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Page: 1 of: 1

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CONTENTS

	Page
1. PURPOSE.....	5
2. METHOD	5
3. ASSUMPTIONS.....	5
4. USE OF COMPUTER SOFTWARE AND MODELS	8
5. CALCULATION	9
5.1 DATA INPUTS	9
5.2 PRECLOSURE PERIOD.....	11
5.3 POSTCLOSURE PERIOD	12
5.4 NO BACKFILL CASE	17
6. RESULTS.....	18
6.1 PRECLOSURE AND POSTCLOSURE (INNER AND OUTER) WITH BACKFILL REPOSITORY DESIGN	19
6.2 EXTENDED PRECLOSURE CONDITIONS	24
6.3 PRECLOSURE AND POSTCLOSURE (INNER AND OUTER) WITHOUT BACKFILL REPOSITORY DESIGN	25
7. REFERENCES	28
8. ATTACHMENTS.....	29

FIGURES

	Page
Figure 1 Preclosure Period Using Concentric Cylinders.....	11
Figure 2 Postclosure Period Using Concentric Cylinders (with backfill)	13
Figure 3 Effective Thermal Conductivity Parameter for Thermal Radiation Heat Transfer for a Design That Includes Backfill	20
Figure 4 Effective Thermal Conductivity Parameter for Natural Convection Heat Transfer for a Design That Includes Backfill	21
Figure 5 Bulk and Film Temperature Comparison for the Natural Convection Heat Transfer Equations (Kth Outer Term).....	22
Figure 6 Effective Thermal Conductivity Parameter Including both Natural Convection and Thermal Radiation Heat Transfer for a Design That Includes Backfill	23
Figure 7 Effective Thermal Conductivity Parameter for Thermal Radiation Heat Transfer- Extended Preclosure Period	24
Figure 8 Effective Thermal Conductivity Parameter for Thermal Radiation Heat Transfer for a Design Without Backfill.....	25
Figure 9 Effective Thermal Conductivity Parameter for Natural Convection Heat Transfer for a Design Without Backfill.....	26
Figure 10 Effective Thermal Conductivity Parameter Including both Natural Convection and Thermal Radiation Heat Transfer for a Design Without Backfill.....	27

TABLES

	Page
Table 1 Calculation Inputs and Sources.....	10
Table 2 Calculation Design Information (Assumption 3.5).....	19
Table 3 List of Attachments.....	29

1. PURPOSE

The objective of this calculation is to develop a time dependent in-drift effective thermal conductivity parameter that will approximate heat conduction, thermal radiation, and natural convection heat transfer using a single mode of heat transfer (heat conduction). In order to reduce the physical and numerical complexity of the heat transfer processes that occur (and must be modeled) as a result of the emplacement of heat generating wastes, a single parameter will be developed that approximates all forms of heat transfer from the waste package surface to the drift wall (or from one surface exchanging heat with another). Subsequently, with this single parameter, one heat transfer mechanism (e.g., conduction heat transfer) can be used in the models. The resulting parameter is to be used as input in the drift-scale process-level models applied in total system performance assessments for the site recommendation (TSPA-SR). The format of this parameter will be a time-dependent table for direct input into the thermal-hydrologic (TH) and the thermal-hydrologic-chemical (THC) models. This calculation is performed under quality assurance procedure AP-3.12Q, Rev. 0, ICN 3, *Calculations*. The work for this calculation is directed by the development plan TDP-EBS-HS-000001 (CRWMS M&O 1999) which was developed according to procedure AP-2.13Q, *Technical Product Development Planning*.

2. METHOD

The effective thermal conductivity parameter will be used to approximate multiple modes of heat transfer. Basic principles of heat transfer are applied between surfaces that exchange heat with one another. These include principles of heat conduction, natural convection heat transfer, and thermal radiation. The development of the required energy balances and heat transfer rate laws are described in detail in Section 5. The data generated by this calculation was submitted to the technical data management system (TDMS) according to AP-SIII.3Q, *Submittal and Incorporation of Data to the Technical Data Management System*, as specified in the development plan. With regard to the development of this calculation, the control of electronic management of data was evaluated in accordance with AP-SV.1Q, *Control of the Electronic Management of Data*. The evaluation (Andrews 2000) determined that current work processes and procedures are adequate for the control of electronic management of data for this activity.

3. ASSUMPTIONS

The working assumptions applied in this calculation are related to heat transfer geometries, thermal conditions (which dictate surrounding temperatures), and the methods in which different modes of heat transfer may be represented.

- 3.1 It is assumed that, from the standpoint of the governing heat transfer processes, the waste package is concentric within an emplacement drift (preclosure). Furthermore, after drip shield and backfill emplacement, the waste package is concentric within the drip shield, which is concentric within the backfill, which is concentric within the emplacement drift (postclosure). For a no backfill repository design, the backfill is removed and the waste package is concentric within the drip shield, which is concentric within the drift wall

(postclosure).

The basis for this simplification (conceptualization) is that it allows the use of standard textbook or literature published forms of both radiant and natural convection heat transfer rate laws and fluid property correlations (refer to Section 5 of this calculation document for details of the use of the heat transfer rate laws). This assumption is applied in the development of both required energy balances and appropriate rate laws. (The figures in Section 5 illustrate the use of this assumption.) It is emphasized that this conceptualization of the emplacement drift is used only in the development of the effective parameters detailed in this calculation. Other calculations or analysis/model reports (AMR) used in support of TSPA thermal-hydrology utilize the actual emplacement drift geometries (not the concentric assumption).

- 3.2 The resulting temperature data from the enhanced design alternative (EDA) II license application design selection (LADS) thermal-hydrologic (TH) model can be used as an estimate for the in-drift temperature variables required for this calculation (e.g., waste package temperature, drip shield temperature, and drift wall temperature, all as a function of time). EDA II was computed for 50 years of forced ventilation at 50% heat removal efficiency (i.e., a no waste aging case). It is further assumed that energy removed by the forced ventilation process is not available for input into the surrounding host rock (it is removed from the repository system). All remaining energy (50% remaining) is transported through the drift by thermal radiation (during the preclosure period). Therefore, a preclosure effective thermal conductivity that includes the effects of natural convection will not be required since thermal radiation is the dominant mode of heat transfer (input to the host rock) during this period. The preclosure effective thermal conductivity parameter will include only the effects of thermal radiation heat transfer. This assumption is applicable to the preclosure period that precedes either backfilled or no backfill repository postclosure designs described in Section 6.1 and 6.3.

A special case will also be considered for extended periods of ventilation at the same heat removal efficiency. This case will also include only the effects of thermal radiation heat transfer as described in Section 6.2.

The basis for assumption 3.2 is that the temperature data and modeled preclosure heat transfer processes from the LADS EDA II TH calculations represented the most current data available to the project with which to base the development of this parameter.

- 3.3 It is assumed that both thermal radiation and natural convection heat transfer processes may be approximated by a single time dependent parameter that can be applied in a standard Fourier's rate law format for heat transfer by conduction. The effective thermal conductivity will approximate the total rate of heat transfer by radiation and natural convection by a conduction-only mechanism (refer to Section 6).

The basis for assumption 3.3 is that the total rate (including each mode) of heat transfer

obtained by application of the effective thermal conductivity parameter is ensured with the use of individual equivalent rate equations given in Section 5.

- 3.4 The transient nature of the problem is alleviated by considering a series of steady state solutions at each time step with available temperature information. This assumption is applied in Section 5 to the energy balances applied to the effective backfill layer.

The basis for assumption 3.4 is that the transient nature of heat decay is inherently captured when using a series of steady state solutions (at each time point) for the effective thermal conductivity parameter since it is given at enough time points to capture the transient behavior (note the time-dependent nature of the curves given in Sections 6.1, 6.2, and 6.3).

- 3.5 The specific in-drift geometric and thermal properties taken from Buscheck 1999 can be applied to this calculation as well (see Table 2):

- Waste package radius
- Drift wall radius
- Waste package emissivity
- Drift wall emissivity
- Drip shield radius
- Backfill thermal conductivity

Furthermore, the drip shield and backfill emissivities are assumed to be 0.8 (same as waste package) and 0.9, respectively. An assumed effective backfill radius is 1.9 m based on a representative ~ 0.9 m backfill layer thickness taken directly above the drip shield in the discrete-heat-source, drift-scale, thermal (DDT) submodel in LL990301904242.084.

The basis for assumption 3.5 is similar to assumptions 3.1 and 3.2. An effective backfill thickness (obtained from the process-level TH submodel in LL990301904242.084 that includes backfill) is assigned so that standard heat transfer rate law expressions (for thermal radiation and natural convection) can be utilized in the development of the effective thermal conductivity parameter. Since the rate law expressions also require certain geometric and thermophysical properties, the values used in the process-level models (Buscheck 1999) that provided the temperature inputs used in this calculation are the most logical choice to use in developing the effective thermal conductivity parameter. It is noted that the in-drift thermophysical properties and geometries used in this calculation do not correspond to the values in current use for TSPA-SR drift-scale models, hence the assumption. This assumption is applied in Section 6.

4. USE OF COMPUTER SOFTWARE AND MODELS

Microsoft Excel 97 is used to perform the standard mathematical operations required in the implementation of the energy balances and heat transfer rate laws that calculate the in-drift effective thermal conductivity parameter. It is also used to graphically represent the trends of these operations and to visualize the resulting parameter. This software package is appropriate for this application. Samples of user-defined formulas (as implemented in the Excel spreadsheet) are presented in Section 5 of this document. The resulting spreadsheets for this calculation have been submitted to the technical data management system (TDMS) under data tracking numbers (DTNs) SN9907T0872799.002, SN9912T0872799.005, and SN0002T0872799.009.

The spreadsheets implement equations (3) through (6) and (16) for thermal radiation and (7) through (15) for natural convection. The implementation of these equations into the spreadsheets named below has been hand-checked in order to confirm the accuracy of the implementation. Sample calculations used to check the spreadsheet implementation for each case considered are presented in detail in Attachment IV.

The spreadsheet "kth(rad-convht).xls" in DTN: SN9907T0872799.002 contains the calculations for the preclosure and postclosure inner and outer effective thermal conductivities (with and without backfill). The primary emphasis of this spreadsheet is on the backfilled repository design. The spreadsheet "kth(rad-convht)wprec.xls" in DTN: SN9912T0872799.005 contains the effective thermal conductivity results of the extended preclosure period. The spreadsheet "kth(rad-convht)nobf.xls" in DTN: SN0002T0872799.009 contains the working results of the no backfill case preclosure and postclosure inner and outer effective thermal conductivities. The last column (FQ) in the "kth(rad-convht)nobf.xls" worksheet called "EDA-II-noBF-conv" gives the effective thermal conductivity parameter (for natural convection) using the bulk fluid temperature. This is used in the development of the total effective parameter (total includes thermal radiation and natural convection components). The column (FO) details the development of the same parameter using the film fluid temperature. As demonstrated in Section 5.3, the two methods used for evaluating fluid properties (at bulk or film temperature) provide nearly the same result. The primary emphasis of this spreadsheet is on the no backfill repository design. The spreadsheets and their subsequent worksheets used in this calculation are listed as (other worksheets contained in the spreadsheet but not listed below are either supporting or not used):

- kth(rad-convht).xls, version 1.0
 - effective-kth=radiation
 - effective-kth=convection
 - total-time
 - NUFT-input
 - TOUGH-input
 - EDA-II-noBF-rad
 - EDA-II-noBF-conv
- kth(rad-convht)wprec.xls, version 1.0

- preclose
- NUFT-input_preclose
- kth(rad-convht)nobf.xls, version 1.0
 - EDA-II-noBF-rad
 - EDA-II-noBF-conv
 - total-time_noBF
 - nuft-input_noBF
 - tough2-input_noBF

Version 1.0 of the routine named "convfile_gen.f" contained in the TDMS under technical data tracking number (DTN) MO9906SPATHRIP.000 is used to compute the average values (used in this calculation) from input values (see Table 1 below). The testing and verification of this software routine is found in Attachment IV. Also, the software routine "convfile_genprec.f" contained in the TDMS in DTN: SN9912T0872799.005 is used to compute the average values (used in this calculation) from the input values for the special extended preclosure case. The testing and verification of this software routine is also found in Attachment IV.

No models have been used in the calculation to develop the in-drift effective thermal conductivity parameter.

5. CALCULATION

5.1 DATA INPUTS

The temperature inputs for this calculation are from the LADS EDA II thermal hydrology results as discussed in Section 3. The input table below is given with DTNs and input filenames used to compute the average temperatures used in this calculation:

Table 1. Calculation Inputs and Sources¹

Inputs	DTN	Supporting Document
Waste package temperature, drip shield temperature, drift wall temperature--with backfill emplacement (all as a function of time and location)	LL990301904242.084 Input Filenames used: CC_snf_mean_01_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_02_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_11_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_12_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_21_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_31_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_32_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_41_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_42_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_51_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_52_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_61_sandBF_60_c_j4_22_03_02_001_data CC_snf_mean_62_sandBF_60_c_j4_22_03_02_001_data	Buscheck 1999
Extended preclosure ventilation	LL990302204242.087 Input Filenames used: CC_snf_mean_02_sandBF_60_c_j4_22_03_02_001_preClose_data CC_snf_mean_12_sandBF_60_c_j4_22_03_02_001_preClose_data CC_snf_mean_22_sandBF_60_c_j4_22_03_02_001_preClose_data CC_snf_mean_32_sandBF_60_c_j4_22_03_02_001_preClose_data CC_snf_mean_42_sandBF_60_c_j4_22_03_02_001_preClose_data CC_snf_mean_52_sandBF_60_c_j4_22_03_02_001_preClose_data CC_snf_mean_62_sandBF_60_c_j4_22_03_02_001_preClose_data	Buscheck 1999
Waste package temperature, drip shield temperature, drift wall temperature--no backfill emplacement (all as a function of time and location)	LL990302004242.085 Input Filenames used: CC_snf_mean_01_noBF_60_c_j4_22_03_02_0_data CC_snf_mean_11_noBF_60_c_j4_22_03_02_0_data CC_snf_mean_21_noBF_60_c_j4_22_03_02_0_data	Buscheck 1999
convfile_gen.f, convfile_genprec.f ²	MO9906SPATHRIP.000	—

¹ - QA status of input data is not qualified (NQ).

² - The source code for convfile_genprec.f was developed for this calculation and is included with the data submittal in DTN: SN9912T0872799.005

The input temperature values for the backfill/no backfill cases are taken from the repository center region "CC" in DTN: LL990301904242.084 (or DTN: LL990302004242.085) and averaged (results given in the spreadsheets indicated in Section 4 above in worksheet columns A-G) to obtain a single representative time-history curve at each required location (e.g., the waste package surface, drip shield, and drift wall) using the "convfile_gen.f" routine in DTN: MO9906SPATHRIP.000. The temperature values for the extended preclosure case are also taken from the repository center region "CC" in DTN: LL990302204242.087 and averaged (results are given in the spreadsheets indicated in Section 4 above in the specified worksheet columns A-E) to obtain a single representative time-history curve at each required location (e.g., the waste package surface and drift wall) by using the "convfile_genprec.f" routine submitted in DTN: SN9912T0872799.005. This step results in time-histories of average waste package surface temperature, drip shield temperature (for the backfill/no backfill cases only), and drift wall temperature at the center of the repository. The average time-

histories are used in the equations presented in this section to develop the effective thermal conductivity. The center temperatures are selected for this calculation in order to adequately capture the full extent of the initial heating period. Also, the 2-D drift-scale process-level models that utilize the effective thermal conductivity parameter as an input behave as a center representation due to the periodic nature of the modeled domain.

