LLR.20080617.0077

YMP Yucca Mountain Project	**Model** **Error Resolution Document** *Complete only applicable items.*	QA: QA Page 1 of 27

INITIATION

1. Originator: John Case	2. Date: 06/02/2008	3. ERD No. ANL-EBS-MD-000049 ERD 02
4. Document Identifier: ANL-EBS-MD-000049 REV 03 AD 02	5. Document Title: Multiscale Thermohydrologic Model	

6. Description of and Justification for Change (Identify applicable CRs and TBVs):

Editorial corrections and clarifications to ANL-EBS-MD-000049 REV 03 AD 02 are made in response to CR-11935. In addition, deficiencies in data qualification as identified in CR-11936 are addressed. A justification for no impact to results of the subject report, and for other products that use output from this report as direct input, is also included.

See attached pages for details.

CONCURRENCE

	Printed Name	Signature	Date
7. Checker	Charles Haukwa	[signature]	06/19/2008
8. QCS/QA Reviewer	Robert E. Spencer	[signature]	6/19/08

APPROVAL

9. Originator	John Case	[signature]	6/19/2008
10. Responsible Manager	Paul Dixon	[signature]	6-19-08

CR 11935 Evaluation

I. Background Information Summary

Condition Report (CR) 11935 documents a set of issues related to ANL-EBS-MD-000049 REV 03 AD 02 (SNL 2008 [DIRS 184433]), which were found during Lead Lab QA surveillance LQA-IS-08-002. This document presents the disposition of those issues, identifying changes to the analysis/model report (AMR), and evaluating the impact of those changes on the conclusions of the AMR.

II. Disposition of Major Issues/ Description of Change

II.1 (Issue 3 from surveillance; p. 4-23): *Were the DST measurements used for validation or as model input? (A note in Table 4.4-2 says validation; should state so in the report's narrative on p.4-23.)*

AMR Changes:

Change the first paragraph in Section 4.4 to read: "The source DTNs for the field measurements in the Large Block Test (LBT) are listed in Table 4.4-1. These DTNs are used for model validation purposes only and are not direct input to the MSTHM, with the exception of DTN: LB990861233129.001 [DIRS 110226], which provides the calibrated hydrologic property set used in the calculations. The source DTNs for the field measurements in the Drift Scale Test (DST) are listed in Table 4.4-2."

Change the footnote of Table 4.4-1 to state: "With the exception of the last DTN (LB990861233129.001 [DIRS 110226]), which provides the calibrated hydrologic property set used in the calculations, these DTNs are used for validation purposes only. Note that DTN: LB990861233129.001 [DIRS 110226] is not used to validate models."

Change the footnote of Table 4.4-2 to state: "With the exception of the last DTN (LB991201233129.001 [DIRS 146894]), which provides boundary conditions for all thermal and thermal-hydrologic models, these DTNs are used for validation purposes only. Note that DTN: LB991201233129.001 [DIRS 146894] is not used to validate models."

II.2 (Issue 7b from surveillance; p. 5-7): *Third paragraph under Section 5.3.1.2. Reference to Table 4.1-2 appears to be incorrect. Intergranular porosity and grain size information is not listed in Table 4.1-2.*

AMR Change:

In the third paragraph of Section 5.3.1.2, change reference to Table 4.1-2 to Section 4.1.3.

II.3 (Issue 8 from surveillance; p. 5-9): *Section 5.3.1.5, Assumption. The bulkhead permeability is assumed as being 1/10th of the open drift. What is the permeability of the open drift?*

AMR Change:

Change first sentence of the assumption to read: "The bulkhead in the Drift Scale Test (DST) is assumed to be extremely permeable (Section 5.3.1.7), with a permeability one-tenth that of the open drift."

II.4 (Issue 17 from surveillance; p. 6-30): *In line 5 of Stage 5 narrative, it should be* $H_{i,LDTH}$ *(and not* $H_{i,j,\,LMTH}$*).*

AMR Change:

Change the second sentence for Stage 5 to read: "Note that the hydrologic parameters from the LDTH submodels are collectively referred to as $\mathrm{H}_{\mathrm{i,LDTH}}$ in Figure 1-1 and Table 1-3."

II.5 (Issue 20 from surveillance; p. 6-40): *Section 6.2.6.5 LDTH Submodel Material Properties. In second paragraph, seventh line from bottom, need to insert the word "effect" after "insignificant".*

AMR Change:

In Section 6.2.6.5, second paragraph, seventh line from bottom, change the text to read: ". . . has an insignificant effect on flow because conditions in these respective continua are in equilibrium within the gas-filled drift."

II.6 (Issue 30 from surveillance; p. 6-140): *Section 6.3.4. Third paragraph on page. Reference to Table 6.3-20 is incorrect. The correct reference is Table 6.3-23.*

AMR Change:

Change the first sentence in the third paragraph of Section 6.3.4 to read: "Calculations performed using $\mu i - \sigma i$, μi, and $\mu i + \sigma i$ (Table 6.3-23) raise the question concerning how much weight (i.e., probability in the epistemic sense) should be applied to these three host-rock thermal conductivity cases."

II.7 (Issue 31 from surveillance; p. 6-145): *First paragraph. Statements made in lines 7-8 and lines 15-16 do not properly convey the intent. "There is a probability of less than 1.0 that…" can apply to just about any situation. Perhaps the intent is to say this probability is very close to 1.0? Editorial. "…high likelihood that…"*

AMR Changes:

Change the fourth sentence of the first paragraph on page 6-145 to read: "It is likely that a few (on the order of 10) waste packages will never experience boiling, while the waste package at the hottest, driest location in the repository may experience boiling at the drift wall for up to 2,176 years."

Change the eighth sentence of the first paragraph on page 6-145 to read: "It is likely that a few (on the order of 10) single waste packages will never experience boiling in the host rock, while the waste package at the hottest, driest location in the repository may have a maximum lateral extent of boiling of 27.9 m, which represents 69% of the lateral extent between the emplacement drift centerline and the midplane in the center of the rock pillar between drifts."

II.8 (Issue 34 from surveillance; p. 159): *Section 6.3.8. Comparison…(SSPA). Figure 6.3-59 purportedly compares TSPA-LA results to SSPA results. It appears that SSPA results were not included in these plots.*

AMR Change:

In Section 6.3.8, replace the second sentence with the following two sentences: "Figure 6.3-59 plots the thermal-hydrologic parameters for all eight waste packages considered in the TSPA-LA. While Figure 5.3-59 pertains specifically to the TSPA-LA, these eight waste package types were also addressed in the SSPA."

II.9 (Issue 36 from surveillance; pp. 6-166 to 6-167): *Section 6.3.11. Influence…Uncertainty. Either the plots in Figure 6.3-63(a) are wrong or the statement that "Liquid-phase saturation is also insensitive to hydrologic properties of the intergranular porosity" is unsupported.*

AMR Change:

Replace the last sentence in Section 6.3.11 on page 6-166 with the following two sentences: "Compared to the variability across the repository and the influence of parametric uncertainty addressed by the MSTHM calculations supporting TSPA-LA, the hydrologic properties of the intragranular porosity of the invert have an insignificant influence on liquid-phase saturation in the invert. This justifies not propagating the influence of invert hydrologic property uncertainty through the MSTHM calculations supporting TSPA-LA."

II.10 (Issue 39b from surveillance; p. 7-3): *Line 8 of 2nd paragraph: Insert "peak" after "median".*

AMR Change:

On line 8 of the second paragraph on page 7-3, insert "peak" after "median."

II.11 (Issue 39c from surveillance; p. 7-3): *Line 10 of 2nd paragraph: Insert "peak" after "median".*

AMR Change:

On line 10 of the second paragraph on page 7-3, insert "peak" after "median."

II.12 (Issue 39d from surveillance; p. 7-3): *Line 3 of 3rd paragraph: Insert "LDTH" after "SMT".*

AMR Change:

On line 3 of the third paragraph on p. 7-3, insert "LDTH" after "SMT."

