in Section 6.6.
3. KTI agreement TEF 2.07 is satisfied by providing the results of post-test ANSYS modeling of the Atlas Facility Ventilation Test. This effort also served to validate the use of heat transfer coefficients to adequately model convection heat transfer inside the drift (see Section 7.1.2).

4. The impacts of moisture, phase change, and mass transport on the ventilation efficiency were determined to be very minimal.

8.2 MODEL OUTPUTS

The primary purpose of the Ventilation Model Report is to present and validate the heat transfer processes which comprise the conceptual model for ventilating waste emplacement drifts. The Ventilation Model Report does not attempt to predict repository performance during the preclosure period. Therefore, all inputs and subsequent outputs are used solely for validation and verification purposes. Future analyses will exercise the ventilation conceptual model against a range of pertinent input parameters such as, but not limited to, surface emissivity, convection heat transfer coefficient, and host rock thermal conductivity. From these analyses will stem the ranges of applicability of the ventilation model to predict repository performance, as well an identification of the model uncertainties.

The DTNs of the developed data from this report are MO0210MWDTVE30.018, MO0210MWDTEM30.019, MO0209MWDANS30.017, MO0210MWDVEN30.005, and MO0212MWDDFC02.005. These DTNs should not be categorized as Technical Product Output for other models or analyses.

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10. ATTACHMENTS

ATTACHMENT I	DECAY HEAT USING MS EXCEL FOR ANSYS CALCULATIONS
ATTACHMENT II	DITTUS-BOELTER MS EXCEL CALCULATIONS FOR CONVECTIVE HEAT TRANSFER COEFFICIENTS
ATTACHMENT III	ANSYS VENTILATION CALCULATIONAL METHOD
ATTACHMENT IV	ANSYS-Coarse VENTILATION INPUT AND OUTPUT FILES
ATTACHMENT V	ANSYS-Refined VENTILATION INPUT AND OUTPUT FILES
ATTACHMENT VI	DriftFlow INPUT AND OUTPUT FILES
ATTACHMENT VII	VENTILATION PHASE 1 POST-TEST ANSYS INPUT AND OUTPUT FILES
ATTACHMENT VIII	ANALYTICAL SOLUTION USING MATHCAD FOR THE CONTRIBUTION OF LATENT HEAT TO THE IN-DRIFT AIR OF A VENTILATED EMPLACEMENT DRIFT USING A SOLUTION FOR STEADY STATE UNSATURATED FLOW TO MOISTURE POTENTIAL BOUNDARY AT THE DRIFT WALL

ATTACHMENT I

DECAY HEAT USING MS EXCEL FOR ANSYS CALCULATIONS

Ventilation Model Report

(1) Estimate of Linear Heat Load Along Emplacement Drift

Waste Package Type		Number of WPs	Fraction of Total	Length (m)	Heat Output Rate (KW) per package	Drift Length Required (meters)	Total Heat Output (kW)	Linear Heat Load (kW/m)
Sec. 4.1.14				Sec. 4.1.14	See Attachment I	see Note 1		
21-PWR	Absorber	4279	0.429	5.305	11.3375	23128.00	48513.16	2.10
21-PWR	Control Rods	87	0.009	5.305	2.3713	470.24	206.30	0.44
12-PWR	Long	158	0.016	5.791	9.5430	930.78	1507.79	1.62
44-BWR	Absorber	2889	0.29	5.275	7.1368	15528.38	20618.22	1.33
24-BWR	Thick Plates	6	0.001	5.245	0.4910	32.07	2.95	0.09
5-DHLW		1249	0.125	3.73	4.0580	4783.67	5068.44	1.06
5-DHLW	Long	414	0.042	5.357	5.8280	2259.20	2412.79	1.07
Naval	Combined	285	0.029	5.888	7.1368	1706.58	2033.99	1.19
DOE/Other		598	0.06	5.57	0.7930	3390.66	474.21	0.14
Total		9965	1			52229.56	80837.86	
Average				5.141				1.5477

Note: Total drift length required for a given type of WPs is determined using:
Total drift length = (Number of WPs)*(WP length + 0.1 m), where 0.1 m is the gap between WPs (see Section 4.1.4).

(2) Thermal Decay for CSNF

Time (years)	21-PWR Absorber Plates	21-PWR Control Rods	12-PWR Long	44-BWR Absorber Plates	24-BWR Thick Absorber Plates	Total Heat of All CSNF WP (kW)	Percentage Decay of All CSNF WP (%)
	kW	kW	kW	kW	kW		
	(Sec 5.1)	(Sec 5.1)	(Sec 5.1)	(Sec 5.1)	(Sec 5.1)		
0	11.3375	2.3713	9.5430	7.1368	0.4910	70848.42	100.00%
0.01	11.3337	2.3709	9.5402	7.1346	0.4910	70825.33	99.97%
0.167	11.2767	2.3639	9.4955	7.0976	0.4897	70466.92	99.46%
0.5	11.1602	2.3495	9.4034	7.0215	0.4870	69732.68	98.43%
1	10.9954	2.3285	9.2722	6.9146	0.4829	68696.08	96.96%
2	10.6890	2.2974	9.0259	6.7223	0.4721	66787.75	94.27%
5	9.9653	2.1785	8.4286	6.2682	0.4445	62274.26	87.90%
10	8.9956	2.0095	7.5901	5.6536	0.4030	56201.90	79.33%
15	8.1887	1.8547	6.8815	5.1467	0.3689	51159.11	72.21%
20	7.5138	1.7241	6.3149	4.7102	0.3341	46909.07	66.21%
25	6.9115	1.6038	5.8009	4.3098	0.3065	43083.23	60.81%
30	6.3792	1.4942	5.3407	3.9701	0.2806	39741.73	56.09%
35	5.9165	1.3980	4.9411	3.6661	0.2578	36811.93	51.96%
40	5.4984	1.3106	4.5868	3.3915	0.2369	34165.86	48.22%
45	5.1192	1.2333	4.2517	3.1491	0.2182	31783.18	44.86%
50	4.7912	1.1649	3.9792	2.9326	0.2033	29705.11	41.93%
60	4.2229	1.0443	3.5026	2.5621	0.1754	26117.01	36.86%
75	3.5654	0.9070	2.9482	2.1366	0.1445	21974.58	31.02%
100	2.8314	0.7545	2.3024	1.6685	0.1111	17365.94	24.51%
150	2.0790	0.5983	1.6766	1.1977	0.0799	12673.63	17.89%
200	1.7291	0.5244	1.3818	0.9878	0.0684	10516.93	14.84%
300	1.3654	0.4452	1.0804	0.7889	0.0583	8331.46	11.76%

Note: Values for 0.167 year are base on linear interpolation (see Attachment I, pg.2).