5.2 PRECLOSURE PERIOD

Consider first the preclosure period in which the waste package exchanges heat directly with the drift wall. Applying assumption 3.1, the resulting heat transfer conceptual configuration is depicted as the following in Figure 1:

For long concentric cylinders, the thermal radiation exchange between the inner cylinder (the waste package-*wp*) and the outer cylinder (the drift wall-*dw*) is the following (Incropera and DeWitt 1985, p. 609, Eqn. 13.25):

$$Q_{wp-dw} = \frac{\sigma A_{wp} (T_{wp}^4 - T_{dw}^4)}{\frac{1}{\epsilon_{wp}} + \frac{1 - \epsilon_{dw}}{\epsilon_{dw}} \left(\frac{r_{wp}}{r_{dw}} \right)} \quad (\text{EQN. 1})$$

where σ is the Stefan-Boltzmann constant ($= 5.67 \times 10^{-8} \text{ W/m}^2\text{-K}^4$, Incropera and DeWitt 1985, p. 524) for thermal radiation, r is the radius, T is the absolute temperature, and ϵ is the emissivity of the material. An equivalent heat transfer by conduction through this same space is (Incropera and DeWitt 1985, p. 76, Eqn. 3.26):

$$Q_k = \frac{2\pi L k_{eff} (T_{wp} - T_{dw})}{\ln\left(\frac{r_{dw}}{r_{wp}}\right)} \quad (\text{EQN. 2})$$

Equating (1) and (2) and solving for k_{eff} gives the effective thermal conductivity parameter during the preclosure period in terms of temperature, in-drift geometry, and radiative properties:

$$k_{eff} = \frac{\sigma r_{wp} (T_{wp}^2 + T_{dw}^2)(T_{wp} + T_{dw}) \ln\left(\frac{r_{dw}}{r_{wp}}\right)}{\frac{1}{\epsilon_{wp}} + \frac{1 - \epsilon_{dw}}{\epsilon_{dw}} \left(\frac{r_{wp}}{r_{dw}}\right)} \quad (\text{EQN. 3})$$

It is noted from equation (3) that the effective thermal conductivity parameter (k_{eff}) is a strong function of temperature. Equation (3) is implemented in the Excel spreadsheets (kth(rad-convht).xls, kth(rad-convht)wprec.xls, and kth(rad-convht)nobf.xls) and used to determine the effective thermal conductivity between the waste package and the drift wall during the preclosure period. As a result of the forced convection process (e.g., the ventilation process that removes 50% of the waste package heat), thermal radiative heat transfer during this period is the primary mode of heat transfer resulting in a net input of energy into the surrounding host rock. Therefore, all remaining heat not removed by the ventilation system is radiated to the surrounding host rock wall. Natural convection will not effectively transport heat from the waste package surface to the drift wall during the forced ventilation period such that an effective thermal conductivity developed for thermal radiation alone is adequate for the preclosure period.

5.3 POSTCLOSURE PERIOD

A similar analysis is required for the case of drip shield and backfill emplacement in the postclosure period. Applying the same assumption of concentric cylinders, the sketch in Figure 1 is modified for the idealized postclosure case to provide Figure 2:

Figure 2 is conceptually similar to Figure 1. However, during postclosure the drip shield and effective backfill are placed concentrically within the emplacement (refer to assumption 3.1). In this case, two effective parameters will be calculated. One will be calculated in-between the waste package and the drip shield (k_{effi}), and the other in-between the backfill and the drift wall (k_{effo}).

An equation similar to equation (3) can be written for k_{effo} between the effective backfill radius (r_b) and the drift wall:

$$k_{effo} = \frac{\sigma r_b (T_b^2 + T_{dw}^2) (T_b + T_{dw}) \ln \left(\frac{r_{dw}}{r_b} \right)}{\frac{1}{\epsilon_b} + \frac{1 - \epsilon_{dw}}{\epsilon_{dw}} \left(\frac{r_b}{r_{dw}} \right)} \quad (\text{EQN. 4})$$

Note, the subscript b refers to the backfill, and dw to the drift wall. Equation (4) contains two unknowns, the effective thermal conductivity and an estimate of the backfill temperature (T_b) based on the conceptualization shown in the sketch in Figure 2. The backfill temperature can be estimated by applying an energy balance between the drip shield and the drift wall:

$$T_b = \frac{\frac{k_b}{\ln \frac{r_b}{r_{ds}}} T_{ds} + \frac{k_{effo}}{\ln \frac{r_{dw}}{r_b}} T_{dw}}{\frac{k_b}{\ln \frac{r_b}{r_{ds}}} + \frac{k_{effo}}{\ln \frac{r_{dw}}{r_b}}} \quad (\text{EQN. 5})$$

Note, the subscript *ds* refers to the drip shield property (e.g., temperature or radius). Equations (4) and (5) are solved iteratively for the backfill temperature and the outer effective thermal conductivity. The method of solution is the following. Guess an initial backfill temperature (e.g., $\{T_{dw} + T_{ds}\} / 2$), substitute this guess into equation (4) to compute an effective thermal conductivity. With the newly computed effective thermal conductivity from equation (4), substitute this value back into equation (5) to compute a new estimate of the backfill temperature. Continue this process until T_b and k_{effo} converge. Convergence requires approximately 4 to 5 iterations of equations (4) and (5). Equations (4) and (5) are implemented in the Excel spreadsheet (kth(rad-convht).xls) used to determine the effective thermal conductivity between the backfill and the drift wall.

The inner effective thermal conductivity (k_{effi}) is of the same form as equation (3). It represents the effective thermal conductivity between the waste package surface and the inner surface of the drip shield:

$$k_{effi} = \frac{\sigma r_{wp} (T_{wp}^2 + T_{ds}^2) (T_{wp} + T_{ds}) \ln \left(\frac{r_{ds}}{r_{wp}} \right)}{\frac{1}{\epsilon_{wp}} + \frac{1 - \epsilon_{ds}}{\epsilon_{ds}} \left(\frac{r_{wp}}{r_{ds}} \right)} \quad (\text{EQN. 6})$$

Equation (6) is implemented in the Excel spreadsheets (kth(rad-convht).xls and kth(rad-convht)nobf.xls) used to determine the effective thermal conductivity between the waste package and the drip shield. Equations (3) – (6) represent the effective thermal conductivities that are required of a conduction heat transfer formulation that approximates the transport of energy by thermal radiation heat transfer processes. An additional mode of heat transfer must be considered during the postclosure period.

During the postclosure period (forced convection by ventilation is not available), a difference in surface temperatures (e.g., between the waste package and the drip shield) will drive fluid motion between the surfaces. The fluid motion is due to buoyancy forces within the fluid. Buoyancy is due to the combined presence of a fluid density gradient (driven by a temperature difference) and a body force (e.g., gravity) that is proportional to the fluid density. Unlike in the preclosure case, the transport of energy by natural convection is now available for rock wall heating (or drip shield heating). This results in a transfer of heat by natural convection processes. The sketch in Figure 2 provides the necessary conceptualization required in developing an effective thermal conductivity to approximate the fluid motion driven by temperature differences.

The natural convection processes occurring between concentric cylinders are described by Kuehn and Goldstein 1978, p. 639. Similar to the case of thermal radiation heat transfer described above, the effective thermal conductivity used to quantify the transport of energy by fluid motion is the conductivity that a stationary fluid must have to transfer the same amount of heat as the moving fluid. The effective thermal conductivity is written in terms of standard natural convection parameters such as the Rayleigh and Nusselt numbers.

The fluid properties in the Rayleigh number are evaluated at a specified bulk fluid temperature (defined below). The working equations for the Rayleigh number are given by Kuehn and Goldstein 1978, p. 636:

$$Ra_{Di} = \frac{g\beta(T_i - \bar{T}_B)D_i^3}{\nu\alpha} \quad (\text{EQN. 7})$$

and,

$$Ra_{Do} = \frac{g\beta(\bar{T}_B - T_o)D_o^3}{\nu\alpha} \quad (\text{EQN. 8})$$

where g is the gravitation acceleration, β is the volumetric thermal expansion coefficient of air, $\left(= \frac{1}{\bar{T}_B + 273} \right)$ for ideal gases, T_i and D_i are the inner cylinder wall temperature and diameter (subscript o is for the outer cylinder), ν is the kinematic viscosity of the fluid (air), and α is the thermal diffusivity of the fluid (air). Equations (7) and (8) and their corresponding fluid properties are evaluated at the bulk fluid temperature ($\bar{T}_B$) defined by Kuehn and Goldstein 1978, pp. 636 and 639. An additional case is considered by evaluating the fluid properties in equations (7) and (8) at the film temperature instead of the bulk temperature, that is for the inner cylinder $T_{film_i} = \frac{(\bar{T}_B + T_i)}{2}$ and for the outer cylinder $T_{film_o} = \frac{(\bar{T}_B + T_o)}{2}$. For either case, the bulk temperature is defined as:

$$\frac{\bar{T}_B - T_o}{T_i - T_o} = \frac{Nu_i}{Nu_i + Nu_o} \quad (\text{EQN. 9})$$

where the Nusselt numbers for fluid convection in equation (9) are based on the inner and outer cylinders and are defined as:

$$Nu_i = \frac{2}{\ln \left[1 + \frac{2}{\left[\left(0.5 Ra_{Di}^{1/4} \right)^{15} + \left(0.12 Ra_{Di}^{1/3} \right)^{15} \right]^{1/15}} \right]} \quad (\text{EQN. 10})$$

and,

$$Nu_o = \frac{-2}{\ln \left[1 - \frac{2}{\left[\left(Ra_{Do}^{1/4} \right)^{15} + \left(0.12 Ra_{Do}^{1/3} \right)^{15} \right]^{1/15}} \right]} \quad (\text{EQN. 11})$$

Equations (10) and (11) are valid for Prandtl numbers of 0.7 and any Rayleigh number (Kuehn and Goldstein 1978, p. 639; Kuehn and Goldstein 1976, pp. 1128 and 1130). The equivalent thermal conductivity ($= k_{effconv}/k_{sf}$) for natural convection is defined as the following:

$$\bar{k}_{eq} = \frac{Nu}{Nu_{cond}} = \frac{k_{effconv}}{k_{sf}} \quad (\text{EQN. 12})$$

where the effective thermal conductivity ($k_{effconv}$) is the required parameter and k_{sf} is the thermal conductivity of the stagnant fluid. The Nusselt number parameters in equation (12) are defined as:

$$Nu_{cond} = \frac{2}{\ln \frac{D_o}{D_i}} \quad (\text{EQN. 13})$$

$$Nu = \left[(Nu_{cond})^{15} + (Nu_{conv})^{15} \right]^{1/15} \quad (\text{EQN. 14})$$

and the convection Nusselt number is:

$$Nu_{conv} = \left[\frac{1}{Nu_i} + \frac{1}{Nu_o} \right]^{-1} \quad (\text{EQN. 15})$$

where Nu_i and Nu_o are based on equations (10) and (11) above. Solution of equations (7)-(15) provides the necessary formulation to compute an effective thermal conductivity that approximates the flow of heat by natural convection using only a standard heat conduction formulation. Equations (7)-(15) are implemented in spreadsheet *kth(rad-convht).xls* (worksheets: effective-kth=convection and EDA-II-noBF-conv) and *kth(rad-convht)nobf.xls* (worksheet: EDA-II-noBF-conv). Since equations (7) and (8) require direct input of the bulk temperature $\bar{T}_B$ (which is not known in

advance), the solution of this group of equations is also iterative. The method of the solution is the following. An initial guess for $\bar{T}_b$ is computed using a simple average of the inner and outer cylinder wall temperatures. With this guessed average value for $\bar{T}_b$, equations (7) and (8) may be evaluated (using either the bulk or the film temperature to evaluate the fluid properties). Substituting equations (7) and (8) into equations (10) and (11), a new approximation for $\bar{T}_b$ can be computed with equation (9). The process is continued until $\bar{T}_b$ converges to its nearly unchanging value. It is noted in Section 6 that the fluid properties in the Rayleigh numbers can be evaluated at either the film temperature or the bulk temperature, as the values are very nearly identical. With $\bar{T}_b$ now established, equations (12) – (15) are evaluated to obtain the effective conduction heat transfer parameter used to approximate the effects of natural convection. With this set of equations, the effective thermal conductivity parameter can be computed at each time point of input temperature data, thus resulting in a sequence of steady state evaluations with the final result a time dependent history (assumption 3.4 is applied at each time step that equations (3) – (15) are applied).

Equation (3) is evaluated to determine the preclosure thermal radiation effective thermal conductivity parameter. Equations (4) and (5) are used to determine the outer postclosure thermal radiation effective thermal conductivity parameter, and equation (6) is used to determine the inner postclosure thermal radiation effective thermal conductivity parameter. Finally, equations (7) – (15) are used to determine both the inner and outer postclosure natural convection effective parameters. The results are given in Section 6.

5.4 NO BACKFILL CASE

This section describes the thermal radiation and natural convection equations implemented for a repository design without backfill. The no backfill case is similar to the case with backfill already described. The preclosure period is identical to that already described. Therefore, the effective thermal conductivity for thermal radiation during the preclosure period is described by equation (3). The preclosure period requires an effective thermal conductivity for thermal radiation only. The postclosure period includes emplacement of only a drip shield at 50 years. Unlike the previous case which described an effective thermal conductivity parameter developed for combined modes of heat transfer with backfill present, backfill is not included such that heat transfer occurs from the waste package to the drip shield and from the drip shield to the drift wall. Conceptually, this case is similar to the backfill case. Only the radiating surface changes for one of the effective thermal conductivity parameters (e.g., the outer coefficient).

The inner effective thermal conductivity parameter is described exactly as before. The thermal radiation component of the effective thermal conductivity is described by equation (6); the natural convection component of the effective thermal conductivity is described by equations (7)-(15) with the inner cylinder (D_i) assigned waste package properties and the outer cylinder (D_o) assigned drip shield properties.

The outer effective thermal conductivity parameter for the no backfill design case is not as complex as the backfill case. For the outer effective thermal conductivity parameter, the thermal radiation component is now operational between the drip shield and the drift wall (instead of between the top of the backfill and the drift wall). The equation is similar in form to equation (4) with the backfill values in that equation replaced by the drip shield values:

$$k_{effo} = \frac{\sigma r_{ds} (T_{ds}^2 + T_{dw}^2) (T_{ds} + T_{dw}) \ln \left(\frac{r_{dw}}{r_{ds}} \right)}{\frac{1}{\epsilon_{ds}} + \frac{1 - \epsilon_{dw}}{\epsilon_{dw}} \left(\frac{r_{ds}}{r_{dw}} \right)} \quad (\text{EQN. 16})$$

The natural convection component for the outer effective thermal conductivity parameter is described by equations (7)-(15) with the inner cylinder (D_i) assigned drip shield properties and the outer cylinder (D_o) assigned drift wall properties. Equations (3), (6), and (16) are implemented in the Excel spreadsheet kth(rad-convht)nobf.xls (in worksheet: EDA-II-noBF-rad). Equations (7) through (15) are implemented in the Excel spreadsheet kth(rad-convht)nobf.xls (in worksheet: EDA-II-noBF-conv).

6. RESULTS

The results presented in this section are based on unqualified data and must be considered as to be verified. This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

The effective thermal conductivity parameters derived for the backfill case pre and postclosure (inner and outer), the special case of the extended ventilation period, and the no backfill case are contained in the TDMS under the data tracking numbers DTN: SN9907T0872799.002, DTN: SN9912T0872799.005, and DTN: SN0002T0872799.009, respectively. The assumptions applied in the development of these parameters are listed in Section 3 and are applied in the formulation described in Section 5. The resulting parameters have been submitted to the TDMS according to procedure AP-SIII.3Q, *Submittal And Incorporation Of Data To The Technical Data Management System*. The data submitted to the TDMS are not qualified (NQ).

6.1 PRECLOSURE AND POSTCLOSURE (INNER AND OUTER) WITH BACKFILL REPOSITORY DESIGN

Each of the effective thermal conductivity parameters is based on the following design information inputs (Buscheck 1999). It is noted that the data contained in Table 2 are derived from input used in the LADS calculations by the thermal hydrology model. The LADS in-drift geometry is used in the development of the parameters described in this calculation since the temperature inputs used to determine the parameters are based on models that use Table 2 data as input. **The geometry information given in Table 2 is not to be directly used by drift-scale models that require in-drift geometry as inputs for TSPA-SR analysis.** The current in-drift geometric properties (for the waste package, drip shield, emplacement drift, etc.) that should be applied in drift-scale models used in support of TSPA-SR are given in CRWMS M&O 2000.

Table 2. Calculation Design Information (Assumption 3.5)

Design Input	Value	Units
Waste package radius	0.815	m
Drift wall radius	2.55	m
Waste package emissivity	0.80	(-)
Drift wall emissivity	1.00	(-)
Drip shield radius	1.00	m
Effective backfill radius	1.90	m
Backfill thermal conductivity	0.67	W/m-K
Backfill emissivity	0.90	(-)
Drip shield emissivity	0.80	(-)

(Buscheck 1999)

Using Table 2 and equation (3), the preclosure (0 – 50 years) effective thermal conductivity as a function of time is computed to approximate the thermal radiation heat transfer between the waste package surface and the drift wall and is shown in Figure 3 (Precl-Effective Kth). As stated in assumption 3.2, the preclosure period requires a thermal radiative component only. The outer postclosure (50 years on) effective thermal conductivity as a function of time is computed using Table 2 and equations (4) and (5) and is also shown in Figure 3 (Postcl-Effective Kth-outer). This parameter represents an approximation of the thermal radiation heat transfer between the backfill material and the drift wall. Finally, the inner postclosure (50 years on) effective thermal conductivity is computed with equation (6) and is shown as a function of time in Figure 3 (Postcl-Effective Kth-inner). This parameter is representative of the inner thermal radiation heat transfer between the waste package surface and the drip shield. Assumption 3.2 is applied in order to develop this conceptual representation of the effective thermal conductivity parameter for thermal radiation heat transfer.