II.13 Issue 45 (p. 7-14): *Section 7.4.2.3. Typographical error in line 8. The word "convection" should be "convention".*

AMR Change:

On line 8 of Section 7.4.2.3, change the word "convection" to "convention."

II.14 (Issue 59 from surveillance; p. 7-63): *Section 7.5.2.7 Vapor…Test Case. In line 5, the phrase "over the regulatory period" should be revised to say "over the 10,000-yr simulation period."*

AMR Change:

In Section 7.5.2.7 (Vapor and Condensate Fluxes at the Edge of the Three-Drift Repository Test Case), on line 5, change the phrase "over the regulatory period" to "over the 10,000-year simulation period."

II.15 (Issue 60 from surveillance; p. 7-72): *Figure 7.5-10. The figure caption has a word mistake. In line 4, it says "…compared with Range of Temperature…" It should say "…compared with the Range of Relative Humidity…"*

AMR Change:

Figure 7.5-10, change the figure caption to read: "Absolute Difference (vs. Time) in Drift-Wall and Drip-Shield Relative Humidity between the MSTHM and D/LMTH Model for the (a,b) PWR1, (c,d) DHLW, (e, f) PWR2, and (g, h) BWR Waste Packages at the Center of the Three-Drift Repository Test Case, as Compared with the Range of Relative Humidity Resulting from Parametric Uncertainty, with and without the Influence of Waste-Package Heat-Output Variability, at the P2WR5C10 Location (Figure 6.3-1)."

II.16 (Issue 61 from surveillance; p. 7-73): *Figure 7.5-11. As in the previous comment, the caption has a word mistake. In line 4, it says "…compared with the Range of*

Temperature…” It should say “…compared with the Range of Liquid-Phase Saturation…”

AMR Change:

Figure 7.5-11, change the figure caption to read: “Absolute Difference (vs. Time) in Drift-Wall and Invert Liquid-Phase Saturation between the MSTHM and D/LMTH Model for the (a,b) PWR1, (c,d) DHLW, (e, f) PWR2, and (g, h) BWR Waste Packages at the Center of the Three Drift Repository Test Case, as Compared with the Range of Liquid-Phase Saturation Resulting from Parametric Uncertainty, with and without the Influence of Waste-Package Heat-Output Variability, at the P2WR5C10 Location (Figure 6.3-1).”

II.17 (Issue 66 from surveillance; p. I-1): *Top of page. There is a typo: “step” should be “step 1”.*

AMR Change:

Page I-1, top of page, change “Step” to “Step 1.”

II.18 (Issue 69 from surveillance; p. IV-3): *Invert Porosity. Line 1 of the paragraph under this heading mentions inter-granular porosity. Should this be intra-granular porosity (see previous paragraph)? Moreover, throughout this paragraph, these terms have not been used consistently to represent a particular variable.*

AMR Change:

Page IV-3, change the first part of the first sentence of the paragraph titled “Invert Porosity” to read: “The matrix porosity or intragranular porosity of the crushed-tuff grains in the invert. . . .”

II.19 (Issue 73 from surveillance; p. VI-3): *Table VI-1. Many entries in this table appear to be in error. See my attached table that shows recalculated values assuming ε_1=0.63 and ε_2 as shown in column 1 of Table VI-1. Should these entries turn out to be incorrect, the text on pp. VI-3, 4 may have to be revised accordingly.*

AMR Change:

Page VI-3, Table VI-1, add the following to the end of the first sentence of the footnote: “, and the ratio A_1/A_2 is equal to 0.457 in Eq. VI-7 (Bird et al. 1960 [DIRS 103524], Equation 14 G, p. 453).”

II.20 (Issue 75 from surveillance; p. X-4): *Vector columns in Eq. X.2. What materials do FM and FFH represent?*

AMR Change:

Page X-4, remove “FM” and “FFH” from the vector columns in Eq. X-2.

II.21 (Issue 77 from surveillance; p. X-14): *X.3. Typo in the last paragraph.* $\varnothing_{inatrix}$ *should be* $\varnothing_{matrix}$.

AMR Change:

Page X-14, last paragraph, second line, change "$\varnothing_{inatrix}$" *to* "$\varnothing_{matrix}$".

II.22 (Issue 79 from surveillance; p. X-26): *Table X-6. The caption (and other text) shows the moisture potential as being non-dimensionalized. Why, then, does it have units of bars (see column 1 of table)?*

AMR Change:

Page X-26, Table X-6, remove "Non-Dimensionalized" from the caption.

II.23 (Issue 80 from surveillance; p. XI-4): *Equation XI-14. Important parentheses are missing making the equation incorrect. Specifically, the part after the large square brackets needs fixing. The expression* $(t + 273/100)^3$ *should be revised as follows:* $((t + 273)/100)^3$

AMR Change:

Page XI-4, Equation XI-14, change $(t + 273/100)^3$ to $((t + 273)/100)^3$.

II.24 (Issue 82 from surveillance; p. XII-13): *Boxes with data. What is the source of data in the two boxes with numbers in them? Presumably, these are percolation flux values for the UZ flow models and MSTHM models. Please verify.*

AMR Change:

Revise the legend of Figure XII-5 on page XII-15. Replace "SMT Model" with "MSTHM," and replace "Tough2 Model" with "3-D UZ Flow Model."

II.25 (Issue 83a from surveillance; p. XII-14): *First paragraph. Reference to Figure XII-3 is incorrect. It should be to Figure XII-4. Additionally, reference to "Figures XII-4 through XII-6" should instead be to "Figures XII-5 through XII-6."*

AMR Change:

Page XII-14, first and second paragraph, change to read: "Develop the CDF by plotting the rank order against the sorted values for mean, lower, and upper percolation cases. The results are shown in Figure XII-4 for the modern or present case. The figure shows the 0.05, 0.30, 0.70, and 0.95 percentiles for the CDF. Perform the analysis for the other cases. These are presented in Figures XII-5 through XII-6."

II.26 (Issue 84 from surveillance; p. XV-5): *Table XV-1. Column headings (units) show a '^' instead of '-' or a '+' sign as a power of 10. I believe it should be* 10^{-3} *in columns 3 and 4 of the table headings.*

AMR Change:

Page XV-5, Table XV-1, change the column headings (units) for columns 3 and 4 from 10^3 to 10^{-3}.

II.27 (Issue 89 from surveillance; p. 6-11[a]): *Section 6.2.14[a]. Current SMT Submodel. Reference to Figure 65.2-18 [a] in line 5 of the first paragraph is incorrect. Do you mean it to be Figure 6.2-19[a]?*

AMR Change:

Page 6-11[a], Section 6.2.14[a], first paragraph, fifth line, change reference from Figure 65.2-18[a] to Figure 6.2-19[a].

II.28 (Issue 94 from surveillance; p. 7-2[a]): *Section 7.4.6[a]. In line 3 of second paragraph, Table 7.4-4 should be Table 7.4-4 [a].*

AMR Change:

Section 7.4.6[a], second sentence of the second paragraph, change to read: "The similarity in locations is seen by comparing Table 7.4-4[a] with Table 7.4-1 of the parent report."

II.29 (Issue 96a from surveillance; p. 7-13[a], 14[a]): *Section 7.4.6[a]. Updated Comparison. The narrative re. comparison of simulated and field-measured temperature histories does not acknowledge that, in some cases, the agreement was better in the previous base case. For example, if you compare Figure 7.4-30 [a], panel (b) with Figure 7.4-14, panel (a) (both for borehole 138, sensor 8 location), the previous base case shows a better agreement.*

AMR Change:

Section 7.4.6[a], page 7-13[a], replace the last sentence of the first paragraph with the following sentence: "A comparison of Figures 7.4-30[a] through 7.4-32[a] with Figures 7.4-13 through 7.4-14 of the parent report results in the following observations for the majority of the comparisons:"

II.30 (Issue 96b from surveillance; p. 7-13[a], 14[a]): *Has the possibility that field measurements and/or instrumentation may themselves be suspect considered?*

AMR Change:

Section 7.4.6[a], page 7-13[a], add the following sentence to the end of the last paragraph: "Additional information on instrument performance is addressed in *Thermal Testing Measurements Report* (SNL 2007 [DIRS 177414])."