(3) Decay of Linear and Volumetric Heat Load

Time (years)	Total Heat of All CSNF WP (kW)	Percentage Decay of All CSNF WP (%)	All WP Linear Heat Load (kW/m)	Volumetric Heat Rate (J/yr-m ³)
	(page II-3)	(page II-3)	(page II-2)	(See Note 4)
0	70848.4208	100.00%	1.5477	2.54E+10
0.01	70825.3276	99.97%	1.5472	2.54E+10
0.167	70466.9161	99.46%	1.5394	2.53E+10
0.5	69732.6750	98.43%	1.5233	2.50E+10
1	68696.0805	96.96%	1.5007	2.47E+10
2	66787.7543	94.27%	1.4590	2.40E+10
5	62274.2638	87.90%	1.3604	2.23E+10
10	56201.9031	79.33%	1.2277	2.02E+10
15	51159.1129	72.21%	1.1176	1.84E+10
20	46909.0735	66.21%	1.0247	1.68E+10
25	43083.2325	60.81%	0.9412	1.55E+10
30	39741.7253	56.09%	0.8682	1.43E+10
35	36811.9330	51.96%	0.8042	1.32E+10
40	34165.8551	48.22%	0.7464	1.23E+10
45	31783.1816	44.86%	0.6943	1.14E+10
50	29705.1059	41.93%	0.6489	1.07E+10
60	26117.0133	36.86%	0.5705	9.37E+09
75	21974.5756	31.02%	0.4800	7.89E+09
100	17365.9444	24.51%	0.3794	6.23E+09
150	12673.6306	17.89%	0.2769	4.55E+09
200	10516.9307	14.84%	0.2297	3.77E+09
300	8331.4641	11.76%	0.1820	2.99E+09

Note: Based on Linear heat load values. For example, in year 0.01,
 $1.5477(\text{kW/m}) \times [1000(\text{J/s})/\text{kW}] \times [365.25 \times 24 \times 60(\text{s/yr})] / [(Pi/4) \times (1.564 \text{ m})^2]$
 $= 2.54\text{E}+10 \quad (\text{J/yr-m}^3)$
 Where 1.564 m is the WP diameter (Section 5.1) used in the calculation.

ATTACHMENT II

**DITTUS-BOELTER MS EXCEL CALCULATIONS FOR CONVECTIVE HEAT
TRANSFER COEFFICIENTS**

Calculating Convective Heat Transfer Coefficients for ANSYS and MULTIFLUX Ventilation Models Using the Dittus-Boelter Correlation

Input Parameter	Value	Source
Constant (pi), dimensionless	3.141592654	Universal Constant
Emplacement Drift Diameter (D), m	5.5	(Sec. 4.1.11)
Waste Package Diameter (d), m	1.564	(Sec. 5.2)
Wetted Perimeter (P), m	22.2	$P = \pi(D + d)$
Cross Section Area (A), m ²	21.84	$A = \pi/4(D^2 - d^2)$
Hydraulic Diameter (Dh), m	3.936	$D_h = 4A/P = D - d$
Air Density (rho), kg/m ³	1.0561	(Sec. 4.1.12)
Air Thermal Conductivity (k), W/m-K	0.0261	(Sec. 4.1.12)
Air Specific Heat (Cp), J/kg-K	1005.7	(Sec. 4.1.12)
Air Dynamic Viscosity (mu), kg/m-s	1.8371E-05	(Sec. 4.1.12)
Air Prandtl Number (Pr), dimensionless	0.7079	(Sec. 4.1.12)
Air Flow Rate (Q), m ³ /s per drift	15	(Sec. 5.7)
Air Flow Velocity (v), m/s	0.69	$v = Q/A$
Reynolds Number (Re), dimensionless	155425.74	$Re = \rho v D_h / \mu$
Nusselt Number (Nu), dimensionless	285.06	$Nu = 0.023 Re^{0.8} Pr^{0.4}$
Conv. Heat Transfer Coef. (h), W/m ² -K	1.89	$h = k Nu / D_h$
or h = 5.96E+07 J/(yr-m²-K)		

Calculating Convective Heat Transfer Coefficients for Ventilation Test Phase 1 Using the Dittus-Boelter Correlation

Input Parameter	Value	Source
Constant (π), dimensionless	3.141592654	Universal Constant
Emplacement Drift Diameter (D), m	1.3716	(Section 4.2.2)
Waste Package Diameter (d), m	0.4064	(Section 4.2.1)
Wetted Perimeter (P), m	5.6	$P = \pi(D + d)$
Cross Section Area (A), m ²	1.35	$A = \pi/4(D^2 - d^2)$
Hydraulic Diameter (Dh), m	0.9652	$D_h = 4A/P = D - d$
Air Density (ρ), kg/m ³	1.0561	(Sec. 4.1.12)
Air Thermal Conductivity (k), W/m-K	0.0261	(Sec. 4.1.12)
Air Specific Heat (Cp), J/kg-K	1005.7	(Sec. 4.1.12)
Air Dynamic Viscosity (μ), kg/m-s	1.8371E-05	(Sec. 4.1.12)
Air Prandtl Number (Pr), dimensionless	0.7079	(Sec. 4.1.12)

Test 2 - Case 5, Test 5 - Case 3

Air Flow Rate (Q), m ³ /s per drift	0.5	(Sec. 4.2.4)
Air Flow Velocity (v), m/s	0.37	$v = Q/A$
Reynolds Number (Re), dimensionless	20583.57	$Re = \rho v D_h / \mu$
Nusselt Number (Nu), dimensionless	56.56	$Nu = 0.023 Re^{0.8} Pr^{0.4}$
Conv. Heat Transfer Coef. (h), W/m ² -K	1.53	$h = k Nu / D_h$

Test 1 - Case 4, Test 3 - Case 1

Air Flow Rate (Q), m ³ /s per drift	1	(Sec. 4.2.4)
Air Flow Velocity (v), m/s	0.74	$v = Q/A$
Reynolds Number (Re), dimensionless	41167.13	$Re = \rho v D_h / \mu$
Nusselt Number (Nu), dimensionless	98.48	$Nu = 0.023 Re^{0.8} Pr^{0.4}$
Conv. Heat Transfer Coef. (h), W/m ² -K	2.66	$h = k Nu / D_h$

Test 4 - Case 5

Air Flow Rate (Q), m ³ /s per drift	2	(Sec. 4.2.4)
Air Flow Velocity (v), m/s	1.48	$v = Q/A$
Reynolds Number (Re), dimensionless	82334.26	$Re = \rho v D_h / \mu$
Nusselt Number (Nu), dimensionless	171.47	$Nu = 0.023 Re^{0.8} Pr^{0.4}$
Conv. Heat Transfer Coef. (h), W/m ² -K	4.64	$h = k Nu / D_h$

ATTACHMENT III
ANSYS VENTILATION CALCULATIONAL METHOD

Calculation of Instantaneous Ventilation Efficiency

The results of Steps 1 through 18 yield the ventilation efficiency as a function of both time and axial position from the drift entrance.