An analogous figure can be developed for the postclosure (50 years on) natural convection effective thermal conductivity. Using equations (7) – (15) and assumption 3.2, Figure 4 is a graphical result of the effective thermal conductivity parameter for natural convection heat transfer (inner and outer components as in the case of thermal radiation heat transfer). Figure 4 is shown on the same scale (in W/m-K) as Figure 3 in order to visualize the relative importance of each heat transfer component during the postclosure period. As indicated by these figures, thermal radiation heat transfer is the dominant mode of heat transfer during the postclosure period as well. For completeness, the natural convection effective thermal conductivity during the postclosure period will be included in the final total effective thermal conductivity parameter. Additionally, as design alternatives work towards lower in-drift and drift wall temperatures, Figure 4 will take on added importance relative to Figure 3 (e.g., natural convection heat transfer will become a more important mode of heat transfer inside the emplacement drift).

In order to determine an appropriate temperature at which to evaluate the fluid properties in equations (7) and (8), the effective thermal conductivity parameter (for natural convection only) obtained from both the bulk temperature and film temperature methods described Section 5.3 are shown as a function of time in Figure 5. From the figure it is noted that the solution method is insensitive to the choice of temperature used to evaluate the fluid properties (as long as either the bulk temperature or the film temperature is used in equations (7) – (15)) as these quantities overlay each other. The same is true of the no backfill case described in Section 6.3.

The final step to determine a total effective thermal conductivity that includes both modes of heat transfer discussed above is the following. Figures (3) are (4) are combined using a parallel network analogy for heat transfer by combined natural convection and thermal radiation. This results in a total effective thermal conductivity that can be used in a less complex conduction heat transfer formulation. Therefore, the resulting effective thermal conductivity parameter in Figure 6 provides an approximation of the total heat transfer rate using a single parameter only. Assumption 3.3 is applied to Figure 6.

The results of Figure 6 are tabulated in both TOUGH2 and NUFT formats in the attachment section given at the end of this calculation. The next section applies similar techniques to compute an effective thermal conductivity for extended preclosure periods (e.g., longer than the 50 years shown in Figure 6). This value can be used in models that require additional ventilation times during the preclosure period.

6.2 EXTENDED PRECLOSURE CONDITIONS

An extended preclosure period may be required for a number of future design alternative considerations. An extended preclosure effective thermal conductivity parameter is based on Figure 1, Table 2, and equation (3), which were previously discussed. The effective thermal conductivity for extended preclosure is shown in Figure 7. Figure 7 is tabulated in a NUFT format in the attachment section at the end of this calculation. As stated in Section 3.2, this effective thermal conductivity is developed to approximate only the effects of thermal radiation heat transfer between the surface of the waste package and the drift wall. Forced ventilation is available throughout this extended preclosure period. Therefore, heat transfer from the source to the receiving surface is by thermal radiation only (remaining energy is removed from the system by forced convection).

6.3 PRECLOSURE AND POSTCLOSURE (INNER AND OUTER) WITHOUT BACKFILL REPOSITORY DESIGN

Using Table 2 and equation (3), the preclosure (0 – 50 years) effective thermal conductivity as a function of time is computed to approximate the thermal radiation heat transfer between the waste package surface and the drift wall and is shown in Figure 8 (Preclosure). As stated in assumption 3.2, the preclosure period requires a thermal radiation component only. The outer postclosure (50 years on) effective thermal conductivity as a function of time is computed using Table 2 and equation (16) and is also shown in Figure 8 (Postclosure-outer). This parameter represents an approximation of the thermal radiation heat transfer between the drip shield and the drift wall. Finally, the inner postclosure (50 years on) effective thermal conductivity is computed with equation (6) and is shown as a function of time in Figure 8 (Postclosure-inner). This parameter is representative of the inner thermal radiation heat transfer between the waste package surface and the inner side of the drip shield. Assumption 3.2 is applied in order to develop this conceptual representation of the effective thermal conductivity parameter for thermal radiation heat transfer.

An analogous figure can be developed for the postclosure (50 years on) natural convection effective thermal conductivity. Using equations (7) – (15) and assumption 3.2, Figure 9 is a graphical result of the effective thermal conductivity parameter for natural convection heat transfer (inner and outer components as in the case of thermal radiation heat transfer). Figure 9 is shown on the same scale (in W/m-K) as Figure 8 in order to visualize the relative importance of each heat transfer component during the postclosure period. As indicated by these figures, thermal radiation heat transfer is the dominant mode of heat transfer during the postclosure period as well. For completeness, the natural convection effective thermal conductivity during the postclosure period will be included in the final total effective thermal conductivity parameter.

The final step to determine a total effective thermal conductivity that includes both modes of heat transfer discussed above is the following. Figures (8) and (9) are combined using a parallel network analogy for heat transfer by combined natural convection and thermal radiation. This results in a total effective thermal conductivity that can be used in a less complex conduction heat transfer formulation.

Therefore, the resulting effective thermal conductivity parameter in Figure 10 provides an approximation of the total heat transfer rate using a single parameter only. Assumption 3.3 is applied to Figure 10.

The tabulated results of Section 6 are given below in the attachment section. The tabulated results are given specifically in NUFT and TOUGH2 formats for use by these process-level model codes. The extended preclosure case (see Attachment II) does not require a TOUGH2 entry since the TOUGH2 models will not be required to simulate the extended preclosure case.

7. REFERENCES

- Andrews, R.W. 2000. "AP-SV.1Q Control of the Electronic Management of Data Evaluation for Natural Systems Analysis/Model Reports." Letter from R.W. Andrews (CRWMS M&O) to S.P. Mellington (DOE/YMSCO), April 11, 2000, LV.PA.RWA.04/00-039, with enclosure. ACC: MOL.20000412.0785.
- AP-2.13Q, Rev. 0, ICN 2. *Technical Product Development Planning*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000329.1182.
- AP-3.12Q, Rev. 0, ICN 3. *Calculations*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20001026.0084.
- AP-SI.1Q, Rev. 2, ICN 4, ECN 1. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20001019.0023.
- AP-SIIL.3Q, Rev. 0, ICN 3. *Submittal and Incorporation of Data to the Technical Data Management System*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000418.0808.
- AP-SV.1Q Rev. 0 ICN 0. *Control of the Electronic Management of Data*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000329.1181.
- Buscheck, T.A. 1999. *Thermohydrologic Calculations for the Site Recommendation/License Application Design Selection, Phase 2*. UCRL-ID-133988. BB0000000-01717-0210-00009 REV 00. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.20000606.0193.
- CRWMS M&O 1999. *Effective Thermal Conductivity for Drift-Scale Models Used in TSPA-SR*. TDP-EBS-HS-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990824.0143.
- CRWMS M&O 2000. *Tabulated In-Drift Geometric and Thermal Properties used in Drift-Scale Models for TSPA-SR*. CAL-EBS-HS-000002 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000718.0219.
- Incropera, F.P. and DeWitt, D.P. 1985. *Introduction to Heat Transfer*. New York, New York: John Wiley & Sons. TIC: 224038.
- Kuehn, T.H. and Goldstein, R.J. 1976. "Correlating Equations for Natural Convection Heat Transfer Between Horizontal Circular Cylinders." *International Journal of Heat and Mass Transfer*, 19, (10), 1127-1134. Oxford, Great Britain: Pergamon Press. TIC: 238411.

Kuehn, T.H. and Goldstein, R.J. 1978. "An Experimental Study of Natural Convection Heat Transfer in Concentric and Eccentric Horizontal Cylindrical Annuli." *Journal of Heat Transfer*, 100, 635-640. New York, New York: American Society of Mechanical Engineers. TIC: 244433.

LL990301904242.084. LADS Phase-II Calculation, EDAIIA. Submittal date: 06/04/1999.

LL990302204242.087. EDA II Ventilation Sensitivity Study. Submittal date: 11/14/2000. URN-0780

LL990302004242.085. LADS Calculations, EDA IIB. Submittal date: 06/04/1999.

MO9906SPATHRIP.000. LADS Thermal-Hydrology: Reformatted EDA5 Thermal Hydrology Results. Submittal date: 06/11/1999.

8. ATTACHMENTS

Table 3. List of Attachments

ATTACHMENT	TITLE	NUMBER OF PAGES
I	Preclosure and Postclosure Effective Thermal Conductivities (With Backfill)	9
II	Extended Preclosure Effective Thermal Conductivity	3
III	Preclosure and Postclosure Effective Thermal Conductivities (Without Backfill)	9
IV	Testing and Verification of Formulas in Excel Spreadsheets	32

ATTACHMENT I
Preclosure and Postclosure Effective Thermal Conductivities (With Backfill)

The effective thermal conductivity parameters for NUFT and TOUGH2 are given in DTN: SN9907T0872799.002.

```
;;Effective Thermal Conductivity inputs for drift-scale TH models using the NUFT code:
;; NDF-07/09/99
;;
;;
;; for 0 to 50 years of preclosure ventilation
;; the effective thermal conductivity includes radiation only since forced convection has
;; removed 50 % of the input energy
;; place near the top of the input deck after usnt
```

```
;;Preclosure
;;Max (W/m-K)=      10.443
;;time (yr)      Keff_prc (W/m-K)-- (rad)
```

```
(modprop
  (tcond (range "dr1 *"))
```

```
(factor
0.      0.400
1y      0.775
1.5y    0.825
2y      0.858
3y      0.899
4y      0.923
5y      0.941
6y      0.956
7y      0.966
8y      0.975
9y      0.982
10y     0.988
11y     0.993
12y     0.997
15y     1.000
20y     0.994
25y     0.979
26y     0.976
27y     0.972
```

30y	0.961
35y	0.941
40y	0.921
50y	0.887)))

;; Note: somewhere in rocktab an entry MUST be made for range "dr1" such that

(tcond tcondLin (solid 10.443) (liquid 10.443) (gas 10.443))

;;Postclosure:

;; for 51 to 900,000 years two effective thermal conductivities are used:

;; inner Kth is in-between the WP and the DS

;; outer Kth is in-between the backfill and the drift wall

;; the effective thermal conductivity includes both radiation and natural convection

;; place near the top of the input deck after usnt

;; inner Kth

(modprop

(tcond (range "dr2*"))

;;Max (W/m-K)= 3.426

;;Time (yr) Keff_inner-total (W/m-K)

(factor

50y	0.887
51y	0.872
52y	0.915
55y	0.984
60y	1.000
65y	0.990
70y	0.968
75y	0.941
76y	0.936
77y	0.931
80y	0.916
90y	0.874
100y	0.833

101y	0.829
105y	0.813
110y	0.796
120y	0.767
130y	0.746
140y	0.729
160y	0.703
180y	0.679
200y	0.659
220y	0.638
250y	0.617
300y	0.587
350y	0.563
400y	0.540
450y	0.519
500y	0.506
550y	0.497
600y	0.491
700y	0.476
800y	0.462
900y	0.450
1000y	0.439
1100y	0.431
1200y	0.423
1300y	0.414
1400y	0.406
1500y	0.398
1600y	0.392
1800y	0.382
2000y	0.370
2200y	0.363
2500y	0.353
3000y	0.342
3500y	0.334
4000y	0.327
4500y	0.321
5000y	0.317
6000y	0.308
7000y	0.302
8000y	0.296
10000y	0.286
15000y	0.267
20000y	0.255
30000y	0.237
40000y	0.228

50000y	0.222
60000y	0.218
80000y	0.212
100000y	0.209
120000y	0.207
150000y	0.205
200000y	0.202
300000y	0.201
400000y	0.199
500000y	0.198
600000y	0.198
700000y	0.197
800000y	0.197
900000y	0.197)))

:: Note: somewhere in rocktab an entry MUST be made for range "dr2" such that

(tcond tcondLin (solid 3.426) (liquid 3.426) (gas 3.426))

:: outer Kth

::Max (W/m-K)= 9.068
 ::Time (yr) Keff_inner-total (W/m-K)

(modprop
 (tcond (range "dr3*"))

(factor	
50y	0.887
51y	0.800
52y	0.849
55y	0.935
60y	0.983
65y	1.000
70y	0.999
75y	0.990
76y	0.987
77y	0.986

80y	0.980
90y	0.963
100y	0.940
101y	0.937
105y	0.924
110y	0.910
120y	0.890
130y	0.879
140y	0.873
160y	0.864
180y	0.847
200y	0.836
220y	0.816
250y	0.800
300y	0.775
350y	0.754
400y	0.731
450y	0.709
500y	0.698
550y	0.692
600y	0.688
700y	0.677
800y	0.664
900y	0.652
1000y	0.642
1100y	0.633
1200y	0.624
1300y	0.615
1400y	0.606
1500y	0.597
1600y	0.590
1800y	0.577
2000y	0.563
2200y	0.552
2500y	0.540
3000y	0.524
3500y	0.512
4000y	0.501
4500y	0.493
5000y	0.486
6000y	0.474
7000y	0.464
8000y	0.455
10000y	0.441
15000y	0.413

20000y	0.395
30000y	0.371
40000y	0.358
50000y	0.350
60000y	0.344
80000y	0.337
100000y	0.333
120000y	0.331
150000y	0.328
200000y	0.325
300000y	0.322
400000y	0.321
500000y	0.321
600000y	0.320
700000y	0.320
800000y	0.319
900000y	0.319)))

:: Note: somewhere in rocktab an entry MUST be made for range "dr3" such that

(tcond tcondLin (solid 9.068) (liquid 9.068) (gas 9.068))

TOUGH2 Input to be performed like the heat table function

Preclosure (0 to 50 yr):

kTH Max (W/m-K)=10.443

0.0E+00	3.153600E+07	4.730400E+07	6.307200E+07
9.460800E+07	1.261440E+08	1.576800E+08	1.892160E+08
2.207520E+08	2.522880E+08	2.838240E+08	3.153600E+08
3.468960E+08	3.784320E+08	4.730400E+08	6.307200E+08
7.884000E+08	8.199360E+08	8.514720E+08	9.460800E+08
1.103760E+09	1.261440E+09	1.576800E+09	
0.400	0.775	0.825	0.858
0.899	0.923	0.941	0.956
0.966	0.975	0.982	0.988
0.993	0.997	1.000	0.994
0.979	0.976	0.972	0.961
0.941	0.921	0.887	

Postclosure-inner (50+ to 900,000 yr):

Kth Max (W/m-K)=3.426

1.576800E+09	1.608336E+09	1.639872E+09	1.734480E+09
1.892160E+09	2.049840E+09	2.207520E+09	2.365200E+09
2.396736E+09	2.428272E+09	2.522880E+09	2.838240E+09
3.153600E+09	3.185136E+09	3.311280E+09	3.468960E+09
3.784320E+09	4.099680E+09	4.415040E+09	5.045760E+09
5.676480E+09	6.307200E+09	6.937920E+09	7.884000E+09
9.460800E+09	1.103760E+10	1.261440E+10	1.419120E+10
1.576800E+10	1.734480E+10	1.892160E+10	2.207520E+10
2.522880E+10	2.838240E+10	3.153600E+10	3.468960E+10
3.784320E+10	4.099680E+10	4.415040E+10	4.730400E+10
5.045760E+10	5.676480E+10	6.307200E+10	6.937920E+10
7.884000E+10	9.460800E+10	1.103760E+11	1.261440E+11
1.419120E+11	1.576800E+11	1.892160E+11	2.207520E+11
2.522880E+11	3.153600E+11	4.730400E+11	6.307200E+11
9.460800E+11	1.261440E+12	1.576800E+12	1.892160E+12
2.522880E+12	3.153600E+12	3.784320E+12	4.730400E+12
6.307200E+12	9.460800E+12	1.261440E+13	1.576800E+13

1.892160E+13	2.207520E+13	2.522880E+13	2.838240E+13
0.887	0.872	0.915	0.984
1.000	0.990	0.968	0.941
0.936	0.931	0.916	0.874
0.833	0.829	0.813	0.796
0.767	0.746	0.729	0.703
0.679	0.659	0.638	0.617
0.587	0.563	0.540	0.519
0.506	0.497	0.491	0.476
0.462	0.450	0.439	0.431
0.423	0.414	0.406	0.398
0.392	0.382	0.370	0.363
0.353	0.342	0.334	0.327
0.321	0.317	0.308	0.302
0.296	0.286	0.267	0.255
0.237	0.228	0.222	0.218
0.212	0.209	0.207	0.205
0.202	0.201	0.199	0.198
0.198	0.197	0.197	0.197