II.31 (Issue 101 from surveillance; p. IV-5[a]): *Waste Package and Drip Shield Properties. The equation for $A_{1/2}$ produces a value of 2.8833m^2 (instead of the 2.9552m^2 shown on the right hand side). If carried to the expressions that follow, one gets rho$_{equiv}$=1,564.2 kg/m^3.*

AMR Change:

Waste Package and Drip Shield Properties, first equation, revise as follows: "$A_{1/2}$ = 0.242 × 0.58 + 0.40 × (0.58 + 0.37) + (0.759 + 0.760 + 0.425) × (0.58 + 0.37 + 0.3165) = 2.9825 m^2."

These dimensions are obtained from the gridblock spacings in the LDTH submodels, which are shown in Figure 6.2-6 of the parent report, and as found in the LDTH-submodel input files (e.g., Output DTN: LL0702PA014MST.069, file: *P3W-13-g_9-LDTH55-P10-02.in.gz*).

II.32 (Issue 102 from surveillance; p. IV-9[a]): *Calculation under item 5. Just below Table IV-2 [a], the expression on the R.H.S. contains (0.332 - 0.331). This should be (0.322 - 0.331).*

AMR Change:

Page IV-9[a], item 5, calculation just below Table IV-2[a], change the expression on the right-hand side to read: "(0.322 – 0.331)."

II.33 (Issue 104 from surveillance; p. VI-2[a]): *Equation VI-5[a]. An "=" is missing after ε_{eff}.*

AMR Change:

Page VI-2[a], Equation VI-5[a], add "=" after ε_{eff}.

II.34 (Issue 107) Table X-4[a]. *Values shown for van Genuchten parameters n and m appear to be incorrect. In each case, the average value listed is greater than maximum value. Further, minimum value (though lower than the average) is greater than or equal to the maximum.*

AMR Change:

Change the table headers to refer to LBTM-2 Average Porosity, LBTM-2 Minimum Porosity, and LBTM-2 Maximum Porosity.

II.35 (Issue 108 from surveillance; p. X-11[a]): *Section X.4[a]. Unsaturated…Invert. Line 2 of the paragraph mentions K_{us}. This is probably K_{uI} for which Eq. X-27 [a] defines a formula.*

AMR Change:

Appendix X[a], change all references to K_{uI} to read $K_{us.}$

The text for the presentation of the relative permeability relationship presented on p. X-11[a] is revised to read:

The relative permeability relationship is given by Fetter (1993 [DIRS 102009], p. 182, Equation 4.17) based upon the van Genuchten parameters and the conversion to hydraulic conductivity:

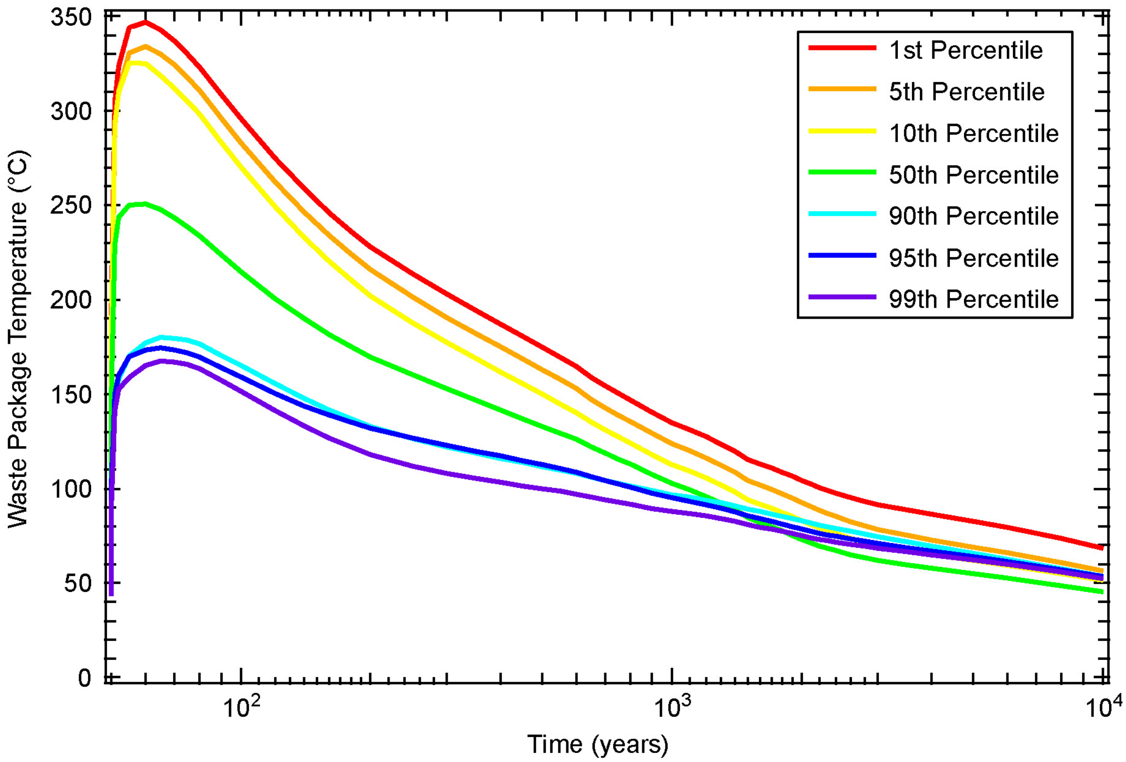
$$K_{us} = \frac{\rho_w g}{\mu_w} k_{sl} \cdot \frac{\{1-(\alpha_I \psi)^{n_I - 1}[1+(\alpha_I \psi)^{n_I}]^{-m_I}\}^2}{[1+(\alpha_I \psi)^{n_I}]^{\frac{m_I}{2}}}$$

where K_{us} is the unsaturated hydraulic conductivity of water in the intragranular/intergranular pore space, ρ_w is the fluid density of water, μ_w is the absolute viscosity of water, g is acceleration due to gravity, α_I is the van Genuchten parameter for the intragranular/intergranular pore space, n_I is the van Genuchten parameter for the intragranular/intergranular pore space, m_I is the van Genuchten parameter for the intragranular/intergranular pore space, k_{sl} is the intrinsic permeability for the intragranular/intergranular pore space of the invert, and ψ is the moisture potential.

II.36 (Issue 111 from surveillance; p. 6-52[a]): *Figure 6.3-86[a] is actually 6.3-85[a], extended to 1 million years.*

AMR Change:

Replace Figure 6.3-86[a] and its associated notes with the corrected information given below:



Source: Output DTNs: LL0702PA015MST.070, LL0702PA017MST.072, LL0702PA019MST.074, LL0702PA021MST.076, LL0702PA023MST.078, LL0702PA025MST.080, LL0702PA029MST.084, and LL0702PA027MST.082. The seven waste package temperature history files are in DTN: MO0707TH2D3DDC.000 [DIRS 182472].

NOTE: The "deltas" for CSNF waste package temperature for the low and high rubble thermal conductivity cases from DTN: LL0702PA027MST.082 are added to the CSNF waste package temperatures from DTNs: LL0702PA015MST.070, LL0702PA017MST.072, LL0702PA019MST.074, LL0702PA021MST.076, LL0702PA023MST.078, LL0702PA025MST.080, and LL0702PA029MST.084, resulting in 274,176 CSNF waste package temperature histories, which are then ranked according to peak CSNF waste package temperature. The 1st, 5th, 10th, 50th, 90th, 95th, and 99th percentile CSNF waste package temperature histories are selected and plotted.