1. Run 2D ANSYS at 0-meters (drift entrance) with $T_{air(Drift_Entrance)} = 25^\circ\text{C}$ which yields $T_{WP(Drift_Entrance)}$ and $T_{DW(Drift_Entrance)}$ for $t = \{0, 0.01, 0.167, 0.5, 1, 2, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 60, 75, 100, 150, 200, 300\}$ years.

2. For $t = 0$ years, calculate total heat input for Segment_1:

$$q_{in(Segment_1)} = q_{WP} L_{Segment_1}$$

3. For $t = 0$ years, calculate total heat output to the air for Segment_1:

$$q_{out(Segment_1)} = q_{WP-air} + q_{DW-air}$$

where

$$q_{WP-air} = hA_{WP} (T_{WP(Drift_Entrance)} - T_{air(Drift_Entrance)})$$

and

$$q_{DW-air} = hA_{DW} (T_{DW(Drift_Entrance)} - T_{air(Drift_Entrance)})$$

4. For $t = 0$ years, calculate the efficiency for Segment_1:

$$\eta = \frac{q_{out(Segment_1)}}{q_{in(Segment_1)}}$$

5. For $t = 0$ years, calculate the segment exit air temperature for Segment_1:

$$T_{air(Segment_1_Exit)} = T_{air(Drift_Entrance)} + \frac{q_{out(Segment_1)}}{\rho_{air} c_p Q_{airflow}}$$

6. Increment to the next time step and repeat Steps 2-5 for $t = 0.01, 0.167, 0.5 \dots 300$ years.
7. Run 2D ANSYS at the beginning Segment_2 with $T_{air(Segment_1_Exit)}$ as calculated from Step 5 for each time step which yields $T_{WP(Segment_2_Entrance)}$ and $T_{DW(Segment_2_Entrance)}$ for $t = \{0, 0.01, 0.167, 0.5, 1, 2, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 60, 75, 100, 150, 200, 300\}$ years.
8. Repeat Steps 2 through 6 for $t = 0, 0.01, 0.167, 0.5 \dots 300$ years.

9. Repeat steps 2 through 8, incrementing the Segment number until the drift exit is reached.

Calculation of Integrated Ventilation Efficiency

The results of Steps 19 through 23 yield a single value of efficiency over the entire drift length and ventilation duration (300 years).

19. Using the results of Steps 1 through 9 (specifically Step 3 for each time step), calculate the sum of the heat output to the air from the waste package and from the drift wall over the entire length of the drift for $t = 0, 0.01, 0.167, 0.5 \dots 300$ years.
20. Calculate the sum of the heat input from the waste package for $t = 0, 0.01, 0.167, 0.5 \dots 300$ years.
21. Integrate the sum of the heat output to the air (Step 19) from $t = 0$ to $t = 300$ years.
22. Integrate the sum of the heat input from the waste package (Step 20) from $t = 0$ to $t = 300$ years.
23. Calculate the “overall” efficiency by dividing the result of Step 21 by Step 22.

ATTACHMENT IV

ANSYS-Coarse VENTILATION INPUT AND OUTPUT FILES

See DTN: MO0210MWDTEM30.019

Compressed Excel files with its name and size are listed as follows:

08/25/02	01:55p	170,175	amr15cs.zip
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amr15cs.zip: Results for an initial linear heat load of 1.55 kW/m, air flow rate of 15 m³/s, and intake air temperature of 25°C. The file contains air, emplacement drift, and waste package temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

Grouped and compressed files of ANSYS runs are listed as follows:

08/26/02	09:30a	486,659	amr.tar.Z
08/25/02	03:44p	168,286,715	amr-10cs.tar.Z
08/25/02	03:50p	168,313,862	amr-15cs.tar.Z
08/25/02	03:52p	168,644,409	amr-5cs.tar.Z

amr.tar.Z: Grouped and compressed file that contains material properties, model configurations, mesh sizes, and etc. of ANSYS runs for all cases analyzed. ANSYS text and binary files.

amr15cs.tar.Z: Grouped and compressed file that contains input and output files of ANSYS runs for an initial linear heat load of 1.55 kW/m, air flow rate of 15 m³/s, and intake air temperature of 25°C. The file contains boundary conditions, loads, and emplacement drift and waste package temperatures. ANSYS text and binary files.

ATTACHMENT V

ANSYS-Refined VENTILATION INPUT AND OUTPUT FILES

See DTN: MO0210MWDTVE30.018

Compressed Excel file with its name and size is listed as follows:

08/25/02 01:54p 529,446 amr15fs.zip

amr15fs.zip: Results for an initial linear heat load of 1.55 kW/m, air flow rate of 15 m³/s, and intake air temperature of 25°C. The file contains air, emplacement drift, and waste package temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

Grouped and compressed file of ANSYS runs is listed as follows:

08/25/02 02:25p 703,669,190 amr15fs.tar.Z

amr15fs.tar.Z: Grouped and compressed file that contains input and output files of ANSYS runs for an initial linear heat load of 1.55 kW/m, air flow rate of 15 m³/s, and intake air temperature of 25°C. The file contains material properties and calculation configurations, and emplacement drift and waste package temperatures. ANSYS text and binary files.

ATTACHMENT VI
DriftFlow INPUT AND OUTPUT FILES

See DTN: MO0212MWDDFC02.005

Grouped and compressed file for the DriftFlow runs is listed as follows:

DriftFlow-Runs.zip 11,974 KB 12/16/2002 12:58 PM

The grouped and compressed file, **DriftFlow-Runs.zip** contains the following folders and file:

DriftFlow-Coarse
DriftFlow-Dry
DriftFlow-20%
DriftFlow-40%
DriftFlow-60%
DriftFlow-80%
DriftFlow-Wet

DriftFlow Results.xls

Excel workbook that contains a summary and comparative plots of the various DriftFlow runs

Each **DriftFlow-xxx** folder contains the following files:

Dimensionless Cylinder Pulse.mcd

MathCAD workbook to calculate the dimensionless pulse of an internally bounded cylinder

Workbook DriftFlow-xxx.xls

Worksheet	Description
<i>Main</i>	Summary of input parameters, and selected output
<i>Detailed Results</i>	Temperature and efficiency output
<i>Peak Temp vs. Time</i>	Plot of maximum temperatures
<i>Flow Rate vs. Time</i>	Plot of flowrate
<i>Energy Balance</i>	Energy balance calculations at specific times and locations
<i>Pulse Responses & Decay Heat</i>	Includes the composite temperature pulse response for 300 years in 1 year increments (column G) and the heat decay for 300 years in 1 year increments (column I)