Postclosure-outer (50+ to 900,000 yr):
Kth Max (W/m-K)=9.068

1.576800E+09	1.608336E+09	1.639872E+09	1.734480E+09
1.892160E+09	2.049840E+09	2.207520E+09	2.365200E+09
2.396736E+09	2.428272E+09	2.522880E+09	2.838240E+09
3.153600E+09	3.185136E+09	3.311280E+09	3.468960E+09
3.784320E+09	4.099680E+09	4.415040E+09	5.045760E+09
5.676480E+09	6.307200E+09	6.937920E+09	7.884000E+09
9.460800E+09	1.103760E+10	1.261440E+10	1.419120E+10
1.576800E+10	1.734480E+10	1.892160E+10	2.207520E+10
2.522880E+10	2.838240E+10	3.153600E+10	3.468960E+10
3.784320E+10	4.099680E+10	4.415040E+10	4.730400E+10
5.045760E+10	5.676480E+10	6.307200E+10	6.937920E+10
7.884000E+10	9.460800E+10	1.103760E+11	1.261440E+11
1.419120E+11	1.576800E+11	1.892160E+11	2.207520E+11
2.522880E+11	3.153600E+11	4.730400E+11	6.307200E+11
9.460800E+11	1.261440E+12	1.576800E+12	1.892160E+12
2.522880E+12	3.153600E+12	3.784320E+12	4.730400E+12
6.307200E+12	9.460800E+12	1.261440E+13	1.576800E+13
1.892160E+13	2.207520E+13	2.522880E+13	2.838240E+13
0.887	0.800	0.849	0.935
0.983	1.000	0.999	0.990

0.987	0.986	0.980	0.963
0.940	0.937	0.924	0.910
0.890	0.879	0.873	0.864
0.847	0.836	0.816	0.800
0.775	0.754	0.731	0.709
0.698	0.692	0.688	0.677
0.664	0.652	0.642	0.633
0.624	0.615	0.606	0.597
0.590	0.577	0.563	0.552
0.540	0.524	0.512	0.501
0.493	0.486	0.474	0.464
0.455	0.441	0.413	0.395
0.371	0.358	0.350	0.344
0.337	0.333	0.331	0.328
0.325	0.322	0.321	0.321
0.320	0.320	0.319	0.319

ATTACHMENT II

Extended Preclosure Effective Thermal Conductivity

The effective thermal conductivity parameter for NUFT is given in DTN: SN9912T0872799.005.

;;"Nuft Input to be performed with the "modprop" function"
;;This assumes a longer preclosure period (1000 years). This is to be used in the multiscale
model only

;;Effective Thermal Conductivity inputs for drift-scale TH models using the NUFT code:
;; NDF-07/09/99
;;
;;
;; for 0 to 1000 years of preclosure ventilation
;; the effective thermal conductivity includes radiation only since forced convection has
;; removed 50 % of the input energy
;; place near the top of the input deck after usnt

;;This is an extended Preclosure period.

;;Max (W/m-K)= 10.47
;;Time (years) Keff_prc (W/m-K)-- (rad only)

(modprop
 (tcond (range "dr1*")

(factor

0.	0.399
1y	0.768
1.5y	0.820
2y	0.854
3y	0.895
4y	0.920
5y	0.938
6y	0.952
7y	0.963
8y	0.972

9y	0.980
10y	0.987
11y	0.992
12y	0.995
15y	1.000
20y	0.994
25y	0.981
26y	0.977
27y	0.974
30y	0.963
35y	0.943
40y	0.924
50y	0.889
51y	0.886
52y	0.883
55y	0.876
60y	0.865
65y	0.854
70y	0.842
75y	0.835
76y	0.834
77y	0.833
80y	0.826
90y	0.802
100y	0.784
101y	0.783
105y	0.779
110y	0.776
120y	0.768
130y	0.757
140y	0.743
160y	0.722
180y	0.711
200y	0.700
220y	0.693
250y	0.684
300y	0.673
350y	0.664
400y	0.656
450y	0.650
500y	0.645
550y	0.640
600y	0.635
700y	0.622
800y	0.609

900y 0.598
1000y 0.592)))

;; Note: somewhere in rocktab an entry MUST be made for range "dr1" such that

(tcond tcondLin (solid 10.47) (liquid 10.47) (gas 10.47))

ATTACHMENT III
Preclosure and Postclosure Effective Thermal Conductivities (Without Backfill)

The effective thermal conductivity parameters for NUFT and TOUGH2 are given in DTN: SN0002T0872799.009.

```
;;"Nuft Input to be performed with the ""modprop"" function"
;;Effective Thermal Conductivity inputs for drift-scale TH models using the NUFT code:
;; NDF-02/08/00
;;
;;
;; for 0 to 50 years of preclosure ventilation
;; the effective thermal conductivity includes radiation only since forced convection has
;; removed 50 % of the input energy
;; place near the top of the input deck after usnt
```

```
;;***No backfill case***
```

```
;;Preclosure:
```

```
;;Max (W/m-K)=      10.568
;;time (yr)      Keff_prc (W/m-K)-- (rad)
```

```
(modprop
  (tcond (range "dr1*")
```

```
(factor
```

0.	0.395
1y	0.777
1.5y	0.825
2y	0.856
3y	0.898
4y	0.921
5y	0.939
6y	0.955
7y	0.966
8y	0.975
9y	0.982
10y	0.988
11y	0.993
12y	0.997
15y	1.000

20y	0.993
25y	0.977
26y	0.974
27y	0.970
30y	0.958
35y	0.936
40y	0.915
50y	0.879)))

;; Note: somewhere in rocktab an entry MUST be made for range "dr1" such that

(tcond tcondLin (solid 10.568) (liquid 10.568) (gas 10.568))

;;Postclosure:

;; for 51 to 900,000 years two effective thermal conductivities are used:

;; inner Kth is in-between the WP and the DS

;; outer Kth is in-between the DS and the drift wall

;; the effective thermal conductivity includes both radiation and natural convection

;; place near the top of the input deck after usnt

;; ** No backfill Case **

;; inner Kth

(modprop

(tcond (range "dr2*"))

Postclosure-inner:

Max (W/m-K)= 2.298

Time (yr) Keff_inner-total (W/m-K)

51y	0.844
52y	0.892
55y	0.951
60y	0.988
65y	1.000
70y	0.995
75y	0.985

76y	0.983
77y	0.981
80y	0.973
90y	0.954
100y	0.932
101y	0.929
105y	0.918
110y	0.905
120y	0.882
130y	0.872
140y	0.864
160y	0.852
180y	0.839
200y	0.830
220y	0.818
250y	0.798
300y	0.763
350y	0.736
400y	0.707
450y	0.689
500y	0.677
550y	0.672
600y	0.667
700y	0.656
800y	0.646
900y	0.637
1000y	0.627
1100y	0.619
1200y	0.611
1300y	0.602
1400y	0.592
1500y	0.582
1600y	0.574
1800y	0.559
2000y	0.543
2200y	0.533
2500y	0.519
3000y	0.503
3500y	0.491
4000y	0.480
4500y	0.472
5000y	0.465
6000y	0.453
7000y	0.444
8000y	0.436

10000y	0.422
15000y	0.395
20000y	0.378
30000y	0.354
40000y	0.341
50000y	0.333
60000y	0.326
80000y	0.318
100000y	0.314
120000y	0.311
150000y	0.307
200000y	0.302
300000y	0.299
400000y	0.297
500000y	0.297
600000y	0.294
700000y	0.294
800000y	0.295
900000y	0.295)))

:: Note: somewhere in rocktab an entry MUST be made for range "dr2" such that

(tcond tcondLin (solid 2.298) (liquid 2.298) (gas 2.298))

::outer kth
 ::Postclosure-outer:

::Max (W/m-K)= 14.407
 ::Time (yr) Keff_outer-total (W/m-K)

(modprop
 (tcond (range "dr3*"))

(factor

51y	0.829
52y	0.878
55y	0.944
60y	0.986
65y	1.000

70y	0.998
75y	0.990
76y	0.988
77y	0.986
80y	0.980
90y	0.963
100y	0.943
101y	0.941
105y	0.929
110y	0.917
120y	0.896
130y	0.886
140y	0.879
160y	0.869
180y	0.857
200y	0.849
220y	0.838
250y	0.818
300y	0.784
350y	0.758
400y	0.729
450y	0.711
500y	0.700
550y	0.694
600y	0.690
700y	0.680
800y	0.670
900y	0.661
1000y	0.651
1100y	0.643
1200y	0.635
1300y	0.626
1400y	0.616
1500y	0.605
1600y	0.597
1800y	0.583
2000y	0.566
2200y	0.555
2500y	0.541
3000y	0.523
3500y	0.510
4000y	0.499
4500y	0.491
5000y	0.484
6000y	0.471

7000y	0.461
8000y	0.452
10000y	0.438
15000y	0.411
20000y	0.393
30000y	0.367
40000y	0.354
50000y	0.346
60000y	0.339
80000y	0.330
100000y	0.325
120000y	0.323
150000y	0.318
200000y	0.315
300000y	0.311
400000y	0.309
500000y	0.307
600000y	0.306
700000y	0.305
800000y	0.305
900000y	0.305)))

;; Note: somewhere in rocktab an entry MUST be made for range "dr3" such that

(tcond tcondLin (solid 14.407) (liquid 14.407) (gas 14.407))

TOUGH2 Input to be performed like the heat table function
 No backfill case
 Preclosure:
 Max (W/m-K)= 10.568

3.153600E+03 3.153600E+07 4.730400E+07 6.307200E+07
 9.460800E+07 1.261440E+08 1.576800E+08 1.892160E+08
 2.207520E+08 2.522880E+08 2.838240E+08 3.153600E+08
 3.468960E+08 3.784320E+08 4.730400E+08 6.307200E+08
 7.884000E+08 8.199360E+08 8.514720E+08 9.460800E+08
 1.103760E+09 1.261440E+09 1.576800E+09
 0.395 0.777 0.825 0.856
 0.898 0.921 0.939 0.955
 0.966 0.975 0.982 0.988
 0.993 0.997 1.000 0.993
 0.977 0.974 0.970 0.958
 0.936 0.915 0.879

Postclosure-inner:
 Max (W/m-K)= 2.298

1.608336E+09 1.639872E+09 1.734480E+09 1.892160E+09
 2.049840E+09 2.207520E+09 2.365200E+09 2.396736E+09
 2.428272E+09 2.522880E+09 2.838240E+09 3.153600E+09
 3.185136E+09 3.311280E+09 3.468960E+09 3.784320E+09
 4.099680E+09 4.415040E+09 5.045760E+09 5.676480E+09
 6.307200E+09 6.937920E+09 7.884000E+09 9.460800E+09
 1.103760E+10 1.261440E+10 1.419120E+10 1.576800E+10
 1.734480E+10 1.892160E+10 2.207520E+10 2.522880E+10
 2.838240E+10 3.153600E+10 3.468960E+10 3.784320E+10
 4.099680E+10 4.415040E+10 4.730400E+10 5.045760E+10
 5.676480E+10 6.307200E+10 6.937920E+10 7.884000E+10
 9.460800E+10 1.103760E+11 1.261440E+11 1.419120E+11
 1.576800E+11 1.892160E+11 2.207520E+11 2.522880E+11
 3.153600E+11 4.730400E+11 6.307200E+11 9.460800E+11
 1.261440E+12 1.576800E+12 1.892160E+12 2.522880E+12
 3.153600E+12 3.784320E+12 4.730400E+12 6.307200E+12
 9.460800E+12 1.261440E+13 1.576800E+13 1.892160E+13
 2.207520E+13 2.522880E+13 2.838240E+13
 0.844 0.892 0.951 0.988

1.000	0.995	0.985	0.983
0.981	0.973	0.954	0.932
0.929	0.918	0.905	0.882
0.872	0.864	0.852	0.839
0.830	0.818	0.798	0.763
0.736	0.707	0.689	0.677
0.672	0.667	0.656	0.646
0.637	0.627	0.619	0.611
0.602	0.592	0.582	0.574
0.559	0.543	0.533	0.519
0.503	0.491	0.480	0.472
0.465	0.453	0.444	0.436
0.422	0.395	0.378	0.354
0.341	0.333	0.326	0.318
0.314	0.311	0.307	0.302
0.299	0.297	0.297	0.294
0.294	0.295	0.295	

Postclosure-outer:

Max (W/m-K)= 14.407

1.608336E+09 1.639872E+09 1.734480E+09 1.892160E+09
2.049840E+09 2.207520E+09 2.365200E+09 2.396736E+09
2.428272E+09 2.522880E+09 2.838240E+09 3.153600E+09
3.185136E+09 3.311280E+09 3.468960E+09 3.784320E+09
4.099680E+09 4.415040E+09 5.045760E+09 5.676480E+09
6.307200E+09 6.937920E+09 7.884000E+09 9.460800E+09
1.103760E+10 1.261440E+10 1.419120E+10 1.576800E+10
1.734480E+10 1.892160E+10 2.207520E+10 2.522880E+10
2.838240E+10 3.153600E+10 3.468960E+10 3.784320E+10
4.099680E+10 4.415040E+10 4.730400E+10 5.045760E+10
5.676480E+10 6.307200E+10 6.937920E+10 7.884000E+10
9.460800E+10 1.103760E+11 1.261440E+11 1.419120E+11
1.576800E+11 1.892160E+11 2.207520E+11 2.522880E+11
3.153600E+11 4.730400E+11 6.307200E+11 9.460800E+11
1.261440E+12 1.576800E+12 1.892160E+12 2.522880E+12
3.153600E+12 3.784320E+12 4.730400E+12 6.307200E+12
9.460800E+12 1.261440E+13 1.576800E+13 1.892160E+13
2.207520E+13 2.522880E+13 2.838240E+13

0.829	0.878	0.944	0.986
1.000	0.998	0.990	0.988
0.986	0.980	0.963	0.943
0.941	0.929	0.917	0.896
0.886	0.879	0.869	0.857

0.849	0.838	0.818	0.784
0.758	0.729	0.711	0.700
0.694	0.690	0.680	0.670
0.661	0.651	0.643	0.635
0.626	0.616	0.605	0.597
0.583	0.566	0.555	0.541
0.523	0.510	0.499	0.491
0.484	0.471	0.461	0.452
0.438	0.411	0.393	0.367
0.354	0.346	0.339	0.330
0.325	0.323	0.318	0.315
0.311	0.309	0.307	0.306
0.305	0.305	0.305	

ATTACHMENT IV

Testing and Verification of Formulas in Excel Spreadsheets

This attachment provides the details of testing and verification of the spreadsheet formulas used in this calculation according to AP-SI.1Q, Rev. 2, ICN 4, *Software Management*, Section 5.1.1. The macros/equations are implemented in the Excel 97 spreadsheets: kth(rad-convht).xls, kth(rad-convht)wprec.xls, and kth(rad-convht)nobf.xls. All spreadsheets are version 1.0. The spreadsheets implement equations (3) through (6) and (16) for thermal radiation and (7) through (15) for natural convection. The results of the calculation are shown in Section 6. The operating system used in this implementation is a Windows NT system.

kth(rad-convht).xls (version 1.0)

Consider application of equation (3) in spreadsheet kth(rad-convht).xls, specifically in the worksheet named: effective-kth=radiation. Selecting the 10 year data point for the preclosure effective thermal conductivity, equation (3) gives a thermal radiation equivalence:

$$k_{eff} = \frac{(5.67 \times 10^{-8})(0.815)[(403.35)^2 + (384.63)^2][403.35 + 384.63] \ln\left(\frac{2.55}{0.815}\right)}{\frac{1}{0.8} + \frac{1-1}{1}\left(\frac{0.815}{2.55}\right)} = 10.32 \frac{W}{m-K}$$

An excerpt from the worksheet is shown below with the sample calculation check shown in bold:

A	B	C	D	E	F	G	H	I	J
Time(years)	Waste Package Temperature (°C)	Waste Package RH	Liq. Sat.	Drift Wall Temperature (°C)					Keff_prc (W/m-K)
7	128.02868	0.44462	0	108.021	0	0			10.09
8	128.94256	0.4397	0	109.4716	0	0			10.18
9	129.71605	0.43542	0	110.657	0	0			10.26
10	130.35469	0.43148	0	111.6323	0	0			10.32
11	130.82026	0.42753	0	112.432	0	0			10.37
12	131.12501	0.42339	0	113.0606	0	0			10.41

Equation (3) has been implemented correctly in the worksheet based on this sample calculation. The postclosure inner effective thermal conductivity parameter, found in worksheet effective-kth=radiation, is computed at the 100 year data point using equation (6) for a thermal radiation equivalence:

$$k_{eff} = \frac{(5.67 \times 10^{-8})(0.815)[(472.07)^2 + (469.17)^2][472.07 + 469.17] \ln\left(\frac{1.0}{0.815}\right)}{\frac{1}{0.8} + \frac{1-0.8}{0.8}\left(\frac{0.815}{1.0}\right)} = 2.71 \frac{W}{m-K}$$

An excerpt from the worksheet is shown below with the sample calculation check shown in bold:

A	B	C	D	E	F	G	H	I	J	K
Time (years)	Waste Package Temperature (°C)	Waste Package RH	Liq. Sat.	Drift Wall Temperature e (°C)	Drip Shield Temperature (°C)	Drip Shield RH				Keff_i_poc
80	215.06618	0.03321	0	145.6744	211.9896	0.03529				3.00
90	207.17575	0.04013	0	143.349	204.1912	0.04265				2.85
100	199.06811	0.04821	0	139.9758	196.169	0.05127				2.71
101	198.28498	0.04917	0	139.4838	195.3898	0.05229				2.70
105	195.11989	0.05315	0	137.4564	192.2517	0.05655				2.64
110	191.56351	0.05804	0	135.3187	188.7287	0.06177				2.58

Equation (6) has been implemented in the worksheet correctly based on this sample calculation. The postclosure outer effective thermal conductivity parameter (with backfill), found in worksheet effective-kth=radiation (in spreadsheet kth(rad-convht).xls), is computed at the 100 year data point using equations (4) and (5):

First, provide an initial guess for the backfill temperature as: $T_b = \frac{139.9758 + 196.169}{2} = 168.0724^\circ\text{C}$.