Figure 6.3-86[a]. Waste Package Temperature Histories and Corresponding Percentiles Showing Ranges for the 21-PWR AP CSNF (pwr1-3) Waste Packages for the Collapsed-Drift Case

II.37 (Issue 112 from surveillance; p. 6-54[a]): *The last paragraph of page 6-54[a] describes the process of developing an equivalent thermal-conductivity versus time relationship to represent the influence of thermal radiation between the drip shield. The text states that the details of the calibration process are found in DTN: LL0705PA032MST.028. This process should be discussed in the body of the report.*

AMR Change:

The text of Section 6.3.18[a] is rewritten starting with the second paragraph to include the following detailed description of the calibration process described in DTN: LL0705PA032MST.028:

6.3.18.1[a] Condensation Analyses

In addition to model validation (Section 7.8[a]), the 3-D pillar scale TH model also provides information for use by *In-Drift Natural Convection and Condensation* (SNL 2007 [DIRS 181648], Section 6.2[a]), to bound the occurrence and rate of drift wall condensation during Stage 2 (when some waste package locations are still at temperatures above boiling). The needed output parameters are vapor flow and condensation along the emplacement drift (see Output DTN: LL0705PA032MST.028). Data from that output DTN are generated for a wide range of percolation flux, including the P10 and P90 percolation flux cases (Section 6.2.16[a]). These calculations were conducted for the P10 and P90 cases for a typical location in the repository, which is the g_9 UZ flow model grid column location (Figure 6.2-17[a]). The local P10 percolation flux values for the g_9 location are 3.6, 6.8, 13.6, and 17.8 mm/yr for the present day, monsoonal, glacial-transition, and post-10,000-year climates, respectively (Output DTN: LL0702PA014MST.069). The local P90 percolation flux values for the g_9 location are 26.8, 75.4, 59.3, and 44.6 mm/yr for the present-day, monsoonal, glacial-transition, and post-10,000-year climates, respectively (Output DTN: LL0702PA018MST.075). To bound the uncertainty in the influence of turbulent natural-convective mixing of water vapor and air in the drift, the 3-D pillar-scale TH model calculations were conducted for a range of gas-phase dispersion coefficient factors: 200, 1,000, 2,000, and 10,000 in the emplacement drift. For the P10 case, a dispersion-coefficient factor of 100,000 was also considered. Note that a dispersion coefficient factor of 1,000 was used in the model confidence-building test case (Section 7.8[a]). The gas-phase dispersion coefficient factor is a multiplier applied to the nominal binary gas-phase diffusion coefficient for an open system, which is determined by the NUFT code as a function of temperature.

6.3.18.2[a] Calibration of In-Drift Effective Thermal Conductivity in Three-Dimensional Pillar-Scale Thermal-Hydrologic Model

As discussed in Section 7.8[a], the 3-D pillar-scale TH model represents in-drift heat transfer by radiation and natural convection using a calibrated “equivalent” thermal conductivity versus time relationship. The calibration process is conducted with a revised version of the 2-D LDTH submodel. Note that the standard LDTH submodel lumps the waste package and drip shield into a monolithic heat source. For the purpose of the calibration the LDTH submodel is revised to include a discrete waste package and a discrete drip shield, just as it is done with the 3-D DDT submodel of the MSTHM. The calibration process is conducted with the following models:

- Target 2-D DDTH Model: This model has exactly the same cross-sectional geometry as the 3-D DDT submodel of the MSTHM. It also represents thermal radiation between the drip shield and the drift wall (called the outer gap), and between the waste package and the drip shield (called the inner gap), just as is done with the 3-D DDT submodel. It also incorporates the effective thermal conductivity for air, representing the influence of natural convection, on the basis of correlations from the FLUENT-code thermal model in *In-Drift Natural Convection and Condensation* (BSC 2004 [DIRS 164327], Appendix J), just as is done with the 3-D DDT submodel.

- Calibration 2-D DDTH Model: This model has the same cross-sectional geometry as the 3-D DDT submodel of the MSTHM, with the exception that the waste-package cross-sectional dimensions are modified for the reasons discussed below. This model does not explicitly represent thermal radiation. Instead it uses time-dependent effective (equivalent) thermal conductivity relationships for the inner and outer air-filled gaps to represent the combined influence of thermal radiation and natural convection in those gaps. The time-dependent relationships are determined by comparing the calibrated-model-predicted temperature differences across the inner and outer gaps with those predicted by the target model.

The generation of the in-drift equivalent thermal conductivity versus time relationship was achieved in a two-step iterative process that proceeds from the outer gap to the inner gap. The first step establishes the equivalent thermal conductivity function for the outer gap, which is the annulus between the drip shield and the drift wall. The second step establishes the equivalent thermal conductivity function for the inner gap, which is the annulus between the waste package and the drip shield. In each step, the equivalent thermal conductivity function within each annulus is changed until the temperature differences between the inner and outer surfaces in the calibration model match those in the target model for each time step in the respective simulations. While conducting this process, it was found that the ratio of inner to outer thermal equivalent conductivity is equal to 1.75 for every time step. Thus, multiplying the outer thermal conductivity by a factor of 1.75 yields a good match for waste package temperature at each time step, as shown in Figure 6.3-88[a].

As discussed in Output DTN: LL0705PA032MST.028 (file: *ReadMe.doc*), the calibration of the equivalent thermal conductivity function for the inner gap required some modifications to the representation of the waste package in the calibration model, which are described below. For waste package heat-generation histories, which result in a quasi-steady heat flux-driven system, temperatures for radiant heat transfer scale to the fourth root of the waste package power. Accordingly, radiant heat transfer is very efficient, causing it to be the dominant mode of heat transfer between the waste package and drip shield. In the standard 3-D DDT submodel, as well as in the target 2-D DDTH model, thermal radiation is calculated between the waste package center and the drip shield. Because of the efficiency of radiant heat transfer, thermal conduction plays a minor role for radial heat transfer from the waste package to the drip shield. However, in the calibration 2-D DDTH model, the absence of thermal radiation causes thermal conduction within the waste package to dominate radial heat transfer from the waste package to the drip shield. During the initial attempts to calibrate the equivalent thermal conductivity function for the inner gap, it was found that the radial temperature difference between the center and surface of the waste package was greater than the radial temperature difference between the waste package and drip shield in the target 2-D DDTH model. Consequently, it was necessary to make modifications to the waste package in the calibration model to reduce the radial temperature difference within the waste package to be less than the target radial temperature difference between the waste package and drip shield. These modifications involved reducing, by a factor of two, the vertical and lateral dimensions of the waste package, which reduces the cross-sectional area by a factor of four. The modifications also required increasing the thermal conductivity of the waste package by a factor of four so that the axial component of heat conductance (thermal conductivity multiplied by the vertical cross-sectional area of the waste package) is conserved. Similarly, the mass density of the waste package was increased by a factor of four to conserve the mass and volumetric heat capacity of the waste package.

The net result of these modifications is that the thermal mass and axial heat conductance are identical between the target and calibration models. The only change in heat transfer in the waste package is the eight-fold reduction in radial temperature difference between the center and surface of the waste package, which enabled the calibration process for the inner gap to yield to a good match. As discussed above, radial thermal conduction in the target model has a negligible influence on radial heat transfer to the drip shield. Therefore, any differences in radial thermal conduction within the waste package between the target and calibration models are irrelevant. What is relevant is the fact that this calibration process, which includes the abovementioned waste package modifications, results in a good match in radial heat transfer between the target and calibration models, as seen in Figure 6.3-88[a].

The modifications to the waste package in the calibration model result in one additional difference between the target and calibration model, which is the fact that the vertical cross-sectional area for the inner gap between and waste package and drip shield is 1.8572 times greater in the calibration model than in the target model. When applied to the 3-D pillar-scale TH model (Section 7.8[a]), this results in a greater cross-sectional area for which axial vapor transport occurs within the inner gap. As discussed in Section 6.3.18.1[a], there is uncertainty in the gas-phase dispersion coefficient factor, which is the parameter that influences axial vapor transport. To address that uncertainty, a sensitivity study was conducted over a nearly three-orders-of-magnitude range in gas-phase dispersion coefficient factor. A 1.8572-fold increase in cross-sectional area for the inner gap is small compared to the range of uncertainty in the gas-phase dispersion coefficient. Therefore, this difference in cross-sectional area is insignificant compared to the influence of parameter uncertainty addressed in this report.