DriftFlow-xxx Composite Pulse.xls

Worksheet	Description
<i>Dimensionless Cylinder Pulse</i>	Pasted output for the dimensionless pulse for an internally bounded cylinder from <i>Dimensionless Cylinder Pulse.mcd</i>
<i>C&J Fig. 44 p. 338</i>	Plot of the data on worksheet <i>Dimensionless Cylinder Pulse</i>

Ventilation Model Report

<i>Cylinder Pulse</i>	Non-dimensionless cylinder pulse for 300 years in 1 year increments
<i>Slab Pulse</i>	Non-dimensionless slab pulse for 300 years in 1 year increments
<i>Composite Pulse</i>	Composite pulse for 300 years in 1 year increments

DriftFlow-xxx Output.xls

Worksheet	Description
<i>DriftFlow</i>	Output data from a DriftFlow-xxx.xls ventilation model
<i>DriftFlow (2)</i>	Select DriftFlow-xxx.xls output data
<i>Efficiency Calculation</i>	Calculates the integrated ventilation efficiency for a DriftFlow-xxx.xls ventilation model
<i>50m = Segment 1</i>	Plot waste package, drift wall, and drift air temperatures versus time
<i>250m = Segment 3</i>	Plot waste package, drift wall, and drift air temperatures versus time
<i>550m = Segment 6</i>	Plot waste package, drift wall, and drift air temperatures versus time
<i>5 yr</i>	Plot waste package, drift wall, and drift air temperatures versus axial position
<i>50 yr</i>	Plot waste package, drift wall, and drift air temperatures versus axial position
<i>300 yr</i>	Plot waste package, drift wall, and drift air temperatures versus axial position

VMR Decay Curve.xls

Worksheet	Description
<i>Original Data</i>	Waste package heat decay data from Attachment I
<i>Chart 1</i>	Plot of the heat decay versus time
<i>Lookup Table</i>	Used for worksheet <i>Output</i>
<i>Output</i>	Heat decay data for 300 years in 1 year increments

ATTACHMENT VII

VENTILATION PHASE 1 POST-TEST ANSYS INPUT AND OUTPUT FILES

See DTN: MO0209MWDANS30.017

Compressed Excel file with its name and size is listed as follows:

08/25/02	01:48p	2,100,387	vtia.zip
08/25/02	01:50p	5,033,296	vtib.zip
08/25/02	01:51p	3,527,662	vtic.zip
08/25/02	01:52p	3,246,544	vtid.zip
08/25/02	01:52p	3,324,959	vtie.zip

vtia.zip: Results for Test #1 (a linear heat load of 0.18 kW/m and an air flow rate of 1.0 m³/s). The file contains concrete pipe, waste package, and insulation temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

vtib.zip: Results for Test #2 (a linear heat load of 0.18 kW/m and an air flow rate of 0.5 m³/s). The file contains concrete pipe, waste package, and insulation temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

vtic.zip: Results for Test #3 (a linear heat load of 0.36 kW/m and an air flow rate of 1.0 m³/s). The file contains concrete pipe, waste package, and insulation temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

vtid.zip: Results for Test #4 (a linear heat load of 0.36 kW/m and an air flow rate of 2.0 m³/s). The file contains concrete pipe, waste package, and insulation temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

vtie.zip: Results for Test #5 (a linear heat load of 0.36 kW/m and an air flow rate of 0.5 m³/s). The file contains concrete pipe, waste package, and insulation temperatures, and ventilation efficiencies. Compressed Microsoft Excel 97 file.

Grouped and compressed file of ANSYS runs is listed as follows:

08/25/02	03:41p	126,456,851	vti.tar.Z
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vti.tar.Z: Grouped and compressed file that contains input and output files of ANSYS runs for all cases analyzed. The file contains material properties, model configurations, boundary and initial conditions, heat loads, and concrete pipe, waste package, and insulation temperatures. ANSYS text and binary files.

ATTACHMENT VIII

ANALYTICAL SOLUTION USING MATHCAD FOR THE CONTRIBUTION OF LATENT HEAT TO THE IN-DRIFT AIR OF A VENTILATED EMPLACEMENT DRIFT USING A SOLUTION FOR STEADY STATE UNSATURATED FLOW TO MOISTURE POTENTIAL BOUNDARY AT THE DRIFT WALL

Steady State Solution Summary Unsaturated Flow to a Drift Subject to a Moisture Potential Boundary Condition at the Drift Surface

Electronic files with their name and size are listed as follows:

```
Steady State Unsaturated Flow Solution Rev01 mcad7.mcd
10/07/02    01:18p    240,912

Steady State Unsaturated Flow.xls
10/07/02    01:19p    125,440

Output.prn
10/07/02    01:36p    360
```

Develop a steady solution for radial unsaturated flow to the specified moisture potential conditions. Neglect the gravity component of flow, and consider the Van Genuchten constitutive relationships. *Soil Physics* (Jury et al. 1991, Section 3.4) develops the solution for radial flow under unsaturated conditions. In the case of steady state flow under saturated conditions, the water conservation equation for a cylindrical coordinate geometry is given by:

$$\frac{1}{r} \cdot \frac{d}{dr} (r \cdot J_r) = 0$$

Eq. VIII-1

where

r = Radial Coordinate
J_r = Darcy Flux in the Radial Direction

Equation VIII-1 can be integrated once to produce the result:

$$r \cdot J_r = \phi = t_{\text{cons tan t}} = \frac{Q}{(2 \cdot \pi \cdot z_0)}$$

Eq. VIII-2

where

Q = Flow rate per Unit Length along the Tunnel
z₀ = Length Along the Tunnel

The radial flux under Darcy's Law is given by:

$$J_r = -K_s \cdot \frac{dp}{dr}$$

Eq. VIII-3

where

K_s = Saturated Hydraulic Conductivity
p = Pressure or Pressure Head Depending on convention adopted for Darcy's

Law

Writing Darcy's Law for radial flow to the tunnel surface:

$$-K_s \cdot \frac{dp}{dr} = \frac{Q}{2\pi \cdot z_0 \cdot r}$$

Eq. VIII-4

This equation can be integrated after placing all factors explicitly for r on the same side of the equation:

$$dp = \frac{-Q}{2\pi \cdot K_s} \cdot \frac{dr}{r}$$

Eq. VIII-5

Since $p(R_1) = p_1$ and $p(R_2) = p_2$ are specified at the boundary then:

$$\int_{p_1}^{p_2} dp = \frac{Q}{2 \cdot \pi \cdot K_s \cdot z_0} \int_{R_1}^{R_2} \frac{dr}{r}$$

Eq. VIII-6

from which we calculate:

$$Q = \frac{K_s \cdot 2\pi \cdot z_0 \cdot (p_1 - p_2)}{\ln\left(\frac{R_2}{R_1}\right)}$$

Eq. VIII-7

This expression agrees with the formulation presented in *Soil Physics* (Jury et al., 1991, p. 113 Equation 3.92).