Substitute the initial guess for the backfill temperature into equation (4) to compute the effective thermal conductivity:

$$k_{effo} = \frac{(5.67 \times 10^{-8})(1.9)[(441.0724)^2 + (412.9758)^2][441.0724 + 412.9758] \ln\left(\frac{2.55}{1.9}\right)}{\frac{1}{0.9} + \frac{1-1}{1}\left(\frac{1.9}{2.55}\right)} = 8.8954 \frac{W}{m-K}$$

Since the backfill surface temperature is unknown and the initial guess given above is most likely incorrect, iteration is required to determine an abstracted backfill temperature (T_b). The effective thermal conductivity computed above is substituted back into equation (5) to obtain a new backfill temperature and the process continues until the backfill temperature converges to an unchanging value. The new backfill temperature is:

$$T_b = \frac{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)}(196.169) + \frac{8.8954}{\ln\left(\frac{2.55}{1.9}\right)}(139.9758)}{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)} + \frac{8.8954}{\ln\left(\frac{2.55}{1.9}\right)}} = 141.8513^\circ\text{C}$$

It is evident that the initial guess is incorrect. However, the energy balance equation should rapidly converge on the temperature that satisfies conservation of energy. Substituting this temperature result back into equation (4) gives:

$$k_{effo} = \frac{(5.67 \times 10^{-8})(1.9)[(414.8513)^2 + (412.9758)^2][414.8513 + 412.9758]\ln\left(\frac{2.55}{1.9}\right)}{\frac{1}{0.9} + \frac{1-1}{1}\left(\frac{1.9}{2.55}\right)} = 8.0923 \frac{W}{m-K}$$

The process continues as this result is substituted back into equation (5) to obtain a new backfill temperature. The new backfill temperature is:

$$T_b = \frac{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)}(196.169) + \frac{8.0923}{\ln\left(\frac{2.55}{1.9}\right)}(139.9758)}{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)} + \frac{8.0923}{\ln\left(\frac{2.55}{1.9}\right)}} = 142.0306^\circ\text{C}$$

Although this value has not changed much from the previous calculation of T_b , the process continues.

$$k_{effo} = \frac{(5.67 \times 10^{-8})(1.9)[(415.0306)^2 + (412.9758)^2][415.0306 + 412.9758]\ln\left(\frac{2.55}{1.9}\right)}{\frac{1}{0.9} + \frac{1-1}{1}\left(\frac{1.9}{2.55}\right)} = 8.0976 \frac{W}{m-K}$$

The process continues as this result is substituted back into equation (5) to obtain a new backfill temperature. The new backfill temperature is:

$$T_b = \frac{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)}(196.169) + \frac{8.0976}{\ln\left(\frac{2.55}{1.9}\right)}(139.9758)}{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)} + \frac{8.0976}{\ln\left(\frac{2.55}{1.9}\right)}} = 142.0293^\circ\text{C}$$

This value of T_b and the previous value are very close. One final iteration should be sufficient.

$$k_{effo} = \frac{(5.67 \times 10^{-8})(1.9)[(415.0293)^2 + (412.9758)^2][415.0293 + 412.9758]\ln\left(\frac{2.55}{1.9}\right)}{\frac{1}{0.9} + \frac{1-1}{1}\left(\frac{1.9}{2.55}\right)} = 8.0975 \frac{W}{m-K}$$

The backfill temperature is:

$$T_b = \frac{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)}(196.169) + \frac{8.0975}{\ln\left(\frac{2.55}{1.9}\right)}(139.9758)}{\frac{0.67}{\ln\left(\frac{1.9}{1}\right)} + \frac{8.0975}{\ln\left(\frac{2.55}{1.9}\right)}} = 142.0293^\circ\text{C}$$

The temperature has converged with the resulting postclosure outer effective thermal conductivity equal to 8.0975 W/m-K. This hand check is compared to an excerpt from the worksheet as the following:

A	B	...	E	F	...
80	215.06618	...	145.6744	211.9896	...
90	207.17575	...	143.349	204.1912	...
100	199.06811	...	139.9758	196.169	...
101	198.28498	...	139.4838	195.3898	...
105	195.11989	...	137.4564	192.2517	...

...	L	M	N	O	P	Q	R	S
...	9.4231	147.7677	8.4377	148.0035	8.4448	148.0016	8.4448	148.0017
...	9.1834	145.3181	8.2945	145.5215	8.3006	145.52	8.3006	145.52
...	8.8954	141.8513	8.0923	142.0306	8.0976	142.0294	8.0975	142.0294
...	8.8602	141.3569	8.0634	141.5352	8.0686	141.5339	8.0686	141.5339
...	8.7170	139.3214	7.9451	139.4958	7.9502	139.4946	7.9501	139.4946

Equations (4) and (5) have been correctly implemented in the worksheet based on this sample calculation. The thermal radiation component has been verified to be correctly implemented in the

Excel 97 spreadsheet (e.g., kth(rad-convht).xls) for the pre and postclosure backfill case. Now consider the natural convection heat transfer component.

The following sample calculations are used to verify that the natural convection heat transfer equations (7) through (15) have been implemented correctly in the Excel 97 spreadsheets. The method of solution is iterative since the bulk temperature, used to evaluate both the fluid properties and the Rayleigh numbers, is initially unknown. The inner (between waste package and drip shield) and outer (between backfill and drift wall) effective thermal conductivity parameters for the backfill case are given in spreadsheet kth(rad-convht).xls, specifically in worksheet: effective-kth=convection. Consider a sample hand check for the inner effective parameter at the 51 year data point in this worksheet.

Equations (7) and (8) are computed for air as the surrounding fluid. Using as an initial guess for the bulk temperature, $\bar{T}_B$, the average temperature between the waste package and drip shield of 204.3254°C (477.3254K), the fluid properties and the Rayleigh numbers can be evaluated. The thermal diffusivity and kinematic viscosity are interpolated at the bulk temperature. From Incropera and DeWitt, Table A.4, for a total overall temperature range of 250K to 550K (given in increments of 50K; therefore, this specific example happens to be interpolated between 450 and 500K), the diffusivity and viscosity are linearly interpolated from Table A.4 (using the guessed bulk temperature) as:

- $\nu = 3.5888 \times 10^{-5} \text{ m}^2/\text{s}$
- $\alpha = 5.2392 \times 10^{-5} \text{ m}^2/\text{s}$

Equations (7) and (8) become:

$$Ra_{Di} = \frac{9.81 \left(\frac{1}{477.3254} \right) (206.4674 - 204.3254) (2 \times 0.815)^3}{(3.5888 \times 10^{-5}) (5.2392 \times 10^{-5})} = 1.014 \times 10^8$$

$$Ra_{Do} = \frac{9.81 \left(\frac{1}{477.3254} \right) (204.3254 - 202.1834) (2 \times 1.0)^3}{(3.5888 \times 10^{-5}) (5.2392 \times 10^{-5})} = 1.8731 \times 10^8$$

The inner (waste package) and outer (drip shield) cylinder Nusselt numbers are computed using equations (10) and (11) as the following:

$$Nu_i = \frac{2}{\ln \left[1 + \frac{2}{\left[\left(0.5(1.014 \times 10^8)^{1/4} \right)^{15} + \left(0.12(1.014 \times 10^8)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 57.6194$$

$$Nu_o = \frac{-2}{\ln \left[1 - \frac{2}{\left[\left((1.8731 \times 10^8)^{1/4} \right)^{15} + \left(0.12(1.8731 \times 10^8)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 115.9874$$

These values are now used to compute a new guess for the bulk fluid temperature. The calculational process described above continues until the bulk fluid temperature converges to its unchanging value. The (new) bulk temperature is computed from equation (9) as the following:

$$\bar{T}_B = (206.4674 - 202.1834) \frac{57.6194}{57.6194 + 115.9874} + 202.1834 = 203.6053^\circ\text{C}$$

The new bulk temperature is now used to redefine the fluid properties in equations (7) and (8) and the process continues until temperature convergence. Five more iterations show that the bulk fluid temperature does not significantly change from the fourth to the fifth iteration. Therefore, the calculated information at the fourth iteration step is selected. Once the bulk temperature is fixed, equations (12) through (15) are evaluated to obtain the effective thermal conductivity used to represent natural convection heat transfer in the emplacement drift.

Using the last complete iteration step (corresponding to the fourth full iteration) for the inner and outer cylinder Nusselt numbers, equation (15) is:

$$Nu_{conv} = \left[\frac{1}{62.1676} + \frac{1}{107.4591} \right]^{-1} = 39.3834$$

$$Nu_{cond} = \frac{2}{\ln \frac{1}{0.815}} = 9.7767$$

$$Nu = \left[(39.3834)^{15} + (9.7767)^{15} \right]^{1/15} = 39.3834$$

The effective thermal conductivity is computed by linearly interpolating for the fluid thermal

conductivity at the final bulk fluid temperature (Incropera and DeWitt, Table A.4):

- $k_{sf} = 0.0391 \text{ W/m-K}$

$$k_{effconv} = \frac{39.3834}{9.7767} \times 0.0391 = 0.1576 \text{ W/m-K}$$

The worksheet implementation of the hand check calculation above is given in the excerpt from the worksheet as shown below.

A	B	...	E	F	...	H			
51	206.46742	...	114.199	202.1834	...	118.0426264			
52	214.72256	...	123.064	210.5884	...	126.6512633			
55	227.41558	...	137.5837	223.7383	...	140.7725912			
60	230.25741	...	145.4693	226.8273	...	148.3233297			

I	J	K	L	M	N	O	P	Q
Tavgb	nu	alpha	Radi	Rado		Nui		Nuo
204.3254	3.5888E-05	5.2392E-05	1.0140E+08	1.8731E+08	56.62486	57.61907	116.99	115.9871
212.6555	3.6954E-05	5.3975E-05	9.0658E+07	1.6747E+08	54.63869	55.6327	113.7607	112.7577
225.577	3.8608E-05	5.6430E-05	7.1913E+07	1.3284E+08	50.78012	51.77369	107.3595	106.3563
228.5424	3.8999E-05	5.7008E-05	6.5344E+07	1.2071E+08	49.27902	50.27239	104.8188	103.8156

R	...	BC	BD	BE	BF	BG
Tavgbnw		Nuconv	Nucond	Nu	Kair	keq
203.60526	...	39.38339	9.77674	39.38339	3.91E-02	0.1576
211.95427	...	38.11131	9.77674	38.11131	3.97E-02	0.1547
224.94231	...	35.61849	9.77674	35.61849	4.06E-02	0.1478
227.94641	...	34.64217	9.77674	34.64217	4.08E-02	0.1445

The natural convection heat transfer equations have been correctly implemented for the inner effective thermal conductivity.

Similar sample check calculations have been performed for the outer effective thermal conductivity parameter used to approximate natural convection heat transfer. In the case, the inner cylinder is the backfill top surface, the outer cylinder is the drift wall. The hand check proceeds as before. Consider the 51 year data point in the same worksheet.

Equations (7) and (8) are computed for air as the surrounding fluid. Using as an initial guess for the bulk temperature, $\bar{T}_B$, the average temperature between the top of backfill and drift wall of 116.1208°C (389.1208 K), the fluid properties and the Rayleigh numbers can be evaluated. The thermal diffusivity and kinematic viscosity are interpolated at the bulk temperature. From Incropera and DeWitt, Table A.4, for a total temperature range of 250K to 550K (given in increments of 50K; therefore, this specific example happens to be interpolated between 350 and 400K), the diffusivity

and viscosity are linearly interpolated from Table A.4 (using the guessed bulk temperature) as:

- $\nu = 2.5215 \times 10^{-5} \text{ m}^2/\text{s}$
- $\alpha = 3.6472 \times 10^{-5} \text{ m}^2/\text{s}$

Equations (7) and (8) become:

$$Ra_{Di} = \frac{9.81 \left(\frac{1}{389.1208} \right) (118.0426 - 116.1208) (3.8)^3}{(2.5215 \times 10^{-5}) (3.6472 \times 10^{-5})} = 2.89089 \times 10^9$$

$$Ra_{Do} = \frac{9.81 \left(\frac{1}{389.1208} \right) (116.1208 - 114.199) (5.1)^3}{(2.5215 \times 10^{-5}) (3.6472 \times 10^{-5})} = 6.9885 \times 10^9$$

The inner (backfill top) and outer (drift wall) cylinder Nusselt numbers are computed using equations (10) and (11) as the following:

$$Nu_i = \frac{2}{\ln \left[1 + \frac{2}{\left[\left(0.5 (2.89089 \times 10^9)^{1/4} \right)^{15} + \left(0.12 (2.89089 \times 10^9)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 171.9775$$

$$Nu_o = \frac{-2}{\ln \left[1 - \frac{2}{\left[\left((6.9885 \times 10^9)^{1/4} \right)^{15} + \left(0.12 (6.9885 \times 10^9)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 288.722$$

These values are now used to compute a new guess for the bulk fluid temperature. The calculational process described above continues until the bulk fluid temperature converges to its unchanging value. The (new) bulk fluid temperature is computed from equation (9) as the following:

$$\bar{T}_B = (118.0426 - 114.199) \frac{171.9775}{171.9775 + 288.722} + 114.199 = 115.6338^\circ\text{C}$$

As before, the new bulk temperature is now used to redefine the fluid properties in equations (7) and

(8) and the process continues until bulk fluid temperature convergence. Five more iterations show that the bulk fluid temperature does not significantly change from the fourth to the fifth iteration. Therefore, the calculated information at the fourth iteration step is selected. Once the bulk temperature is fixed, equations (12) through (15) are evaluated to obtain the effective thermal conductivity used to represent natural convection heat transfer in the emplacement drift.

Using the last complete iteration step (corresponding to the fourth full iteration) for the inner and outer cylinder Nusselt numbers, equation (15) is:

$$Nu_{conv} = \left[\frac{1}{182.7947} + \frac{1}{273.4268} \right]^{-1} = 109.5542$$

$$Nu_{cond} = \frac{2}{\ln \frac{2.55}{1.9}} = 6.7972$$

$$Nu = \left[(109.5542)^{15} + (6.7972)^{15} \right]^{1/15} = 109.5542$$

The effective thermal conductivity is computed by linearly interpolating for the fluid thermal conductivity at the final bulk fluid temperature (Incropera and DeWitt, Table A.4):

- $k_{sf} = 0.0329 \text{ W/m-K}$

$$k_{effconv} = \frac{109.5542}{6.7972} \times 0.0329 = 0.5303 \text{ W/m-K}$$

The worksheet implementation of the hand check calculation above for the outer thermal conductivity parameter for natural convection is given in the excerpt from the worksheet as shown below.