II.38 (Issue 113 from surveillance; p. VIII-2): *The first sentence of the section "Typical Waste Package Determination" incorrectly indicates that the typical waste package determination is based on the duration of boiling at the drift wall.*

AMR Change:

Page VIII-2, change the first sentence of the section "Typical Waste Package Determination" to read: "The most typical package is selected by compiling for each waste package type and bin member, peak waste package temperature, and duration of boiling **on the waste package**."

II.39 (Issue QA-1 from surveillance; Section 2[a]): *The Quality Assurance section (Section 2[a]) does not identify the methods used to control the electronic management of data as required by SCI-PRO-006, Attachment 2, Section 2.*

AMR Change:

Change Section 2[a] to include the following paragraphs:

> This addendum was prepared in accordance with *Technical Work Plan for: Additional Multiscale Thermohydrologic Modeling* (BSC 2006 [DIRS 178297) and SCI-PRO-006, *Models;* IM-PRO-003, *Software Management;* SCI-PRO-004, *Managing Technical Product Inputs;* IM-PRO-002 *Control of the Electronic Control of Information*; and reviewed in accordance with SCI-PRO-003, *Document Review.*
>
> As discussed in the TWP (BSC 2006 [DIRS 178297]), the initial planning of the analysis presented herein was originally intended for a revision of the parent report. However, it was later decided to present the analysis in an addendum to the parent report. This is a deviation from the planning done in the TWP.
>
> The work scope described in this Addendum has been determined to be subject to the U.S. Department of Energy's (DOE's) *Quality Assurance Requirements and Description* (DOE 2007 [DIRS 182051]).
>
> Planning and preparation of this addendum was initiated under the Bechtel SAIC Company (BSC) Quality Assurance Program. Therefore, forms and associated documentation prepared prior to October 2, 2006, the date this work transitioned to the Lead Laboratory, were completed in accordance with BSC procedures. Forms and associated documentation executed on or after October 2, 2006, were prepared in accordance with Lead Laboratory procedures.

II.40 (Issue QA-4 from surveillance; SNL 2007 [DIRS 179466] and Table 4-1[a]): *Table 4-1[a] indicates this document contains repository emplacement-drift layout (elevations and end-point coordinates for each emplacement drift). Review of the reference revealed that this information was not directly included in the document, rather Section 4.1.1 of the reference identified other references where this information may reside (e.g., 800-IED-WIS0-01701-000-00B). This document reference was not in CDIS; it was superseded by drawing 00C. Review of revision 00C showed that endpoint coordinates and elevations were documented on the drawing. Table 4-1[a] of the AMR specifies an end-to-end waste package spacing of 0.1 m referencing Table 4-1 of the reference. The surveillance team was unable to trace this value through Table 4-1 of the reference. Table 4-1a of the AMR specifies the duration of waste package emplacement to be 23 years, referencing Table 4-2 of the reference. The surveillance team was unable to trace this value to the referenced table. The note in Figure 6-2.13[a] states "The heated repository footprint is shaded in red lines and outlined in black, as discussed in SNL 2007 [DIRS 179466]." This reference provides no discussion of the footprint though it provides a reference to a superseded IED that specifies drift elevations and end-point coordinates on which Figure 6-2.13[a] could be based. This should be clarified. Figure 6-2.1-19[a] identifies contingency drifts. The surveillance team could not trace this information to the cited reference. Drawing 800-IED-WIS0-01701-000-00C (Rev. 00B of this drawing was referenced by the source) included coordinates that encompasses these drifts, but does not delineate the specific drifts that constitute contingency drifts.*

AMR Changes:

(1) The source of the first item of Table 4-1[a] is revised to state: "The TDIP (SNL 2007 [DIRS 179466], Table 4-1) is the source for the model. This TDIP obtained the values for the elevations and end-point coordinates from 800-ED-WIS0-01701-000-00B, which is not considered an input to the model.

(2) Table 4-1[a], Page 4-6[a], under subtitle "Waste Package Heat-Generation and Ventilation Heat-Removal Efficiency: Design Information," remove (fourth row) the line pertaining to duration of waste package emplacement.

(3) Figure 6.2-19[a], page 6-21[a], add footnote to read as follows: "The drifts shown in purple are not contingency drifts per se, but are included in the MSTHM calculations to represent the contingency area."

II.41 (Issue QA-6 from surveillance; Table 4-1[a]): *Table 4-1[a] of the AMR specified 4'4" (1.321 m) as the distance from the bottom of the drift to the invert referencing Table 4-1 of the source. The surveillance team could not locate the value in Table 4-1 of the source, however 52" (4'4") was specified in Figure 4-1 of the source. Figure 4-1 of the source should be referenced for this information for enhanced traceability rather than Table 4-1 (though Table 4-1 references the entire Figure 4-1 as drawing 800-IED-MGR0-00501-000-00B. Table 4-1 should clarify that the specified drip shield length is "with overlap" and the drip shield width is an "outside" width, as indicated in the reference. Table 4-3[a] specified the bulk density of LBTM material to be 1842 kg/m3 referencing Table 4-1 of the source. The source references drawing 800-IED-MGR0-00601-000-00A (the document TMRB-2007-030 was also referenced which was not in CDIS). This drawing was superseded by Rev. 00B. Rev. 00B specifies an average bulk density of 1300 kg/m3. Therefore, the reported value was not consistent with the referenced value.*

[The average bulk density of the invert ballast listed in Table 4-3[a] is 115 lb/ft^3 (1,842 kg/m^2), which is the same value found in 800-IED-MGR0-00601-000-00B.]

AMR Change:

Table 4-1[a], last row, change "Drip shield width" to "Outside drip-shield width."

II.42 (Issue QA-7 from surveillance; p. IV-7[a]): SNL 2007 [DIRS 179394]. *Total System Performance Assessment Data Input Package for Requirements Analysis for TAD Canister and Related Waste Package Overpack Physical Attributes Basis for Performance Assessment. TDR-TDIP-ES-000006 REV 00. Las Vegas, Nevada: Sandia National Laboratories. Page IV-7[a] references Table 4-2 of the source as providing data on weight, thickness, and length of the drip shield. Table 4-2 is titled, "Surrogate TAD Canister Vessel and Internals." The table does not provide drip shield data.*

AMR Change:

Page IV-7[a], under subtitle "Waste Package and Drip Shield Thermal Properties," in second from the last paragraph, change the reference from "(SNL 2007 [DIRS 179394], Tables 4-1 and 4-2])" to "(SNL 2007 [DIRS 179354], Tables 4-1 and 4-2])."

II.43 (Issue QA-18 from surveillance; DTN: MO0702GLOBAL.000 and Figure 6.3-73[a]): *MO0702GLOBAL.000 is identified in Figure 6.3-73[a]. This DTN was not located in the ATDT, nor was it referenced anywhere else in the AMR. Should be DTN: MO0702PAGLOBAL.000.*

AMR Change:

Page 6-32[a], Figure 6.3-73[a], High/low host-rock K_{th} DTN, change to read: "MO0702PAGLOBAL.000."

II.44 (Comment No. 5 p. 5-3 Last Paragraph). *Assertion that 100m-120m is "small" compared to 300 m is not defensible. Another way to state this concern is that travel time from the repository to the water table is shortened by 30%.*

AMR Change:

The sentence is deleted from the AMR. Note that the context of this statement is that such a change in the water table will result in small changes in liquid saturation at the repository horizon. The small change in liquid-phase saturation would cause insignificant changes to repository temperature and relative humidity.

II.45 (Comment No. 9 p. 6-7 Top Lines). *This statement is counter-intuitive. The gap between waste packages represents even more longitudinal variability.*

AMR Change:

Change the sentence to read on the top lines of p. 6-7 to read: "The small end-to-end waste package spacing of 0.1 m (Table 4.1-2) used in the TSPA-LA repository design limits this longitudinal variability, because it allows effective radiation heat transfer between adjacent waste packages (Section 6.3.1.2)."