Now consider the unsaturated flow case. The pressure gradient becomes a moisture potential gradient. For unsaturated flow, the unsaturated hydraulic conductivity is a strong nonlinear function of the moisture potential $\tilde{\psi}$. The boundary conditions for flow are represented in Figure VIII-1.

Figure VIII-1. Geometry for Unsaturated Flow Calculation

Neglecting the elevation head:

$$H_1 = \frac{p_1}{\gamma_w} + 0 = -\psi_1$$

Eq. VIII-8

$$H_2 = \frac{p_2}{\gamma_w} + 0 = -\psi_2$$

Eq. VIII-9

where

H_1	=	Total Potential at the Drift Surface R1
H_2	=	Total Potential at the Outer Boundary R2
ψ_1	=	Moisture Potential at Radius R1 Set by the RH in the Drift
ψ_2	=	Moisture Potential at Radius R2 Set by Undisturbed State of Capillary Equilibrium
γ_w	=	Unit Weight of Water

Writing Darcy's Law for unsaturated radial flow:

$$-K(\psi) \cdot \frac{dH}{dr} = \frac{Q}{2\pi \cdot z_0 \cdot r}$$

Eq. VIII-10

Noting that if we neglect the elevation head:

$$H \approx \psi$$

$$-K(\psi) \cdot \frac{dH}{dr} = \frac{Q}{2\pi \cdot z_0 \cdot r}$$

Eq. VIII-11

The convention is adopted that moisture potential is in units of head (Jury et al., 1991, p. 51). Now the Van Genuchten constitutive relation can be invoked. From *Contaminant Hydrogeology* (Fetter 1993, p. 182), the constitutive relation is:

$$K(\psi) = \frac{K_s \cdot \left\{ 1 - (\alpha\psi)^{n-1} \cdot [1 + (\alpha\psi)^n]^{-m} \right\}^2}{[1 + (\alpha\psi)^n]^{\frac{m}{2}}}$$

Eq. VIII-12

where

$$\begin{aligned} n &= 1/(1-m) \\ \alpha &= \text{Van Genuchten Parameter} \\ m &= \text{Van Genuchten Parameter} \end{aligned}$$

Substituting in the constitutive relation into Darcy's Law:

$$\frac{K_s \cdot \left\{ 1 - (\alpha\psi)^{n-1} \cdot [1 + (\alpha\psi)^n]^{-m} \right\}^2}{[1 + (\alpha\psi)^n]^{\frac{m}{2}}} \cdot \frac{d\psi}{dr} = \frac{Q}{2\pi \cdot z_0 \cdot r}$$

Eq. VIII-13

Equation VIII-13 can be integrated in the same manner:

$$\int_{\psi_1}^{\psi_2} \frac{K_s \cdot \left\{ 1 - (\alpha\psi)^{n-1} \cdot [1 + (\alpha\psi)^n]^{-m} \right\}^2}{[1 + (\alpha\psi)^n]^{\frac{m}{2}}} \cdot d\psi = \frac{Q}{2\pi \cdot z_0} \cdot \int_{R_1}^{R_2} \frac{dr}{r} = \frac{Q}{2\pi \cdot z_0} \cdot \ln\left(\frac{R_2}{R_1}\right)$$

Eq. VIII-14

Note that the sign convention in the constitutive law is positive while in Darcy's Law it is negative. Note that ψ_1 and ψ_2 are expressed in units of head consistent with sign convention presented by *Soil Physics* (Jury et al., 1991 p. 151). Substituting in the definition of hydraulic conductivity (Fetter 1993, p. 181):

$$K_s = \frac{\rho \cdot g \cdot k}{\mu}$$

Eq. VIII-15

where

k = intrinsic permeability (m²)
 μ = fluid viscosity (N·s/m²)

$$Q = \frac{-2\pi \cdot z_0 \cdot \frac{\rho \cdot g \cdot k}{\mu} \cdot \int_{\psi_1}^{\psi_2} \frac{\left(1 - (\alpha\psi)^{n-1} \cdot \left(1 + (\alpha\psi)^n\right)^{-m}\right)^2}{\left(1 + (\alpha\psi)^n\right)^{\frac{m}{2}}} \cdot d\psi}{\ln\left(\frac{R_2}{R_1}\right)}$$

Eq. VIII-16

Now consider the boundary conditions, and the geometry for the problem. Assume that the RH is 30 percent (Section 5.10) in the ventilated drift and use the Kelvin Equation to calculate moisture potential (Jury et al., 1991, p. 60):

$$RH = \exp\left(\frac{M_w \cdot \psi_1}{\rho_w \cdot R \cdot T}\right)$$

Eq. VIII-17

Input properties for analysis. The properties for water are obtained from *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996, p. 846):

Density of water

$$\rho_w := 1000 \cdot \frac{\text{kg}}{\text{m}^3}$$

$$\rho_w = 1.000 \frac{\text{gm}}{\text{cm}^3}$$

Molecular weight of water

$$M := 18 \cdot \frac{\text{gm}}{\text{mole}}$$

The universal gas constant is given by is obtained from *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996, Backcover):

Gas Constant

$$R := 8.314510 \cdot \frac{\text{joule}}{\text{moleK}}$$

Nominal temperature

$$T := (273.16 + 25) \cdot K$$

Substituting into Equation VIII-16:

$$\psi(RH, T) := \frac{\rho_w \cdot R \cdot T}{M} \cdot \ln\left(\frac{RH}{100}\right)$$

$$\psi(30, T) = -1.658 \times 10^8 \text{ kgm}^{-1} \text{ s}^{-2}$$

The moisture potential is expressed in bars. Calculate the moisture potential in units of head:

$$\psi_1 := \frac{\psi(30, T)}{\rho_w \cdot g}$$

$$\psi_1 = -1.691 \times 10^6 \text{ cm}$$

Input the properties for the tuff surrounding the tunnel (DTN: LB990861233129.001):

Properties :=

	Unit	$k_m \text{ (m}^2\text{)}$	ϕ_m	$\alpha_m \text{ (1/Pa)}$	m_m	S_{lm}	S_{ism}
0	TSw34	4.07E-18	0.110	3.86E-6	0.291	0.19	1.00
1	TSw35	3.04E-17	0.131	6.44E-6	0.236	0.12	1.00
2	TSw36	5.71E-18	0.112	3.55E-6	0.380	0.18	1.00
		0	1	2	3	4	5

From *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996, p. 846)

Viscosity of Water at 300 K:

$$\mu_w := 8.55 \cdot 10^{-4} \cdot \frac{\text{N} \cdot \text{s}}{\text{m}^2}$$

Consider the matrix of the TSw35 unit. Convert the air-entry parameter (cm^{-1}):

$$k := \text{Properties}_{1,2} = 3.040 \times 10^{-17} \text{ m}^2$$

$$\alpha := \text{Properties}_{1,4} = \rho_w \cdot g = 6.315 \times 10^{-4} \text{ cm}^{-1}$$

$$m' := \text{Properties}_{1,3} = 0.236$$

$$\theta_r = \text{Properties}_{1,1} \cdot \text{Properties}_{1,4} = 0.016$$

$$\theta_s = \text{Properties}_{1,1} \cdot \text{Properties}_{1,5} = 0.131$$

$$n := \frac{1}{1 - m'}$$

$$n = 1.309$$

$$z_0 := 1 \cdot \text{mm}$$

$$z_0 = 1.000 \times 10^{-3} \text{ m}$$

The moisture potential in the surrounding formation at a radius $r = R_2$ is calculated in the following manner. The matrix saturation is estimated based upon measurements on core samples. The retention relationship (Fetter, 1993, p. 172, Equation 4.9) is used to calculate the moisture potential.