A	B	...	E	F	...	H	...
51	206.46742	...	114.199	202.1834	...	118.0426264	...
52	214.72256	...	123.064	210.5884	...	126.6512633	...
55	227.41558	...	137.5837	223.7383	...	140.7725912	...
60	230.25741	...	145.4693	226.8273	...	148.3233297	...

BH	BI	BJ	BK	BL	BM	BN
Tavgb	nu	alpha	Radi	Rado		Nui
116.1208	2.5215E-05	3.6472E-05	2.8908E+09	6.9884E+09	170.9776	171.9757
124.8576	2.6175E-05	3.7940E-05	2.4437E+09	5.9075E+09	161.6718	162.6698
139.1782	2.7867E-05	4.0468E-05	1.8465E+09	4.4639E+09	147.27	148.2677
146.8963	2.8790E-05	4.1842E-05	1.5187E+09	3.6713E+09	137.994	138.9916

BO	BP	BQ	...
	Nuo	Tavgbnw	
289.7223	288.7211	115.6338	...
277.6976	276.6964	124.3921	...
258.7842	257.7829	138.7481	...
246.3805	245.3792	146.5013	...

...	DB	DC	DD	DE	DF
	Nuconv	Nucond	Nu	Kair	keq
...	109.5542	6.7972E+00	109.5542	3.2944E-02	0.5310
...	104.1808	6.7972E+00	104.1808	3.3610E-02	0.5151
...	95.80743	6.7972E+00	95.80743	3.4629E-02	0.4881
...	90.36317	6.7972E+00	90.36317	3.5171E-02	0.4676

The difference in the hand calculation result (0.5303) compared to the spreadsheet calculated result (0.5310) is a negligible error associated with round-off. The hand calculation uses only four digits (refer to the hand calculations shown above) during computations while the spreadsheet formulation uses more than four when computing each value. The natural convection heat transfer equations have been correctly implemented for the outer effective thermal conductivity. This concludes the testing and verification of the Excel 97 spreadsheet called kth(rad-convht).xls.

Range of Validity for kth(rad-convht).xls

The range of validity for this spreadsheet routine kth(rad-convht).xls is fixed for an overall temperature range of 250K to 550K for any single component (e.g., waste package, drip shield, etc.) temperature. Component temperatures outside of the given temperature range will result in fluid properties (kinematic and thermal diffusivity and thermal conductivity) not interpolated correctly by the spreadsheet.

convfile_gen.f (version 1.0) and convfile_genprec.f (version 1.0)

The software routine file names convfile_gen.f (version 1.0) and convfile_genprec.f (version 1.0) are used to take the source data (see Table 1) and compute the average result which provides the basis for the development of the effective thermal conductivity. The results of the averaging step are given in columns A-G (A-E only in the extended preclosure case, kth(rad-convht)wprec.xls) in the spreadsheets: kth(rad-convht).xls, kth(rad-convht)wprec.xls, and kth(rad-convht)nobf.xls. The worksheets (within the spreadsheets) containing the averaged data (e.g., the output from the software

routines) are the following:

- kth(rad-convht).xls
 - effective-kth=radiation
 - effective-kth=convection
 - EDA-II-noBF-rad
 - EDA-II-noBF-conv
- kth(rad-convht)wprec.xls
 - preclose
- kth(rad-convht)nobf.xls
 - EDA-II-noBF-rad
 - EDA-II-noBF-conv

A SUN workstation compiler and computer operating system (e.g., SUN OS 5.7 FORTRAN 77) was used in the implementation of both software routines. The software routines convfile_gen.f and convfile_genprec.f are nearly the same. The file convfile_genprec.f reads fewer data points (57 instead of 94, refer to the line "parameter (npts=57)" or "parameter (npts=94)" statement in the source code) from the source files and it does not need to read/compute average values for the drip shield (since it does not exist in the extended preclosure ventilation case).

The source routine for **convfile_genprec.f** is hand checked at a single time point to ensure its correct implementation. Excerpts of the source data files are shown below, with an excerpt of the result of the averaging routine taken directly from the spreadsheet kth(rad-convht)wprec.xls data.

An overall description of this software routine is the following.

- 1) Read input information indicated in Table 1 for the extended preclosure case.
- 2) Compute a weighted average based on the fraction represented by each data set.
- 3) Perform this operation at each time point for specified variables (e.g., waste package temperature) for every input file.
- 4) Write the output to be read into the excel spreadsheets used to generate the parameters described in this calculation.

Use of this routine requires minor runtime intervention by the user and an additional driver file in which the filenames of the input data reside. This is illustrated as the following. The driver input file contains the following input file and required header information:

```
CC_csnf
CC_snf_mean_02_sandBF_60_c_j4_22_03_02_001_preClose_data
CC_snf_mean_12_sandBF_60_c_j4_22_03_02_001_preClose_data
CC_snf_mean_22_sandBF_60_c_j4_22_03_02_001_preClose_data
CC_snf_mean_32_sandBF_60_c_j4_22_03_02_001_preClose_data
CC_snf_mean_42_sandBF_60_c_j4_22_03_02_001_preClose_data
```

CC_snf_mean_52_sandBF_60_c_j4_22_03_02_001_preClose_data
CC_snf_mean_62_sandBF_60_c_j4_22_03_02_001_preClose_data

The header label "CC_csnf" MUST be at the top of the file and should be seven characters or less. The name of each input file must reside in this driver file. The names of the input files (e.g., CC_snf_mean_*) should not exceed 70 characters. The name of the driver file can be anything as long as it does not exceed 70 characters. The driver file and the input files must reside in the directory in which the routine is being executed. The runtime response for this software routine is the following.

'How many bins are there?'
'What is the name of the output file?'
'What is the name of the input file?'

The answer to the first question is seven since there are a total of seven input files to be processed (shown above) by the routine. The answer to the second question can be anything as long as it does not exceed 70 characters. The name of the driver input file (the third question) is describe above and should be limited to 70 characters or less. In summary, execution of this routine requires the seven input files (from Table 1) plus the input driver file.

A test of the routine is given as the following. Excerpts of the actual input files are given below. Only excerpts are shown due to the size of the input files.

MSTHM version MSTHM_rev_6.0
creation date Wed Sep 15 11:28:04 1999
EXTfile creation date: Thu Mar 4 09:56:38 1999
file: CC_snf_mean_02_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 0; (0..9)
t(RH = 0.85) > 200.00
t(RH = 0.85) <= 230.00

temperature bin 2; (0..2)
T(5000y) > 79.00
T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)
average WP location: h@m.i.r#8:11:1
average WP type: snfl

LADS phase-II multi-scale TH calculation for EDA IIA preclosure
TSPA-VA base-case mean alpha_f Ix1 property set
line load
sand invert using VA sand properties
VA heat-generation curves with no additional waste aging
ventilation for 50 yr at 50 percent heat-removal efficiency
AML = 60 MTU/acre
Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m^2)

fraction of zone CC represented by data set = 0.127595
area of repository represented by data set = 100627.50 (m^2)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
							RH_dripShield
0.0	17.856014	1.000000	0.985779	0.000000	17.856014		
0.998505	N/A	N/A					
1.0	103.171173	0.382648	0.499222	0.000000	77.857162		
0.998903	N/A	N/A					
1.5	110.599358	0.416657	0.271140	0.000000	86.362106		
0.998827	N/A	N/A					
2.0	115.144272	0.440716	0.124069	0.000000	91.764679		
0.998446	N/A	N/A					
3.0	121.608360	0.453112	0.032189	0.000000	98.257423		
0.994178	N/A	N/A					
4.0	124.609680	0.458373	0.012061	0.000000	101.902779		
0.969396	N/A	N/A					
5.0	126.705994	0.447100	0.005649	0.000000	104.646240		
0.916197	N/A	N/A					
6.0	128.731018	0.429862	0.004781	0.000000	107.282684		
0.855392	N/A	N/A					
7.0	129.592987	0.426188	0.004526	0.000000	108.928490		
0.823252	N/A	N/A					
8.0	130.487366	0.422335	0.004411	0.000000	110.301117		
0.799763	N/A	N/A					
9.0	131.254684	0.418580	0.004392	0.000000	111.499939		
0.779089	N/A	N/A					
10.0	131.941650	0.414302	0.004545	0.000000	112.548050		
0.760251	N/A	N/A					
11.0	132.433731	0.409418	0.004851	0.000000	113.403030		
0.741046	N/A	N/A					

MSTHM version MSTHM_rev_6.0
creation date Wed Sep 15 11:28:04 1999
EXTfile creation date: Thu Mar 4 09:56:38 1999
file: CC_snf_mean_12_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 1; (0..9)
t(RH = 0.85) > 230.00
t(RH = 0.85) <= 260.00

temperature bin 2; (0..2)
T(5000y) > 79.00
T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)
average WP location: h@m.i.r#7:11:1
average WP type: snf5

LADS phase-II multi-scale TH calculation for EDA IIA preclosure
TSPA-VA base-case mean alpha_f Ix1 property set
line load
sand invert using VA sand properties
VA heat-generation curves with no additional waste aging
ventilation for 50 yr at 50 percent heat-removal efficiency
AML = 60 MTU/acre
Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m²)

fraction of zone CC represented by data set = 0.288542

area of repository represented by data set = 227558.36 (m²)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
		RH_dripShield					
0.0	18.025698		1.000000	0.985640	0.000000		18.025698
0.998040		N/A	N/A				
1.0	98.390724		0.435608	0.497847	0.000000		76.912987
0.998443		N/A	N/A				
1.5	105.957527		0.467282	0.298519	0.000000		85.283508
0.998397		N/A	N/A				
2.0	110.600700		0.487664	0.160690	0.000000		90.482376
0.998214		N/A	N/A				
3.0	116.518723		0.498770	0.057727	0.000000		96.358566
0.996937		N/A	N/A				
4.0	119.789017		0.508409	0.022876	0.000000		99.968811
0.990535		N/A	N/A				
5.0	121.897888		0.507501	0.010280	0.000000		102.507545
0.965992		N/A	N/A				
6.0	123.386620		0.498015	0.005801	0.000000		104.202560
0.935616		N/A	N/A				
7.0	124.478981		0.489852	0.004651	0.000000		105.986229
0.894996		N/A	N/A				
8.0	125.547707		0.480863	0.004331	0.000000		107.630211
0.858312		N/A	N/A				
9.0	126.469978		0.472298	0.004148	0.000000		108.901680
0.830781		N/A	N/A				
10.0	127.198334		0.466165	0.004107	0.000000		109.940079
0.809110		N/A	N/A				
11.0	127.719971		0.460993	0.004087	0.000000		110.740723
0.791738		N/A	N/A				

MSTHM version MSTHM_rev_6.0

creation date Wed Sep 15 11:28:04 1999

EXTfile creation date: Thu Mar 4 09:56:38 1999

file: CC_snf_mean_22_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 2; (0..9)

t(RH = 0.85) > 260.00

t(RH = 0.85) <= 290.00

temperature bin 2; (0..2)

T(5000y) > 79.00

T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)

average WP location: h@m.i.r#9:14:1

average WP type: snf3

LADS phase-II multi-scale TH calculation for EDA IIA preclosure

TSPA-VA base-case mean alpha_f Ix1 property set

line load

sand invert using VA sand properties

VA heat-generation curves with no additional waste aging

ventilation for 50 yr at 50 percent heat-removal efficiency
 AML = 60 MTU/acre
 Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m²)

fraction of zone CC represented by data set = 0.268980

area of repository represented by data set = 212131.05 (m²)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
							RH_dripShield
0.0	19.095760		1.000000	0.984587	0.000000		19.095760
	0.998874	N/A	N/A				
1.0	104.337517		0.386807	0.468709	0.000000		79.127792
	0.999245	N/A	N/A				
1.5	111.179878		0.419165	0.243751	0.000000		87.017662
	0.999181	N/A	N/A				
2.0	115.444756		0.441646	0.106166	0.000000		92.077103
	0.998773	N/A	N/A				
3.0	121.321236		0.454214	0.029753	0.000000		98.085640
	0.993634	N/A	N/A				
4.0	124.308907		0.459461	0.012927	0.000000		101.664604
	0.971000	N/A	N/A				
5.0	126.554947		0.450702	0.006412	0.000000		104.520737
	0.923346	N/A	N/A				
6.0	128.586578		0.433172	0.005203	0.000000		106.841026
	0.871439	N/A	N/A				
7.0	129.613861		0.430597	0.005016	0.000000		108.856461
	0.834274	N/A	N/A				
8.0	130.541275		0.428205	0.005025	0.000000		110.308884
	0.811959	N/A	N/A				
9.0	131.332336		0.426433	0.005140	0.000000		111.518349
	0.795076	N/A	N/A				
10.0	131.983276		0.424465	0.005363	0.000000		112.522583
	0.780510	N/A	N/A				
11.0	132.471970		0.422606	0.005695	0.000000		113.354874
	0.767006	N/A	N/A				

MSTHM version MSTHM_rev_6.0

creation date Wed Sep 15 11:28:04 1999

EXTfile creation date: Thu Mar 4 09:56:38 1999

file: CC_snf_mean_32_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 3; (0..9)

t(RH = 0.85) > 290.00

t(RH = 0.85) <= 320.00

temperature bin 2; (0..2)

T(5000y) > 79.00

T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)

average WP location: h@m.i.r#5:15:1

average WP type: snf6

LADS phase-II multi-scale TH calculation for EDA IIA preclosure
 TSPA-VA base-case mean alpha_f Ix1 property set

line load
sand invert using VA sand properties
VA heat-generation curves with no additional waste aging
ventilation for 50 yr at 50 percent heat-removal efficiency
AML = 60 MTU/acre
Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m²)
fraction of zone CC represented by data set = 0.133778
area of repository represented by data set = 105504.01 (m²)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
							RH_dripShield
0.0	19.095604	1.000000	0.984741	0.000000	19.095604		
0.998033	N/A	N/A					
1.0	92.966461	0.363004	0.591610	0.000000	67.935547		
0.998309	N/A	N/A					
1.5	102.814064	0.403026	0.502505	0.000000	78.844292		
0.998368	N/A	N/A					
2.0	108.205292	0.426894	0.336999	0.000000	84.948441		
0.998216	N/A	N/A					
3.0	114.495621	0.450224	0.147986	0.000000	91.795624		
0.997649	N/A	N/A					
4.0	118.841469	0.464141	0.069914	0.000000	96.537674		
0.992958	N/A	N/A					
5.0	121.846382	0.470638	0.030992	0.000000	100.057129		
0.975329	N/A	N/A					
6.0	123.790573	0.468665	0.017182	0.000000	102.436821		
0.948581	N/A	N/A					
7.0	125.612900	0.456920	0.011694	0.000000	104.680008		
0.904622	N/A	N/A					
8.0	127.218040	0.446339	0.008741	0.000000	107.067238		
0.854822	N/A	N/A					
9.0	128.521301	0.437416	0.007737	0.000000	108.878860		
0.819443	N/A	N/A					
10.0	129.444305	0.433998	0.007032	0.000000	110.170189		
0.800059	N/A	N/A					
11.0	130.123932	0.431331	0.006500	0.000000	111.186836		
0.784661	N/A	N/A					

MSTHM version MSTHM_rev_6.0
creation date Wed Sep 15 11:28:04 1999
EXTfile creation date: Thu Mar 4 09:56:38 1999
file: CC_snf_mean_42_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 4; (0..9)
t(RH = 0.85) > 320.00
t(RH = 0.85) <= 350.00

temperature bin 2; (0..2)
T(5000y) > 79.00
T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)
average WP location: h@m.i.r#7:11:1
average WP type: snf4