II.46 (Comment No. 47 p. 7-18 Third Bullet). *The statement pertains to distances greater than 12 m from the borehole collar. However, the same sort of scattering is also seen in Figure 7.4-4 at shorter distances. What is the explanation in that instance?*

[Note that third bullet on page 7-18 pertains specifically to lateral boreholes. As can be seen in Table 7.4-1, boreholes 139 and 143 are the only lateral boreholes for which temperature profiles are being compared. Note that Figure 7.4-4 pertains to a vertical borehole (as seen in Table 7.4-1). Consequently, the reviewer's comment in the surveillance is not relevant, since the third bullet pertains specifically to lateral boreholes.]

AMR Change:

At the end of the third bullet on page 7-18, add the following statement: "Note that Boreholes 139 and 143 are the only lateral boreholes for which temperature profiles are compared."

II. 47 (Comment No. 73 P. VI-1 Table VI-1). *Many entries in this table appear to be in error. See my attached table that shows recalculated values assuming $\varepsilon 1 = 0.63$ and $\varepsilon 2$ as shown in column 1 of Table VI-1. Should these entries turn out to be incorrect, the text on pp. VI-3,4 may have to revised accordingly.*

AMR Change:

At the end of the first sentence of the footnote to Table VI-1 (page VI-3), insert the phrase: ", and the ratio A_1/A_2 is equal to 0.457 in Eq. VI-7."

II.48 (Issue QA-9 from surveillance) *DTN SN0404T050102.011 [DIRS 169129] Thermal Conductivity of the Potential Repository Horizon, Rev. 3 Submittal date: 04/27/2004. Also used in Rev. 03 Need help tracing data in Table IV-3a[a].*

[Note that the wet and dry thermal conductivity values for the four repository horizon units (tsw33, tsw34, tsw35, tsw36, and tsw37) are obtained from DTN: MO0612MEANTHER.000, as indicated in the short footnote a on p. IV-14[a].]

AMR Change:

The long footnote will be edited to state: "The wet and dry thermal conductivity values for the four repository horizon units (tsw33, tsw34, tsw35, tsw36, and tsw37) are obtained from Output DTN: MO0612MEANTHER.000 (file: *Repository Unit Mean Kthermal.xls*, worksheet: "Summary"). The bulk density values are obtained from Table 7-10 of DTN: SN0404T0503102.011 [DIRS 169129] (files: *Tptpll1.zip*, *tptpll2.zip*, *tptpll3.zip*, *tptpln1.zip*, *tptpln2.zip*, *tptpln3.zip*, *tptpmn1.zip*, *tptpmn2.zip*, *tptpmn3.zip*, *tptpul1.zip*, *tptpul2.zip*, and *tptpul3.zip*). The bulk density values are rounded to three significant figures."

II.49 (Issue QA-10 from surveillance). *DTN GS020183351030.001 [DIRS 163107]. Uncompacted Bulk Density for Analyses Performed 02/02/00 to 05/23/00 on Potential Backfill Materials Used in the Engineered Barrier System. Submittal date: 1/22/2002. Also used in Rev. 03 Table 4-1[a] lists the bulk density of the invert as 1270 kg/m3 referencing fill zz_sep_262417.txt, Table S02025_001, rows 321-370 of the DTN. Review of the DTN showed that this data resided in GS02018335103_001_s02025_001.txt. Data were the same, but the referenced file name was different.*

AMR Change:

Change the text in Table 4-1 to read: "The source for the bulk density for crushed tuff is DTN: GS02018335103.001 [DIRS 163107], file: *gs020183351030_001_s02025_001*, txt rows 321 through 370."

II.50 (Issue QA-11 from surveillance) SNL 2007 [DIRS 179567]. *Total System Performance Assessment Data Input Package for Requirements Analysis for DOE SNF/HLW and Navy SNF Waste Package Overpack Physical Attributes Basis for Performance Assessment. TDR-TDIP-ES-000009 REV 00. Could not trace Table 4-1[a] values through this source. Tracked to superseded drawing 800-IED-WIS0-0201-000-00A. Could not find data in drawing 00B. Need to show how values were calculated from the drawing.*

AMR Change:

The text in Table 4-1[a] is changed to read: "The values for waste package mass density and specific heat are from *Total System Performance Assessment Data Input Package for Requirements Analysis for DOE SNF/HLW and Naval SNF Waste Package Physical Attributes Basis for Performance Assessment* (SNL 2007 [DIRS 179567], Table 4-1, Parameter No. 03-11, Waste Package Dimensions and Component Masses). That source obtained the values from Table 2 of Drawing 800-IED-WIS0-00801-000-00B, which is not considered an input to this model.""

II.51 (Issue QA-13 from surveillance) *DTN LB0205REVUZPRP.001 [DIRS 159525] Fracture Properties for UZ Model Layers Developed from Field Data. Submittal date: 5/14/2002. Also used in Rev. 03 ch1V1 and ch[23456]V1 data from Table IV-5[a] do not appear to match the DTN.*

AMR Change:

No change required. As discussed in Section 6.1.4 (page 6-4) of *Calibrated Properties Model* (MDL-NBS-HS-000003 REV02), fractures are absent and liquid flow occurs only through the matrix in the vitric portions of the CHn.

The following editorial corrections were identified subsequent to the surveillance, and are included here for completeness:

II.52 Page 6-40, Section 6.2.6.5, fourth sentence from the last, change to read: "This partitioning, which is taken to be 50% matrix continuum and 50% fracture continuum, has an insignificant effect on flow because conditions in these respective continua are in equilibrium within the gas-filled drift."

II.53 Page 6-40, Section 6.2.6.5, remove last paragraph that reads: "The input files require the assumptions described in Sections 5.1.1, 5.1.2, 5.2.3, 5.3.1.1, 5.3.1.2, 5.3.1.7, 5.3.1.8, 5.3.2.3, and 5.3.2.4. The process of generating the LDTH submodel material properties files is described in Appendix IV."

II.54 Page 8-9, second paragraph, first and second sentences, change to read: "Results from the FLUENT thermal model, which is the thermal model in *In-Drift Natural Convection and Condensation* (BSC 2004 [DIRS 164327]), are applied in the MSTHM to generate the in-drift effective thermal conductivity versus time relationship that captures the time-dependent influence of in-drift natural convection on the MSTHM results. Consequently, as documented in Section 7.6, there is excellent agreement between the MSTHM and FLUENT thermal model in predicting average temperature differences between the waste-package, drip-shield, and drift-wall surfaces."

II.55 The following references are added to Section 9.1:

182051 DOE (U.S. Department of Energy) 2007. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 19. Washington, D. C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20070717.0006.

181648 SNL (Sandia National Laboratories) 2007. *In-Drift Natural Convection and Condensation*. MDL-EBS-MD-000001 REV 00 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050330.0001; DOC.20051122.0005; DOC.20070907.0004.

177414 SNL 2007. *Thermal Testing Measurements Report*. TDR-MGR-HS-000002 REV 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070307.0010.

III. Inputs and/or Software

There is no change to the input values or to the software.

IV. Impact/Results and Conclusion

The errors addressed in the sections above are typographical errors and the corrected text completes the needed clarification. There is no impact to the results or conclusions of ANL-EBS-MD-000049 REV 03 AD 02. Moreover, documents that use information from ANL-EBS-MD-000049 REV 03 AD 02 as direct input (see Table 1) have been evaluated for impacts from these changes, and it has been determined that there are no impacts.

CR 11936 Evaluation

I. Background Information Summary

Condition Report 11936 documents another set of issues related to ANL-EBS-MD-000049 REV 03 AD 02 that were also identified during Lead Lab QA surveillance LQA-IS-08-002. This section presents the disposition of those issues, identifying changes to the AMR, and evaluating the impact of those changes on the conclusions of the AMR.