Characterization of Hydrogeologic Units Using Matrix Properties (Flint 1998, p. 17) described the test method (ASTM R97-47 1977) for matrix properties. After initial sample weighing, core samples were saturated with CO₂ after evacuation of air under a vacuum to enable the saturation of small internal pores. The samples were then submersed in distilled, de-aired water. Samples were removed, dried with a damp towel, and weighed to determine the saturated weight. The sample was suspended in a beaker of water in a wire basket to determine volume displacement, dried for 48 hours in a relative humidity oven at 60 °C and 65 percent relative humidity, and reweighed. The samples were then dried at 105 °C for at least 48 hours to obtain a standard dry weight. Test determinations were made for matrix porosity (fM), bulk density (r), and grain density (rG) for both RH and oven dry weights. The table below presents the source for the matrix saturation for 377 measurements from several boreholes. The saturation can be determined from the initial weighing and the properties.

Borehole	DTN Core Data
USW SD-7	GS951108312231.009
USW UZ-7A	GS951108312231.011
USW NRG-7/7A	GS951108312231.010
USW NRG-6	GS000508312231.006
USW SD-9	GS950408312231.004
USW UZ-14	GS950408312231.005

The average saturation from these 377 measurements is 0.76 (Steady State Unsaturated Flow.xls, Worksheet: Matrix Saturation).

Calculate the average volumetric moisture content:

$$\theta := 0.76 \cdot \theta_s$$

$$\theta = 0.100$$

The retention relationship (Fetter, 1993, p. 172, Equation 4.9) is used to calculate the moisture potential:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (\alpha \cdot \psi)^n\right]^m}$$

Eq. VIII-17

$$n = \frac{1}{1 - m}$$

Eq. VIII-18

Solve for m:

$$m' := \frac{-(-n + 1)}{n}$$

$$m' = 0.236$$

Solve for moisture potential in terms of volumetric moisture content:

$$\psi := \frac{\left[-1 + \left[\frac{-(-\theta_s + \theta_r)}{(\theta - \theta_r)} \right]^{\left(\frac{1}{m'}\right)} \right]^{\left(\frac{1}{n}\right)}}{\alpha}$$

Eq. VIII-19

$$\psi = 3.529 \times 10^3 \text{ cm}$$

The calculated value is 3530 cm.

$$\psi_2 := \psi$$

Input the geometry of the drift. Assume a radius of influence of 6 m. Note that subsequently this value is varied to assess the sensitivity to the radius of influence:

$$R_1 := 2.75 \cdot \text{m}$$

$$R_2 := 6 \cdot \text{m}$$

$$k = 3.040 \times 10^{-17} \text{m}^2$$

$$\psi_1 = -1.691 \times 10^4 \text{m}$$

$$\psi_2 = 35.292 \text{m}$$

Calculate the steady state flux rate at the wall (Equation VIII-15):

$$Q := -2 \cdot \pi \cdot z_0 \cdot \frac{\rho_w \cdot g \cdot k}{\mu_w} \cdot \frac{\int_{|\psi_1|}^{|\psi_2|} \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n \right]^{-m'} \right]^2}{\left[1 + (\alpha \cdot \psi)^n \right]^{\frac{m'}{2}}} d\psi}{\ln \left(\frac{R_2}{R_1} \right)}$$

$$z_0 = 1.000 \times 10^{-3} \text{m}$$

$$R_1 = 2.750 \text{m}$$

$$Q = 2.653 \times 10^{-13} \text{m}^3 \text{s}^{-1}$$

$$z_0 = 0.100 \text{cm}$$

$$R_2 = 6.000 \text{m}$$

$$k = 3.040 \times 10^{-13} \text{cm}^2$$

$$\text{Flux} := \frac{Q}{2 \cdot \pi \cdot R_1 \cdot z_0}$$

$$\text{Flux} = 0.484 \frac{\text{mm}}{\text{yr}}$$

$$\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m} = 1.327 \times 10^3 \frac{\text{gal}}{\text{yr}}$$

Calculate the latent heat transfer by multiplying by the latent heat of vaporization. From *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996, p. 846):

$$2.334 \cdot 10^3 \cdot \frac{\text{J}}{\text{kg}} \cdot 1000 \cdot 1000 \frac{\text{kg}}{\text{m}^3} \cdot (\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m}) = 371.475 \text{ W}$$

Note that the factor of 1000 is for kJ in the reference.

Calculate the total energy for 300 years:

$$2.334 \cdot 10^3 \cdot \frac{\text{J}}{\text{kg}} \cdot 1000 \cdot 1000 \cdot \frac{\text{kg}}{\text{m}^3} \cdot (\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m}) \cdot 300 \cdot \text{yr} = 3.517 \times 10^{12} \text{ J}$$

Compare this calculation with the average line loading used in the ventilation analysis. The heat load is calculated out to three hundred years, and the average value for the line loading is determined during this period (Attachment II).

Initial Heat Load	1.5477	kW/m					
Time (yr)	Decay (%)	Heat Load	Area				
0	100.00%	1.5477	0		Average	0.412514	
0.01	99.97%	1.547196	0.015474				
0.167	99.46%	1.539366	0.25777				
0.5	98.43%	1.523326	0.767708				
1	96.96%	1.500682	1.52371				
2	94.27%	1.458994	3.003548				
5	87.90%	1.360396	7.232632				
10	79.33%	1.227743	13.70298				
15	72.21%	1.117583	19.56629				
20	66.21%	1.024739	24.9221				
25	60.81%	0.941163	29.83686				
30	56.09%	0.868167	34.36018				
35	51.96%	0.804165	38.54101				
40	48.22%	0.746361	42.41733				
45	44.86%	0.694311	46.01901				
50	41.93%	0.648915	49.37707				
60	36.86%	0.570532	55.47431				
75	31.02%	0.48004	63.35359				
100	24.51%	0.379363	74.09613				
150	17.89%	0.276858	90.50166				
200	14.84%	0.229745	103.1667				
300	11.76%	0.182003	123.7541				

$$123 \cdot 1000 \cdot \frac{\text{W}}{\text{m}} \cdot \text{yr} \cdot 600 \cdot \text{m} = 2.329 \times 10^{15} \text{J}$$

$$\frac{3.517 \cdot 10^{12} \text{J}}{2.329 \cdot 10^{15} \text{J}} = 0.151\%$$

The latent heat transfer is approximately 0.151% and is a small percentage of the waste package heat loading. Repeat the calculation for a higher farfield saturation. Consider a saturation of the mean (0.76) plus one standard deviation (0.15).