LADS phase-II multi-scale TH calculation for EDA IIA preclosure
 TSPA-VA base-case mean alpha_f Ix1 property set
 line load
 sand invert using VA sand properties
 VA heat-generation curves with no additional waste aging
 ventilation for 50 yr at 50 percent heat-removal efficiency
 AML = 60 MTU/acre
 Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m²)

fraction of zone CC represented by data set = 0.129024

area of repository represented by data set = 101754.84 (m²)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
			RH_dripShield				
0.0	18.025698		1.000000	0.985640	0.000000		18.025698
0.998040		N/A	N/A				
1.0	108.723129		0.350396	0.425605	0.000000		80.405167
0.998433		N/A	N/A				
1.5	115.738930		0.383728	0.209774	0.000000		88.642296
0.998291		N/A	N/A				
2.0	119.980904		0.406302	0.097656	0.000000		93.781044
0.997604		N/A	N/A				
3.0	125.452621		0.420271	0.025561	0.000000		99.555779
0.991641		N/A	N/A				
4.0	128.144318		0.422774	0.008489	0.000000		102.972168
0.959855		N/A	N/A				
5.0	129.857986		0.414000	0.004782	0.000000		105.404495
0.909082		N/A	N/A				
6.0	131.247314		0.404895	0.004284	0.000000		107.467567
0.863150		N/A	N/A				
7.0	131.996277		0.401343	0.004025	0.000000		109.080574
0.828559		N/A	N/A				
8.0	132.782013		0.396732	0.003889	0.000000		110.409615
0.801170		N/A	N/A				
9.0	133.473389		0.391920	0.003883	0.000000		111.567787
0.777150		N/A	N/A				
10.0	134.019928		0.388001	0.003998	0.000000		112.519028
0.757600		N/A	N/A				
11.0	134.397171		0.382664	0.004263	0.000000		113.286621
0.736586		N/A	N/A				

MSTHM version MSTHM_rev_6.0

creation date Wed Sep 15 11:28:04 1999

EXTfile creation date: Thu Mar 4 09:56:38 1999

file: CC_snf_mean_52_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 5; (0..9)

t(RH = 0.85) > 350.00

t(RH = 0.85) <= 380.00

temperature bin 2; (0..2)

T(5000y) > 79.00

T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)

average WP location: h@m.i.r#6:13:1

average WP type: snf4

LADS phase-II multi-scale TH calculation for EDA IIA preclosure
TSPA-VA base-case mean alpha_f Ix1 property set
line load
sand invert using VA sand properties
VA heat-generation curves with no additional waste aging
ventilation for 50 yr at 50 percent heat-removal efficiency
AML = 60 MTU/acre
Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m²)

fraction of zone CC represented by data set = 0.031970

area of repository represented by data set = 25213.34 (m²)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
							RH_dripShield
0.0	18.992054		1.000000	0.984765	0.000000		18.992054
0.997706		N/A	N/A				
1.0	109.912895		0.352865	0.416516	0.000000		81.594933
0.997963		N/A	N/A				
1.5	117.064301		0.386558	0.193401	0.000000		89.967667
0.997354		N/A	N/A				
2.0	121.368340		0.406695	0.085767	0.000000		95.168480
0.991347		N/A	N/A				
3.0	126.702141		0.408951	0.022803	0.000000		100.805298
0.959003		N/A	N/A				
4.0	129.353928		0.399329	0.007942	0.000000		104.181778
0.900840		N/A	N/A				
5.0	131.060608		0.388649	0.004973	0.000000		106.607117
0.848480		N/A	N/A				
6.0	132.437683		0.382967	0.004131	0.000000		108.657921
0.812325		N/A	N/A				
7.0	133.096329		0.384001	0.003777	0.000000		110.180618
0.788595		N/A	N/A				
8.0	133.663300		0.381877	0.003753	0.000000		111.290909
0.768676		N/A	N/A				
9.0	134.098923		0.378727	0.003988	0.000000		112.193329
0.749162		N/A	N/A				
10.0	134.377060		0.372007	0.004494	0.000000		112.876160
0.725500		N/A	N/A				
11.0	134.548645		0.350906	0.006369	0.000000		113.438103
0.674978		N/A	N/A				

MSTHM version MSTHM_rev_6.0

creation date Wed Sep 15 11:28:04 1999

EXTfile creation date: Thu Mar 4 09:56:38 1999

file: CC_snf_mean_62_sandBF_60_c_j4_22_03_02_001_preClose_data

RH bin 6; (0..9)

t(RH = 0.85) > 380.00

t(RH = 0.85) <= 410.00

temperature bin 2; (0..2)

T(5000y) > 79.00

T(5000y) <= 200.00

zone 1 of 6: Center-Center (CC)
average WP location: h@m.i.r#5:14:1
average WP type: snf4

LADS phase-II multi-scale TH calculation for EDA IIA preclosure
TSPA-VA base-case mean alpha_f Ix1 property set
line load
sand invert using VA sand properties
VA heat-generation curves with no additional waste aging
ventilation for 50 yr at 50 percent heat-removal efficiency
AML = 60 MTU/acre
Ix1 infiltration based on Flint infiltration map (7.8 mm/yr avg infiltration)

area of zone CC = 788649.0 (m²)
fraction of zone CC represented by data set = 0.020110
area of repository represented by data set = 15860.00 (m²)

time	T_wp	RH_wp	x.air.gas_dr	S.liquid.in	T_dw	RH_dw	T_dripShield
							RH_dripShield
0.0	19.218489		1.000000	0.984591	0.000000		19.218489
0.997791		N/A	N/A				
1.0	110.313187		0.353852	0.413377	0.000000		81.995224
0.998023		N/A	N/A				
1.5	117.385910		0.387204	0.189547	0.000000		90.289276
0.997438		N/A	N/A				
2.0	121.652893		0.407705	0.084212	0.000000		95.453033
0.992191		N/A	N/A				
3.0	127.030739		0.409280	0.023391	0.000000		101.133896
0.958076		N/A	N/A				
4.0	129.971817		0.397128	0.009734	0.000000		104.799667
0.893651		N/A	N/A				
5.0	132.042526		0.384585	0.006641	0.000000		107.589035
0.836060		N/A	N/A				
6.0	133.762711		0.377951	0.005300	0.000000		109.982956
0.796971		N/A	N/A				
7.0	134.687866		0.376992	0.004631	0.000000		111.772156
0.769226		N/A	N/A				
8.0	135.401550		0.374644	0.004505	0.000000		113.029160
0.748971		N/A	N/A				
9.0	135.920868		0.373138	0.004670	0.000000		114.015274
0.732876		N/A	N/A				
10.0	136.289856		0.367081	0.005246	0.000000		114.788963
0.710665		N/A	N/A				
11.0	136.525986		0.352771	0.006632	0.000000		115.415436
0.673602		N/A	N/A				

The file names and numbers in bold above are selected to check the averaging routine used to compute the input data required in this parameter development. The average (drift wall) temperature is hand computed as the following:

$$\begin{aligned}
 dwT(9 \text{ years}) &= 0.127595 \times 111.499939 + 0.288542 \times 108.901680 + 0.26898 \times 111.518349 \\
 &\quad + 0.133778 \times 108.878860 + 0.129024 \times 111.567787 \\
 &\quad + 0.031970 \times 112.193329 + 0.020110 \times 114.015274 = 110.48593^{\circ}\text{C}
 \end{aligned}$$

This is compared to (an excerpt of) the information given in the worksheet preclose:

Inputs:

CC_snf_mean_0	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data
CC_snf_mean_1	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data
CC_snf_mean_2	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data
CC_snf_mean_3	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data
CC_snf_mean_4	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data
CC_snf_mean_5	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data
CC_snf_mean_6	2_sandBF_60_c_j4_22	_03_02_001_preClos	e_data

output:

CC_snf_sandBF time(years),T	_60_c_j4_22_03_02_0 (C),RH,SI, dwT(C)	01_preClose_newave	rage
0.0001	18.48987	1	0 18.48987
1	101.81576	0.39073	0 77.1306
1.5	109.38082	0.42431	0 85.70986
2	113.9396	0.44647	0 91.00991
3	119.8788	0.45967	0 97.10559
4	123.08159	0.46616	0 100.8319
5	125.28101	0.46125	0 103.6011
6	127.03338	0.44984	0 105.7489
7	128.11496	0.44431	0 107.6085
8	129.1355	0.43846	0 109.2003
9	130.00022	0.43308	0 110.4859
10	130.68343	0.42894	0 111.5223
11	131.17801	0.42432	0 112.3519

The average waste package temperature is checked at the same time.

$$\begin{aligned}
 T(9 \text{ years}) &= 0.127595 \times 131.254684 + 0.288542 \times 126.469978 + 0.26898 \times 131.332336 \\
 &\quad + 0.133778 \times 128.521301 + 0.129024 \times 133.473389 \\
 &\quad + 0.031970 \times 134.098923 + 0.020110 \times 135.920868 = 130.00022^\circ\text{C}
 \end{aligned}$$

The results of this comparison indicate that the software routine, convfile_genprec.f, is performing the averaging calculation correctly.

Range of Validity for convfile_genprec.f

The written format of the input files for this routine must be identical to the files listed in Table 1 for the extended preclosure ventilation case: LL990302204242.087. The number of sequential (time) points from the input data that this routine can process (without changing the parameter "npts" and recompiling) is 54.

The source routine for convfile_gen.f is hand checked at a single time point to ensure its correct

implementation. The procedure is similar to the process shown above. However, the routine test case is for source input data and averaged (output) results from another analysis (as contained in the TDMS under DTN: MO9906SPATHRIP.000). The test case input files are of the same format as the input files processed in this calculation. Therefore, this testing procedure is considered applicable as a method to ensure that the input files used in this calculation are correctly averaged. The point of this test case is to ensure correct implementation of the software routine and to show that it computes averages correctly based on weights of the given input data. Excerpts of the testing data input files are shown below, with an excerpt of the result of the averaging routine also shown. Direct comparisons to hand calculations are shown in bold.

An overall description of this software routine is the following.

- 1) Read input information indicated in Table 1 for the extended preclosure case.
- 2) Compute a weighted average based on the fraction represented by each data set.
- 3) Perform this operation at each time point for specified variables (e.g., drip shield temperature) for every input file.
- 4) Write the output to be read into the excel spreadsheets used to generate the parameters described in this calculation.

Use of this routine requires minor runtime intervention by the user and an additional driver file (created by the user) in which the filenames of the input data reside. This is illustrated as the following for the no backfill case described in Table 1. (An analogous procedure is followed for specifying the driver file for the backfill case as listed in Table 1 as well.) The driver input file contains the following input file and required header information:

```
CC_snf
CC_snf_mean_01_noBF_60_c_j4_22_03_02_0_data
CC_snf_mean_11_noBF_60_c_j4_22_03_02_0_data
CC_snf_mean_21_noBF_60_c_j4_22_03_02_0_data
```

The header label "CC_snf" MUST be at the top of the file and should be seven characters or less. The name of each input file must reside in this driver file. The names of the input files (e.g., CC_snf_mean_*) should not exceed 70 characters. The name of the driver file can be anything as long as it does not exceed 70 characters. The driver file and the input files must reside in the directory in which the routine is being executed. The runtime response for this software routine is the following.

```
'How many bins are there?'
'What is the name of the output file?'
'What is the name of the input file?'
```

The answer to the first question is three (3) since there are a total of three input files to be processed (shown above) by the routine (note: in the case of backfill, the answer to this question is 13 as indicated in Table 1). The answer to the second question can be anything as long as it does not

exceed 70 characters. The name of the driver-input file (the third question) is described above and should be limited to 70 characters or less. In summary, execution of this routine requires the three input files (from Table 1) plus the input driver file. An analogous process is followed for the backfill case files listed in Table 1.

A test case for the software routine is given as the following. The test case input files have the same format as the files (i.e., CC_snf_mean_01_noBF_60_c_j4_22_03_02_0_data, etc.) used in this calculation. Excerpts of the test case input files and output are given below. Only excerpts are shown due to the size of the files.

```
creation date  Sat Feb 20 15:13:57 1999
file: CC_snf_mean_02_noBF_150_c_j4_17_03e_05_0_data
RH bin 0 of 9
temperature bin 2 of 2
zone 6 of 6: Center Center (CC)
```

```
LADS phase-II multi-scale TH calculation for EDA V
TSPA-VA base-case mean alpha_f Ix1 property set
line load with no backfill
2-m-diameter drip shield emplaced at 75 yr
VA heat-generation curves with 25 yr additional waste aging
ventilation for 75 yr at 50 percent heat-removal efficiency
AML = 150 MTU/acre
Ix0.5 infiltration based on Flint infiltration map (3.9 mm/yr avg
infiltration)
```

```
area of zone CC = 788649.0 (m^2)
fraction of zone CC represented by data set = 0.525883
area of repository represented by data set = 414737.12 (m^2)
```

time(years)	temp(C)	RH	Xair	Sliquid	dw T
dw RH	ds T	ds RH			
...					
80.0	141.18	0.274070	0.001347	0.000000	130.539993
0.372850	136.619995	0.311970			
90.0	145.60	0.221580	0.001765	0.000000	135.770004
0.292360	141.550003	0.247990			
100.0	147.59	0.225100	0.001762	0.000000	138.410004
0.290670	143.880005	0.249160			
101.0	147.51	0.225500	0.001762	0.000000	138.389999
0.290670	143.839996	0.249370			
105.0	147.21	0.227050	0.001762	0.000000	138.350006
0.290670	143.679993	0.250190			

```
creation date  Sat Feb 20 15:13:57 1999
file: CC_snf_mean_12_noBF_150_c_j4_17_03e_05_0_data
RH bin 1 of 9
temperature bin 2 of 2
zone 6 of 6: Center Center (CC)
```

```
LADS phase-II multi-scale TH calculation for EDA V
TSPA-VA base-case mean alpha_f Ix1 property set
```

line load with no backfill
 2-m-diameter drip shield emplaced at 75 yr
 VA heat-generation curves with 25 yr additional waste aging
 ventilation for 75 yr at 50 percent heat-removal efficiency
 AML = 150 MTU/acre
 Ix0.5 infiltration based on Flint infiltration map (3.9 mm/yr avg
 infiltration)

area of zone CC = 788649.0 (m²)
fraction of zone CC represented by data set = 0.352455
 area of repository represented by data set = 277963.28 (m²)

time(years)	temp(C)		RH	Xair	Sliquid	dw T
dw RH	ds T		ds RH			
...	...					
80.0	144.48		0.248780	0.000726	0.000000	132.199997
0.353280	138.850006		0.291380			
90.0	148.47		0.205540	0.000944	0.000000	137.169998
0.281680	143.470001		0.235710			
100.0	150.72		0.196580	0.001189	0.000000	140.210007
0.262330	146.169998		0.222230			
101.0	150.70		0.197020	0.001189	0.000000	140.270004
0.262330	146.199997		0.222450			
105.0	150.57		0.198650	0.001189	0.000000	140.449997
0.262330	146.240005		0.223300			

creation date Sat Feb 20 15:13:57 1999
file: CC_snf_mean_22_noBF_150_c_j4_17_03e_05_0_data
 RH bin 2 of 9
 temperature bin 2 of 2
 zone 6 of 6: Center Center (CC)

LADS phase-II multi-scale TH calculation for EDA V
 TSPA-VA base-case mean alpha_f Ix1 property set
 line load with no backfill
 2-m-diameter drip shield emplaced at 75 yr
 VA heat-generation curves with 25 yr additional waste aging
 ventilation for 75 yr at 50 percent heat-removal efficiency
 AML = 150 MTU/acre
 Ix0.5 infiltration based on Flint infiltration map (3.9 mm/yr avg
 infiltration)

area of zone CC = 788649.0 (m²)
fraction of zone CC represented by data set = 0.038416
 area of repository represented by data set = 30296.74 (m²)

time(years)	temp(C)		RH	Xair	Sliquid	dw T
dw RH	ds T		ds RH			
...	...					
80.0	144.92		0.242110	0.000629	0.000000	132.649994
0.343500	139.289993		0.283380			
90.0	148.95		0.203200	0.000793	0.000000	137.649994
0.278150	143.949997		0.232880			
100.0	151.38		0.191480	0.001140	0.000000	140.869995
0.255340	146.839996		0.216430			

101.0	151.37	0.191910	0.001140	0.000000	140.949997
0.255340	146.880005	0.216640			
105.0	151.28	0.193540	0.001140	0.000000	141.160004
0.255340	146.949997	0.217500			

creation date Sat Feb 20 15:13:57 1999
file: CC_snf_mean_32_noBF_150_c_j4_17_03e_05_0_data
 RH bin 3 of 9
 temperature bin 2 of 2
 zone 6 of 6: Center Center (CC)

LADS phase-II multi-scale TH calculation for EDA V
 TSPA-VA base-case mean alpha_f Ix1 property set
 line load with no backfill
 2-m-diameter drip shield emplaced at 75 yr
 VA heat-generation curves with 25 yr additional waste aging
 ventilation for 75 yr at 50 percent heat-removal efficiency
 AML = 150 MTU/acre
 Ix0.5 infiltration based on Flint infiltration map (3.9 mm/yr avg
 infiltration)

area of zone CC = 788649.0 (m^2)
fraction of zone CC represented by data set = 0.083226
 area of repository represented by data set = 65636.10 (m^2)

time(years)	temp(C)	RH	Xair	Sliquid	dw T
dw RH	ds T	ds RH			
80.0	143.55	0.254410	0.000888	0.000000	131.250000
0.362210	137.889999	0.298420			
90.0	147.50	0.210200	0.001290	0.000000	136.179993
0.288640	142.479996	0.241390			
100.0	149.88	0.199330	0.001641	0.000000	139.360001
0.266540	145.320007	0.225660			
101.0	149.92	0.199810	0.001641	0.000000	139.470001
0.266540	145.399994	0.225890			
105.0	149.94	0.201560	0.001641	0.000000	139.800003
0.266540	145.600006	0.226790			

The average drip shield temperature is computed by hand at the 100 year data point given above.

$$dsT(100 \text{ years}) = 0.525883 \times 143.880005 + 0.352455 \times 146.169998 + 0.038416 \times 146.839996 \\ + 0.083226 \times 145.320007 = 144.9178^{\circ}\text{C}$$

This input check is compared to (an excerpt of) the resulting information obtained from the averaging routine, convfile_gen.f, (DTN: MO9906SPATHRIP.000 filename: CC_snf_noBF_150_c_j4_17_03e_05_0_newaverage):

Inputs:

```

CC_snf_mean_02_noBF_150_c_j4_17_03e_05_0_data
CC_snf_mean_12_noBF_150_c_j4_17_03e_05_0_data
CC_snf_mean_22_noBF_150_c_j4_17_03e_05_0_data
CC_snf_mean_32_noBF_150_c_j4_17_03e_05_0_data
output:
CC_snf_noBF_150_c_j4_17_03e_05_0_newaverage
time(years),T(C),RH,Sl, dwT(C), dsT(C), dsRH

```

...