II. Disposition of Major Issues/ Description of Change

All of these issues are related to data qualification, as stated in CR-11936:

> An ongoing surveillance by Lead Lab QA (LQA-IS-08-002) has identified non-compliant data qualification in Addendum 1 to the multiscale AMR. The 3 data items identified were qualified for use in the AMR without having an approved plan as required by SCI-PRO-001, Section 6.1, and SCI-PRO-006, Section 6.2.1.L.3.b.

Note that the following discussions present the qualification for McAdams 1954 [DIRS 161435], Arya et al. 1999 [DIRS 176802], and Kunii and Smith 1960 [DIRS 153166]. The following criteria were used to assess the external data, consistent with the data qualification plan (Attachment 1) for each of the three sets of information:

- Data must appropriately demonstrate properties of interest.
- Data must be demonstrated to be reliable as judged by the experience of the originators and reputation of the originating organization.
- Prior uses of the data and associated verification process.
- Data must be sufficiently extensive to cover the context of this application.

II.1 (Issue QA-12 from surveillance; McAdams 1954 [DIRS 161435]): *External Source. Also used in Rev. 03 as an indirect input. Data traceability ok. The procedure in place at the time of issuance of Addendum 01 to the MultiScale Model, SCI-PRO-006 Rev. 05, required that the external source qualification be documented in an Appendix. This qualification was documented in Section 4.1.1.2[a]. Attachment 2 of SCI-PRO-001 (referenced for use in SCI-PRO-006) required that the qualification team be identified. The team was not identified in the qualification documentation. The qualification justification was adequate. Data traceability was OK.*

AMR Change:

The qualification discussion for emissivity of stainless steel obtained from McAdams (1954 [DIRS 161435]), and documented in Section 4.1.1.2[a], is revised as follows:

The emissivity for 316 stainless steel from McAdams (1954 [DIRS 161435]) is qualified for its intended use to represent the drift wall in the multiscale model (as updated in this addendum) because it is specific to the material, and directly demonstrates thermal radiation properties of interest. The monograph by McAdams (1954 [DIRS 161435]) is a prominent work in heat transfer and is listed in the McGraw-Hill Series in Chemical Engineering. The monograph was sponsored by the Committee on Heat Transmission of the National Research Council, and has been used as a source in approximately 10 other controlled project documents. This source is therefore demonstrated to be reliable as judged by the reputation of the originating authors and organization, and by prior uses of the data by other project investigators.

The emissivity value ε = 0.44 (from McAdams 1954 [DIRS 161435]) is used to represent drift openings lined with 316 stainless-steel, and is less than the value of 0.90 used in a previous version of the multiscale model for the unlined drift wall (Table 4.1-1 and Section 5.3.2.7 of the parent report). Other project documents use different emissivity values for 316 stainless steel:

- ε = 0.62 (000-00C-WIS0-03100-000-00B, Table 11)
- ε = 0.90 (ANL-EBS-MD-000030 Rev. 04, Table 6-9)
- ε = 0.92 (000-00C-WIS0-03100-000-00B, Section 6.2.7).

If the stainless steel drift lining becomes dirty or its surface is altered, the emissivity could be greater than the value qualified here. Quantitative comparison of thermal results using values of 0.44 and 0.90 (Appendix VI[a]) shows that the lower value (0.44) could overestimate the peak drip shield temperature (and by inference the peak waste package temperature) but not by more than approximately 3°C. The limited effect of drift-wall emissivity is explained because temperature differences for radiant heat transfer in the drift are proportional to the fourth root of the waste package thermal power. As discussed in the parent report (Section 6.2.13.6) variations in drift wall emissivity produce variations in drip shield temperature which are small compared to the influence of uncertainty in host-rock thermal conductivity, a dominant parameter in the multiscale model.

In summary, the emissivity value of 0.44 from McAdams (1954 [DIRS 161435]) sufficiently covers the context of its application in the multiscale model because: (1) modeling of thermal-hydrologic response in the repository drifts has limited sensitivity to this value, (2) use of a low value tends to slightly overestimate in-drift temperature, and (3) the temperature difference (between low and high values) is small compared to the temperature effect from dominant parametric uncertainties in the multiscale model.

Based on the assessment made above, data from McAdams (1954 [DIRS 161435]) are qualified for use as direct input to this report.

II.2 (Issue QA-16 from the surveillance; first item: Arya et al. 1999 [DIRS 176802]): *External source. The procedure in place at the time of issuance of Addendum 01 to the MultiScale Model, SCI-PRO-006 Rev. 05, required that the external source qualification be documented in an Appendix. This qualification was documented in Section 4.1.1.2[a]. Attachment 2 of SCI-PRO-001 (referenced for use in SCI-PRO-006) required that the qualification team be identified. The team was not identified in the qualification documentation. The qualification justification was weak, but adequate. Data traceability was OK.*

AMR Change:

The qualification discussion for the capillary retention scaling parameter of Arya et al. 1999 [DIRS 176802], as documented in Section 4.1.1.1[a], is revised as follows:

> The capillary retention scaling parameter was developed by Arya et al. (1999 [DIRS 176802]) for sand. It is used in the multiscale model for estimating capillary retention properties for the LTBM-2 invert ballast material (Appendix X[a]). The intent of the original work was estimation of capillary retention properties for granular media, which is the specific application needed for the multiscale model, so the data directly demonstrate the properties of interest.
>
> The sensitivity of in-drift thermal-hydrologic responses to the capillary properties of the invert ballast was evaluated in Section 6.3.11 of the parent report. The capillary retention scaling parameter is used to estimate retention in the intergranular porosity of the invert ballast. The LTBM-2 material has many large pores and limited water retention at repository conditions, so its physical properties (e.g., thermal conductivity) are not very sensitive to intergranular water retention, as is noted for other candidate ballast materials in Section 6.3.11. Water content in the invert ballast material is dominated by the *intragranular* retention properties, which are measured separately on samples of host rock, and are also not important to predicted invert thermal-hydrologic conditions as shown in Section 6.3.11. The multiscale model is therefore insensitive to use of the capillary retention scaling parameter (Arya et al. 1999 [DIRS 176802]) for estimating intergranular retention properties of the invert ballast (although the approach is realistic and technically appropriate). Accordingly, the data are sufficiently extensive and cover the context of the application to the multiscale model.
>
> The referenced source for the capillary retention scaling parameter in Table 4-3[a] is the article "Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media," presented in *Proceedings of the International Workshop on Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media* (Arya et al. 1999 [DIRS 176802]), which was an event held at the U.S. Salinity Laboratory in Riverside, California. The proceedings were edited by the well-known soil scientists M. Th. van Genuchten and F. J. Leij. Accordingly, this source is demonstrated to be reliable as judged by the reputation of the originating authors and organization.

Based on the assessment made above, data from Arya et al. (1999 [DIRS 176802]) are qualified for use as direct input for estimating invert ballast capillary retention properties (Appendix X[a]).

II.3 (Issue QA-16 from the surveillance; second item: Kunii and Smith 1960 [DIRS 153166]): *External source. The procedure in place at the time of issuance of Addendum 01 to the MultiScale Model, SCI-PRO-006 Rev. 05, required that the external source qualification be documented in an Appendix. This qualification was documented in Section 4.1.1.2[a]. Attachment 2 of SCI-PRO-001 (referenced for use in SCI-PRO-006) required that the qualification team be identified. The team was not identified in the qualification documentation. The qualification justification was weak, but adequate. Data traceability was OK.*

AMR Change:

The qualification discussion for the data from Kunii and Smith 1960 [DIRS 153166] used for estimating effective thermal conductivity of drift collapse rubble, documented in Section 4.1.1.3[a], is revised as follows:

The data from Kunii and Smith (1960 [DIRS 153166]) are implemented in calculations presented in Appendix X[a] and Table 4-3[a]. The predictive equation has two intrinsic parameters: β and γ. The β parameter is the ratio of the characteristic length between two neighboring solid particles divided by the particle diameter. As stated by the authors, the value will range from 0.9 to 1.0 for almost all packed beds. A value of 1.0 is selected for analysis representing loose or open packing, which is appropriate for collapse rubble. The γ parameter is the ratio of the effective thickness of the fluid (air) film adjacent to the surface of two solid particles divided by particle diameter. This ratio is set to 0.67 for spherical particles, consistent with its use by the authors (Kunii and Smith 1960 [DIRS 153166], p. 72).