$$0.76 + 0.15 = 0.910$$

$$\theta := 0.91 \cdot \theta_s$$

Substituting into Equation VIII-19:

$$\psi := \frac{\left[-1 + \left[\frac{-(-\theta_s + \theta_r)}{(\theta - \theta_r)} \right]^{\left(\frac{1}{m'}\right)} \right]^{\left(\frac{1}{n}\right)}}{\alpha}$$

$$\psi = 1.044 \times 10^3 \text{ cm}$$

The calculated value is 1040 cm.

$$\psi_2 := \psi$$

Calculate the steady state flux rate at the wall (Equation VIII-15):

$$Q := -2 \cdot \pi \cdot z_0 \cdot \frac{\rho_w \cdot g \cdot k}{\mu_w} \cdot \frac{\int_{|\psi_1|}^{|\psi_2|} \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n \right]^{-m'} \right]^2}{\left[1 + (\alpha \cdot \psi)^n \right]^{\frac{m'}{2}}} d\psi}{\ln\left(\frac{R_2}{R_1}\right)}$$

$$z_0 = 1.000 \times 10^{-3} \text{ m}$$

$$R_1 = 2.750 \text{ m}$$

$$Q = 1.237 \times 10^{-12} \text{ m}^3 \text{ s}^{-1}$$

$$z_0 = 0.100 \text{ cm}$$

$$R_2 = 6.000 \text{ m}$$

$$k = 3.040 \times 10^{-13} \text{ cm}^2$$

$$\text{Flux} := \frac{Q}{2 \cdot \pi \cdot R_1 \cdot z_0}$$

$$\text{Flux} = 2.259 \frac{\text{mm}}{\text{yr}}$$

$$\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m} = 6.186 \times 10^3 \frac{\text{gal}}{\text{yr}}$$

Calculate the latent heat transfer by multiplying by the latent heat of vaporization. From *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996, p. 846):

$$2.334 \cdot 10^3 \cdot \frac{\text{J}}{\text{kg}} \cdot 1000 \cdot 1000 \cdot \frac{\text{kg}}{\text{m}^3} \cdot (\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m}) = 1.732 \times 10^3 \text{ W}$$

Calculate the total energy for 300 years:

$$2.334 \cdot 10^3 \cdot \frac{\text{J}}{\text{kg}} \cdot 1000 \cdot 1000 \cdot \frac{\text{kg}}{\text{m}^3} \cdot (\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m}) \cdot 300 \cdot \text{yr} = 1.640 \times 10^{13} \text{ J}$$

$$\frac{1.64 \cdot (10^{13} \cdot \text{J})}{2.329 \cdot 10^{15} \text{ J}} = 0.704 \%$$

The latent heat transfer is approximately 0.704% and is a small percentage of the waste package heat loading.

The calculation of the farfield moisture potential from the saturation on core measurements, and the Van Genuchten retention relationship may be compared with measurements made in the ECRB.

Water-potential measurements along three horizontal boreholes in the ECRB Cross Drift are summarized in *In Situ Field Testing of Processes AMR* (BSC 2001, Section 6.10.2.2). The water potential as a function of depth and time are presented in DTN: LB0110ECRBH2OP.001. Low water potentials close to the drift increase rapidly over a distance of several meters, and remain close to saturation values along the deeper profile. As discussed subsequently, these qualitative observations are in agreement with the calculation of the moisture potential profile presented subsequently.

Among the monitored boreholes, the borehole located at CD 15+00 in the Tptpl unit has the lowest water potential (driest condition) close to the driftwall. The borehole at CD 20+00 also shows lower water potentials up to a distance of about 1.5 m from the borehole collar. The borehole located furthest into the ECRB Cross Drift at CD 25+00 did not show large drops in saturated potential closer to the collar, nor did the borehole show any increases in water

potentials following the installation of the bulkhead doors. The following table summarizes the measurements at ECRB Station 15+00 on 07/29/2000.

DEPTH (m)	WATER POTENTIAL (m)
0.62	-258.8
1.12	-90.7
1.62	-10.4
2.12	-24.23
2.62	-36.78
3.12	-4.62
3.62	3.51
4.12	-12.49
4.62	-13.52
5.12	-7.62
5.62	-9.99

The calculation of farfield moisture potential from the average and high saturation values on core samples, and the Van Genuchten relationship (-1000 to -3500 cm) presented above are in approximate agreement with water potential measurements made at Station 15+00 at depths of 2 to 5 meters in the ECRB drift.

Repeat the calculation for different radii of influence. Consider a radius of influence of 4.75 m (Flow path length of 2 m) and the farfield moisture potential of 3529 cm.

$$\psi_1 = -1.691 \times 10^6 \text{ cm}$$

$$\psi_2 := 3529 \cdot \text{cm}$$

$$R_2 := 4.75 \cdot \text{m}$$

Restate the flow rate equation (Equation VIII-15):

$$Q := -2 \cdot \pi \cdot z_0 \cdot \frac{\rho_w \cdot g \cdot k}{\mu_w} \cdot \frac{\int_{|\psi_1|}^{|\psi_2|} \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n \right]^{-m'} \right]^2}{\left[1 + (\alpha \cdot \psi)^n \right]^{\frac{m'}{2}}} d\psi}{\ln \left(\frac{R_2}{R_1} \right)}$$

$$z_0 = 1.000 \times 10^{-3} \text{ m}$$

$$R_1 = 2.750 \text{ m}$$

$$Q = 3.787 \times 10^{-13} \text{ m}^3 \text{ s}^{-1}$$

$$z_0 = 0.100 \text{ cm}$$

$$R_2 = 4.750 \text{ m}$$

$$k = 3.040 \times 10^{-13} \text{ cm}^2$$

$$\text{Flux} := \frac{Q}{2 \cdot \pi \cdot R_1 \cdot z_0}$$

$$\text{Flux} = 0.692 \frac{\text{mm}}{\text{yr}}$$

$$\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m} = 1.894 \times 10^3 \frac{\text{gal}}{\text{yr}}$$

Calculate the latent heat transfer by multiplying by the latent heat of vaporization. From *Fundamentals of Heat and Mass Transfer* (Incropera and DeWitt 1996, p. 846):

$$2.334 \cdot 10^3 \cdot \frac{\text{J}}{\text{kg}} \cdot 1000 \cdot 1000 \frac{\text{kg}}{\text{m}^3} \cdot (\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m}) = 530.311 \text{ W}$$

Calculate the total energy for 300 years:

$$2.334 \cdot 10^3 \cdot \frac{\text{J}}{\text{kg}} \cdot 1000 \cdot 1000 \cdot \frac{\text{kg}}{\text{m}^3} \cdot (\text{Flux} \cdot \pi \cdot 5.5 \cdot \text{m} \cdot 600 \cdot \text{m}) \cdot 300 \cdot \text{yr} = 5.020 \times 10^{12} \text{ J}$$

$$\frac{5.021 \cdot (10^{12} \cdot \text{J})}{2.329 \cdot 10^{15} \text{ J}} = 0.216 \%$$

The percentage is less than one percent for a radius of influence extending 4.75 m out. The following table presents a summary of the percentages for various radii of influence.