80.00	142.68120	0.26229	0.00000
131.26261	137.61151	0.30248	
90.00	146.89546	0.21427	0.00000
136.36707	142.39348	0.24253	
100.00	149.02642	0.21161	0.00000
139.21522	144.91780	0.23645	
101.00	148.98024	0.21203	0.00000
139.23808	144.91553	0.23667	
105.00	148.77486	0.21363	0.00000
139.31602	144.86482	0.23750	

...

The results of this comparison indicate that the software routine, convfile_gen.f, is performing the averaging calculation correctly. Therefore, it can be applied to the input data sets used to develop the no backfill/with backfill parameters presented in this calculation.

Ranges of Validity convfile_gen.f

The written format of the input files for this routine must be identical to the files listed in Table 1 for the design cases: LL990301904242.084 (with backfill) and LL990302004242.085 (no backfill). The number of sequential (time) points from the input data that this routine can process (without changing the parameter "npts" and recompiling) is 94.

Other Spreadsheet Hand Checks (kth(rad-convht)wprec.xls and kth(rad-convht)nobf.xls)

Consider the special case of extended preclosure period (> 50 years). Consider application of equation (3) in the Excel 97 spreadsheet, kth(rad-convht)wprec.xls, specifically in the worksheet named: preclose. Selecting the 15 year data point for the extended preclosure effective thermal conductivity parameter, equation (3) gives a thermal radiation equivalence of:

$$k_{eff} = \frac{(5.67 \times 10^{-8})(0.815)[(404.65148)^2 + (387.124)^2][404.65148 + 387.124] \ln\left(\frac{2.55}{0.815}\right)}{\frac{1}{0.8} + \frac{1-1}{1}\left(\frac{0.815}{2.55}\right)} = 10.47 \frac{W}{m-K}$$

An excerpt from the worksheet itself is shown below with the sample calculation check shown in bold:

A	B	...	E	...	J
Time(years)	Waste Package Temperature (°C)		Drift Wall Temperature (°C)		Keff_prc (W/m-K)
11	131.17801	...	112.3519	...	10.383
12	131.52878	...	113.0366	...	10.423
15	131.65148	...	114.124	...	10.471
20	130.28672	...	114.0285	...	10.412
25	127.86001	...	112.769	...	10.267

Equation (3) has been implemented correctly in the worksheet (preclosure) based on this sample calculation.

Final verification and testing are performed for the Excel 97 spreadsheet, kth(rad-convht)nobf.xls, specifically for the worksheet named: EDA-II-noBF-rad (*note: this same worksheet is contained in both spreadsheets: kth(rad-convht)nobf.xls and kth(rad-convht).xls*). The spreadsheets compute the effective thermal conductivity parameters for the no backfill design. The preclosure (thermal radiation) effective thermal conductivity parameter is computed, as before, with equation (3). Although the value of this parameter (without backfill) is similar to the preclosure parameter determined in the backfill case, it is slightly different since the source input files are different. Using equation (3), the effective thermal conductivity parameter for radiation heat transfer at the 30 year data point is:

$$k_{eff} = \frac{(5.67 \times 10^{-8})(0.815)[(398.5416)^2 + (384.3262)^2][398.5416 + 384.3262] \ln\left(\frac{2.55}{0.815}\right)}{\frac{1}{0.8} + \frac{1-1}{1}\left(\frac{0.815}{2.55}\right)} = 10.12 \frac{W}{m-K}$$

An excerpt from the worksheet EDA-II-noBF-rad (from either spreadsheet) is used to verify this calculation:

A	B	...	E	...	P
Time(years)	Waste Package Temperature (°C)		Drift Wall Temperature (°C)		Keff_prc (W/m-K) (
27	127.51823 ...		112.7028	...	10.25
30	125.54161 ...		111.3262	...	10.12
35	122.11365 ...		108.7909	...	9.89

Equation (3) has been correctly implemented into the spreadsheets.

The postclosure inner and outer effective thermal conductivity parameters are also spot checked to ensure correct implementation in the spreadsheets: kth(rad-convht)nobf.xls and kth(rad-convht).xls. The inner effective thermal conductivity parameter (between waste package and drip shield) is computed using equation (6). Selecting the year 77 data point from the worksheet named EDA-II-noBF-rad, the hand check is the following for the thermal radiative equivalence:

$$k_{eff} = \frac{(5.67 \times 10^{-8})(0.815)[(433.1465)^2 + (427.0393)^2][433.1465 + 427.0393] \ln\left(\frac{1.0}{0.815}\right)}{\frac{1}{0.8} + \frac{1-0.8}{0.8}\left(\frac{0.815}{1.0}\right)} = 2.0695 \frac{W}{m-K}$$

An excerpt from the worksheet EDA-II-noBF-rad (from either spreadsheet) is used to verify this calculation:

A	B	...	E	F	...	Q
Time (years)	Waste Package Temperature (°C)		Drift Wall Temperature (°C)	Drip Shield Temperature (°C)		Keff_i_poc (W/m-K)
77	160.14649 ...		142.5542	154.0393	...	2.06945

Equation (6) has been correctly implemented into this spreadsheet. The final check of the worksheet named EDA-II-noBF-rad in the Excel 97 spreadsheet kth(rad-convht)nobf.xls (or kth(rad-convht).xls) is for the outer effective thermal conductivity. The radiative equivalent effective thermal conductivity at 77 years is checked using equation (16):

$$k_{effo} = \frac{(5.67 \times 10^{-8})(1)[(415.5542)^2 + (427.0393)^2][415.5542 + 427.0393] \ln\left(\frac{2.55}{1}\right)}{\frac{1}{0.8} + \frac{1-1}{1}\left(\frac{1}{2.55}\right)} = 12.7027 \frac{W}{m-K}$$

An excerpt from the worksheet EDA-II-noBF-rad (from either spreadsheet) is used to verify this calculation:

A	B	...	E	F	...	Q
Time (years)	Waste Package Temperature (°C)		Drift Wall Temperature (°C)	Drip Shield Temperature (°C)		Keff_i_poc (W/m-K)
77	160.14649	...	142.5542	154.0393	...	2.06945
						12.7027

Equation (16) has been correctly implemented into the spreadsheets. The natural convection component is also checked for the no backfill case. This check proceeds as before (as in the backfill case) with the appropriate spreadsheet formulation copied directly from the spreadsheet kth(rad-convht).xls into the spreadsheet kth(rad-convht)nobf.xls. Minor alterations of the geometric terms in equations (7), (8), and (13) have been made (e.g., the outer effective thermal conductivity parameter for natural convection without backfill requires the drip shield diameter instead of the effective backfill diameter). A few sample checks are given as the following for the 10,000 year data point. Note that the worksheet EDA-II-noBF-conv in spreadsheet kth(rad-convht).xls is the general form of the result. It uses the *bulk* fluid temperature to evaluate the fluid properties. The worksheet EDA-II-noBF-conv in the spreadsheet kth(rad-convht)nobf.xls contains the same formulation as kth(rad-convht).xls for the inner effective parameter. However, it contains an evaluation of the outer effective parameter using the *film* fluid temperature to compute fluid properties as a comparison to the method in worksheet EDA-II-noBF-conv in spreadsheet kth(rad-convht).xls that uses the bulk fluid temperature. Additionally, the final result of the bulk fluid temperature evaluation in worksheet EDA-II-noBF-conv in spreadsheet kth(rad-convht).xls is copied into column FQ of the worksheet EDA-II-noBF-conv in the spreadsheet kth(rad-convht)nobf.xls; this is what is used in the final calculation result (given in Attachment III).

Using an initial guess for the bulk temperature, $\bar{T}_B$, the average temperature between the waste package and drip shield of 47.89494°C (320.8949K), the fluid properties and the Rayleigh numbers can be evaluated. The thermal diffusivity and kinematic viscosity are interpolated at the bulk temperature. From Incropera and DeWitt, Table A.4, for a total temperature range of 250K to 550K (given in increments of 50K; therefore, this specific example happens to be interpolated between 300 and 350K), the diffusivity and viscosity are linearly interpolated from Table A.4 (using the guessed bulk temperature) as:

- $\nu = 1.7992 \times 10^{-5} \text{ m}^2/\text{s}$
- $\alpha = 2.5592 \times 10^{-5} \text{ m}^2/\text{s}$

Implementation of equations (7) and (8) into worksheet EDA-II-noBF-conv found in spreadsheet kth(rad-convht).xls (or kth(rad-convht)nobf.xls) becomes:

$$Ra_{Di} = \frac{9.81 \left(\frac{1}{320.8949} \right) (48.2335 - 47.8949) (2 \times 0.815)^3}{(1.7992 \times 10^{-5}) (2.5592 \times 10^{-5})} = 9.7358 \times 10^7$$

$$Ra_{Do} = \frac{9.81 \left(\frac{1}{320.8949} \right) (47.8949 - 47.5564) (2 \times 1.0)^3}{(1.7992 \times 10^{-5}) (2.5592 \times 10^{-5})} = 1.7979 \times 10^8$$

The inner (waste package surface) and outer (drip shield) cylinder Nusselt numbers (required to compute the inner effective thermal conductivity for natural convection) are computed using equations (10) and (11) as the following:

$$Nu_i = \frac{2}{\ln \left[1 + \frac{2}{\left[\left(0.5(9.7358 \times 10^7)^{1/4} \right)^{15} + \left(0.12(9.7358 \times 10^7)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 56.8880$$

$$Nu_o = \frac{-2}{\ln \left[1 - \frac{2}{\left[\left((1.7979 \times 10^8)^{1/4} \right)^{15} + \left(0.12(1.7979 \times 10^8)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 114.7950$$

An excerpt from the worksheet EDA-II-noBF-conv from kth(rad-convht).xls (or kth(rad-convht)nobf.xls) is:

A Time (years)	B Waste Package Temperature (°C)	...	E Drift Wall Temperature (°C)	F Drip Shield Temperature (°C)	...
8000	51.88158	...	50.40383	51.16503	...
10000	48.23348	...	46.85384	47.5564	...
15000	41.03813	...	39.94578	40.49607	...

O Tavgb	P nu	Q alpha	R Radi	S Rado	T
51.52331	1.8357E-05	2.6129E-05	97784365	180632792	55.97219
47.89494	1.7992E-05	2.5592E-05	97338998	1.7981E+08	55.89069
40.7671	1.7275E-05	2.4538E-05	86575222	159926631	53.84451

U Nui	V	W Nuo
56.96634	115.9334	114.9305
56.88483	115.8011	114.7982
54.83843	112.4574	111.4545

The implementation of the natural convection equations in the spreadsheets is verified to be correct for the inner effective thermal conductivity parameter for the no backfill case.

The final check is for the outer effective thermal conductivity parameter. From the spreadsheet kth(rad-convht).xls, the worksheet EDA-II-noBF-conv is considered. The final result of this calculation is also copied into the spreadsheet kth(rad-convht)nobf.xls specifically in the worksheet EDA-II-noBF-conv (refer to column FQ).

Using an initial guess for the bulk temperature, $\bar{T}_b$, the average temperature between the drip shield and drift wall of 47.2051°C (320.2051K), the fluid properties and the Rayleigh numbers can be evaluated. The thermal diffusivity and kinematic viscosity are interpolated at the bulk temperature. From Incropera and DeWitt, Table A.4, for a total temperature range of 250K to 550K (given in increments of 50K; therefore, this specific example happens to be interpolated between 300 and 350K), the diffusivity and viscosity are linearly interpolated from Table A.4 (using the guessed bulk temperature) as:

- $\nu = 1.7923 \times 10^{-5} \text{ m}^2/\text{s}$
- $\alpha = 2.5490 \times 10^{-5} \text{ m}^2/\text{s}$

Implementation of equations (7) and (8) into worksheet EDA-II-noBF-conv found in spreadsheet kth(rad-convht).xls (or kth(rad-convht)nobf.xls) becomes:

$$Ra_{Di} = \frac{9.81 \left(\frac{1}{320.2051} \right) (47.5564 - 47.2051) (2 \times 1.0)^3}{(1.7923 \times 10^{-5}) (2.5490 \times 10^{-5})} = 1.8846 \times 10^8$$

$$Ra_{Do} = \frac{9.81 \left(\frac{1}{320.2051} \right) (47.2051 - 46.8538) (2 \times 2.55)^3}{(1.7923 \times 10^{-5}) (2.5490 \times 10^{-5})} = 3.125 \times 10^9$$

The inner (drip shield surface) and outer (drift wall) cylinder Nusselt numbers (required to compute the outer effective thermal conductivity for natural convection) are computed using equations (10) and (11) as the following:

$$Nu_i = \frac{2}{\ln \left[1 + \frac{2}{\left[\left(0.5 (1.8846 \times 10^8)^{1/4} \right)^{15} + \left(0.12 (1.8846 \times 10^8)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 70.1902$$

$$Nu_o = \frac{-2}{\ln \left[1 - \frac{2}{\left[\left((3.125 \times 10^9)^{1/4} \right)^{15} + \left(0.12 (3.125 \times 10^9)^{1/3} \right)^{15} \right]^{1/15}} \right]} = 235.6124$$

and equation (13) is checked as the following,

$$Nu_{cond} = \frac{2}{\ln \frac{2.55}{1.0}} = 2.1365$$

An excerpt from the worksheet EDA-II-noBF-conv from kth(rad-convht).xls is:

A	B	...	E	F	...
Time	Waste Package		Drift Wall	Drip Shield	
(years)	Temperature (°C)		Temperature	Temperature (°C)	
			(°C)		
8000	51.88158	...	50.40383	51.16503	...
10000	48.23348	...	46.85384	47.5564	...
15000	41.03813	...	39.94578	40.49607	...

BW	BX	BY	BZ	CA	CB	CC
Tavgb	nu	alpha	Radi	Rado		Nui
50.78443	1.8283E-05	2.6020E-05	1.9392E+08	3.2155E+09	69.84342	70.83872
47.20512	1.7923E-05	2.5490E-05	1.8845E+08	3.1248E+09	69.19435	70.18961
40.22093	1.7220E-05	2.4457E-05	1.6370E+08	2.7143E+09	66.09012	67.08515

CD	CF	...	EJ	...
	Nuo		Nucond	
238.3144	237.313	50.57882	2.1365E+00	...
236.6107	235.6093	47.0151	2.1365E+00	...
228.3967	227.3952	40.07114	2.1365E+00	...

The implementation of the natural convection equations in the spreadsheets is verified to be correct for the outer effective thermal conductivity parameter for the no backfill case.

This completes the testing and verification of the spreadsheets used in this calculation. All spreadsheet implemented equations and macros have been thoroughly checked and found to be correct in each case.

Range of Validity

The range of validity for the spreadsheet routine kth(rad-convht)wprec.xls and kth(rad-convht)nobf.xls is fixed for an overall temperature range of 250K to 550K for any single component (e.g., waste package, drip shield, etc.) temperature. Component temperatures outside of the given temperature range will result in fluid properties (kinematic and thermal diffusivity and thermal conductivity) not interpolated correctly by the spreadsheet.