The predictive equation and the β and γ parameters from Kunii and Smith (1960 [DIRS 153166], p. 72) are specific to aggregate materials such as the collapse rubble, with considerable uncertainty associated with particle size and shape, as represented in the high and low rubble conductivity cases developed in Appendix X[a]. Thus the data appropriately demonstrate the properties of interest. They are applied in a manner that propagates the uncertainty attendant to rubble properties, and so are sufficiently extensive to cover the context of the application.

The data are published in the peer-reviewed scientific journal *American Institute of Chemical Engineers Journal*, which has been in publication since 1955. The authors have published other articles on thermal property estimation for particulate media, including corroborative experimental measurements (e.g., Yagi and Kunii 1957 [DIRS 170330]). The estimation approach has also been used in other project reports (e.g., BSC 2004 [DIRS 170033]) using the same parameter values. This source is therefore demonstrated to be sufficiently reliable based on the reputation of the authors and of the journal publication, and on the prior uses of the data by other project investigators.

Based on the assessment made above, the data from Kunii and Smith (1960 [DIRS 153166]) are qualified for use as direct input to this report.

III. Inputs and/or Software

There is no change to the input values or to the software.

IV. Impact/Results and Conclusion

Typographical errors have been corrected and clarifications provided (CR-11935). Data qualification has been documented consistent with the applicable implementing procedures (CR-11936). There is no impact from these changes to the results or conclusions of the subject AMR. Other documents which use information from the subject AMR as direct input, as indicated in Table 1, were also evaluated and found not to be impacted.

Table 1. Product Documents Evaluated to Determine Impact of Changes

CAL-DS0-NU-000001 REV 00A	STEADY-STATE CRITICALITY CONSEQUENCE MODEL REPORT
CAL-MGR-NU-000012 REV 0A	PROBABILITY OF POSTCLOSURE CRITICALITY
ANL-WIS-PA-000001 REV 02	EBS RADIONUCLIDE TRANSPORT ABSTRACTION
ANL-EBS-PA-000002 REV 05	SCREENING OF FEATURES, EVENTS, AND PROCESSES IN DRIP SHIELD AND WASTE PACKAGE DEGRADATION
ANL-WIS-PA-000002 REV 05	ENGINEERED BARRIER SYSTEM FEATURES, EVENTS, AND PROCESSES
ANL-EBS-GS-000002 REV 01	GEOCHEMISTRY MODEL VALIDATION REPORT: EXTERNAL ACCUMULATION MODEL
000-3DR-MGR0-00100-000-006 REV 00	PROJECT DESIGN CRITERIA DOCUMENT
TDR-MGR-MD-000037 REV 01	POSTCLOSURE MODELING AND ANALYSES DESIGN PARAMETERS
ANL-EBS-MD-000075 REV 01	THERMAL MANAGEMENT FLEXIBILITY ANALYSIS
TDR-TDIP-ES-000006 REV 00	TOTAL SYSTEM PERFORMANCE ASSESSMENT DATA INPUT PACKAGE FOR REQUIREMENTS ANALYSIS FOR TRANSPORTATION AGING AND DISPOSAL CANISTER AND RELATED WASTE PACKAGE PHYSICAL ATTRIBUTES BASIS FOR PERFORMANCE ASSESSMENT
TDR-TDIP-ES-000009 REV 00	TOTAL SYSTEM PERFORMANCE ASSESSMENT DATA INPUT PACKAGE FOR REQUIREMENTS ANALYSIS FOR DOE SNF/HLW AND NAVAL SNF WASTE PACKAGE PHYSICAL ATTRIBUTES BASIS FOR PERFORMANCE
ANL-NBS-HS-000057 REV 00	POSTCLOSURE ANALYSIS OF THE RANGE OF DESIGN THERMAL LOADINGS
ANL-DS0-NU-000001 REV 00	SCREENING ANALYSIS OF CRITICALITY FEATURES, EVENTS, AND PROCESSES FOR LICENSE APPLICATION
ANL-WIS-MD-000024 REV 01	POSTCLOSURE NUCLEAR SAFETY DESIGN BASES
ANL-WIS-MD-000027 REV 00	FEATURES, EVENTS, AND PROCESSES FOR THE TOTAL SYSTEM PERFORMANCE ASSESSMENT: ANALYSES
CAL-DN0-NU-000002 REV 00C	WASTE PACKAGE FLOODING PROBABILITY EVALUATION

Attachment 1. Qualification Plan for Data Items Identified in CR-11936

Data Qualification Plan

Complete only applicable items.

QA: QA

Page 1 of 1

Section I. Organizational Information

Qualification Title

1. The capillary retention scaling parameter from Arya et al. (1999 [DIRS 176802])
2. The emissivity of stainless steel from McAdams (1954 [DIRS 161435]), and
3. The β and γ parameters from Kunii and Smith (1960 [DIRS 153166], p. 72

Requesting Organization

Sandia National Laboratories, Lead Lab

Section II. Process Planning Requirements

1. List of Unqualified Data to be Evaluated

1. Arya, L.M.; Leij, F.J.; and van Genuchten, M.Th. 1999. "Relationship Between Particle-Size Distribution and Soil Water Retention." *Proceedings of the International Workshop on Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part 2, Riverside, California, October 22-24, 1997.* van Genuchten, M.Th.; Leij, F.J.; and Wu, L., eds. Pages 931-946. Riverside, California: University of California. TIC: 247322.
2. McAdams, W.H. 1954. *Heat Transmission.* 3rd Edition. New York, New York: McGraw-Hill. TIC: 242359.
3. Kunii, D. and Smith, J.M. 1960. "Heat Transfer Characteristics of Porous Rocks." *American Institute of Chemical Engineers Journal, 6,* (1), 71-78. New York, New York: American Institute of Chemical Engineers. TIC: 249321.

2. Type of Data Qualification Method(s) [Including rationale for selection of method(s) (Attachment 3) and qualification attributes (Attachment 4)]

The method for qualification of all the external sources of data is the "Technical Assessment".

3. Data Qualification Team and Additional Support Staff Required

Thomas Buscheck (Chairman), and
Ernest Hardin

4. Data Evaluation Criteria

1. The extent to which the data demonstrate the properties of interest (e.g., physical, chemical, geologic, mechanical).
2. Prior uses of the data and associated verification processes.
3. Data must be demonstrated to be reliable as judged by the experience of the originators and reputation of the originating organization.
4. Data must be sufficiently extensive to cover the context of this application.

5. Identification of Procedures Used

SCI-PRO-006, *Models*

6. Plan coordinated with the following known organizations providing input to or using the results of the data qualification

No other organizations presently use the information to be qualified (Natural Systems, In-Package/Waste Form, TSPA/EBS Transport, Engineered Systems). Other LA-supporting models use emissivity values for SS316 (e.g., 0.62 from 000-00C-WIS0-03100-000-00B, Table 11) and for the drift wall (0.90 from ANL-EBS-MD-000030 Rev. 04, Table 6-9; also 0.92 from 000-00C-WIS0-03100-000-00B, Section 6.2.7). Note that the use of 0.44 instead of a larger value (0.90 was used in the previous version) for the drift wall in the multiscale model slightly overestimates drip shield temperature, as addressed in ANL-EBS-MD-000049 Rev. 03 AD02, Appendix VI[a].

Section III. Approval

Qualification Chairperson Printed Name	Qualification Chairperson Signature	Date
Thomas A. Buscheck	*Thomas A. Buscheck*	5/28/2008
Responsible Manager Printed Name	**Responsible Manager Signature**	**Date**
Paul R. Dixon	*Paul*	5-28-08

SCI-PRO-001.1-R1