4.75m	0.216%
-------	--------

6.00m	0.151%
10.00m	0.091%
20.00m	0.059%

$$\psi_2 = 35.290 \text{ m}$$

$$\psi_2 := 3529 \cdot \text{cm}$$

$$R_2 := 6 \cdot \text{m}$$

Solve for the base case flow. Construct the moisture potential profile surrounding the drift.
Restate the flow equation (Equation VIII-15):

$$Q = 3.787 \times 10^{-13} \text{ m}^3 \text{ s}^{-1}$$

$$Q := -2 \cdot \pi \cdot z_0 \cdot \frac{\rho_w \cdot g \cdot k}{\mu_w} \cdot \frac{\int_{|\psi_1|}^{|\psi_2|} \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n\right]^{-m'}\right]^2}{\left[1 + (\alpha \cdot \psi)^n\right]^{\frac{m'}{2}}} d\psi}{\ln\left(\frac{R_2}{R_1}\right)}$$

$$Q = 2.653 \times 10^{-13} \text{ m}^3 \text{ s}^{-1}$$

In order to solve for the moisture profile, we solve the transcendental equation presented below, and then solve for ψ as a function of r for a given flow rate.

Define a transcendental equation based upon Equation VIII-15:

$$\psi_1 = -1.691 \times 10^6 \text{ cm}$$

$$F(\psi, r) := \frac{-1.0 \rho_w \cdot g \cdot k}{\mu_w} \cdot \int_{|\psi_1|}^{\psi} \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n\right]^{-m'}\right]^2}{\left[1 + (\alpha \cdot \psi)^n\right]^{\frac{m'}{2}}} d\psi - \frac{Q}{2 \cdot \pi \cdot z_0} \cdot \ln\left(\frac{r}{R_1}\right)$$

Once ψ is determined for each value of r , then the volumetric moisture content can be determined for each value ψ from the basic Van Genuchten retention relationship. The Van Genuchten retention relationship is given by (Fetter 1993, p. 172, Equation 17):

$$\theta(\psi) := \theta_r + \frac{(\theta_s - \theta_r)}{\left[1 + (\alpha \cdot |\psi|)^n\right]^m}$$

$$\theta_r = 0.016$$

$$\theta_s = 0.131$$

$$\frac{\rho_w \cdot g}{\mu_w} \cdot k = 3.487 \times 10^{-8} \frac{\text{cm}}{\text{s}}$$

Plot the retention relationship, and the hydraulic conductivity relationship for the TSw35 unit.

$$\psi := 100 \cdot \text{cm}, 110 \cdot \text{cm}.. 100000 \cdot \text{cm}$$

Figure VIII-2. Moisture Potential Relationship for TSw35

Define the unsaturated hydraulic conductivity relationship from Equation VIII-12:

$$K_r(\psi) := \frac{\rho_w \cdot g}{\mu_w} \cdot k \cdot \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n \right]^{-m'} \right]^2}{\left[1 + (\alpha \cdot \psi)^n \right]^{\frac{m'}{2}}}$$

Figure VIII-3. Unsaturated Hydraulic Conductivity Relationship

Develop the profile for the moisture content in the following manner:

1. Select the radius.
2. Plot the transcendental equation as a function of ψ , and estimate the root.

$$r := 5.50 \cdot m$$

$$\psi := 1000 \cdot \text{cm}, 2000 \cdot \text{cm}.. 500000 \cdot \text{cm}$$

Figure VIII-4. Transcendental Equation Extracting the Moisture Potential

3. Estimate the root from the plot. Use the estimated root with the root function. Make multiple substitutions to reduce the error.

$$\psi := 3818 \cdot \text{cm}$$

$$r = 5.500 \text{ m}$$

$$\psi_{\text{ans}} := \text{root}(F(\psi, r), \psi)$$

$$\psi_{\text{ans}} = 3.818 \times 10^3 \text{ cm}$$

$$F(\psi_{\text{ans}}, r) = 6.825 \times 10^{-19} \text{ m}^2 \text{ s}^{-1}$$

4. Check the answer by substituting into Equation VIII-15.

$$Q := -2 \cdot \pi \cdot z_0 \cdot \frac{\rho_w \cdot g \cdot k}{\mu_w} \cdot \frac{\int_{|\psi_1|}^{\psi_{ans}} \frac{\left[1 - (\alpha \cdot \psi)^{n-1} \cdot \left[1 + (\alpha \cdot \psi)^n \right]^{-m'} \right]^2}{\left[1 + (\alpha \cdot \psi)^n \right]^{\frac{m'}{2}}} d\psi}{\ln\left(\frac{r}{R_1}\right)}$$

$$Q = 2.653 \times 10^{-13} \text{ m}^3 \text{ s}^{-1}$$

$$z_0 = 1.000 \times 10^{-3} \text{ m}$$

5. Calculate the moisture content based upon the retention relationship.

$$r = 5.500 \text{ m}$$

$$\theta(\psi_{ans}) = 0.0980$$

6. Place the data into a matrix and export to EXCEL.

$$A := \begin{pmatrix} 2.76 & .049 \\ 2.78 & 0.057 \\ 2.80 & .060 \\ 2.82 & .063 \\ 2.84 & .065 \\ 2.86 & .067 \\ 2.90 & .070 \\ 2.94 & .072 \\ 2.98 & .073 \\ 3.02 & .075 \end{pmatrix}$$

$$B := \begin{pmatrix} 3.25 & .081 \\ 3.50 & .085 \\ 3.75 & .088 \\ 4.0 & .090 \\ 4.25 & .092 \\ 4.50 & .094 \\ 4.75 & .095 \\ 5.0 & .096 \\ 5.25 & .097 \\ 5.5 & .098 \end{pmatrix}$$

$$\theta(3529 \cdot \text{cm}) = 0.100$$

$$C := \text{stack}(A, B)$$

Plot the moisture content profile.

Figure VIII-5. Steady State Moisture Content Profile

Conclusions: Under the assumptions made for the analysis, the latent heat associated with evaporation of porewater is small for a range of farfield moisture potentials, and radii of influence.