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Appendix E
FCT Document Cover Sheet

Name/Title of Deliverable/Milestone: Parameter Uncertainty for Repository Thermal Analysis

Work Package Title and Number: FT-12SN080403 Disposal Research – Design Concepts & Thermal Load Management

Work Package WBS Number: 1.2.08.04 Milestone Number: M4FT12SN0804033

Responsible Work Package Manager

Ernest Hardin EHardin 18April2012

(Name/Signature) (Date Submitted)

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This deliverable was prepared in accordance with Sandia National Laboratories

(Participant/National Laboratory Name)

QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1-2000 ☐ Other:

This Deliverable was subjected to:

☒ Technical Review ☐ Peer Review

Technical Review (TR) **Review Documentation Provided**	**Peer Review (PR)** **Review Documentation Provided**
☐ Signed TR Report, or TR Report No.:	☐ Signed PR Report, or PR Report No.:
☐ Signed TR Concurrence Sheet (attached), or	☐ Signed PR Concurrence Sheet (attached), or
☒ Signature of TR Reviewer(s) below	☐ Signature of PR Reviewers below

Name and Signature of Reviewers

Robert MacKinnon

Robert MacKinnon 04/18/12

(Name/Signature) (Date)

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Parameter Uncertainty for Repository Thermal Analysis

Fuel Cycle Research & Development

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Parameter Uncertainty for Repository Thermal Analysis

Deliverable M4FT-12SN0804033
Work Package FT-12SN080403

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Summary

This report describes three contributions to analysis of uncertainty in maximum repository (peak waste package surface) temperatures:

- Analytical description of overall variance in temperature, as a function of contributions from key parameters of the analytical solution used in previous temperature analyses.
- Compilation of literature data on key parameter values, for various geologic host media and clay-based buffer materials, drawing on international work.
- Correlation between maximum repository temperature and waste package power at emplacement, which is strong even for different combinations of waste package size, SNF burnup, and fuel age.

Results from the analytical treatment of temperature variance include the following:

- Temperature at all times is relatively insensitive to heat capacitance (volumetric heat capacity) given the state of knowledge represented by the assigned parameter variance.
- Buffer thermal conductivity is an important parameter in early time (except for disposal concepts that have no buffer), but the ratio of buffer radius to waste package radius may be a more important parameter depending on how much it is allowed to vary in developing a disposal concept.
- Host rock thermal conductivity is the most important input parameter, especially at later time (e.g., greater than 10 years after emplacement) and where buffers are not used.

Compilation of literature data and selection of uncertainty ranges provide mean and $\pm 1\sigma$ property values for temperature uncertainty analysis based on the analytical solution.

Finally, the study of maximum (peak waste package surface) temperature corroborates earlier findings from FEM simulations of the generic salt repository. Thus the waste package heat output can be used to predict maximum temperature, to a good approximation, for all host media, waste package sizes, SNF burnup, and decay storage duration cases considered.

Revision History

29 March 2012	Draft milestone M4FT-12SN0804033 (internal use only)
FCRD-UFD-2012-000097 Rev. 0, 06April2012	Reviewed and approved for unlimited release (Sandia programmatic review).

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Acronyms

BWR	Boiling-Water Reactor
DOE	U.S. Department of Energy
EBS	Engineered Barrier System
EDZ	Excavation Damage Zone
FEM	Finite Element Method
FY	Fiscal Year
GW-d	Gigawatt-Days
HLW	High Level (Radioactive) Waste
LWR	Light Water Reactor
MT	Metric Ton
MTHM	Metric Tons of Heavy Metal
OCRWM	Office of Civilian Radioactive Waste Management (DOE)
PWR	Pressurized Water Reactor
R&D	Research and Development
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
TAD	Transport/Aging/Disposal
THMC	Thermal-Hydrologic-Mechanical-Chemical
UFD	Used Fuel Disposition
UNF	Used Nuclear Fuel
UOX	Uranium Oxide Fuel
WP	Waste Package
YM	Yucca Mountain

Parameter Uncertainty for Repository Thermal Analysis

1. Introduction

This report is one follow-on to a study of reference geologic disposal design concepts (Hardin et al. 2011a). Based on an analysis of maximum temperatures, that study concluded that certain disposal concepts would require extended decay storage prior to emplacement, or the use of small waste packages, or both. The study used nominal values for thermal properties of host geologic media and engineered materials, demonstrating the need for uncertainty analysis to support the conclusions. This report is a first step that identifies the input parameters of the maximum temperature calculation, surveys published data on measured values, uses an analytical approach to determine which parameters are most important, and performs an example sensitivity analysis. Using results from this first step, temperature calculations planned for FY12 can focus on only the important parameters, and can use the uncertainty ranges reported here.

The survey of published information on thermal properties of geologic media and engineered materials, is intended to be sufficient for use in generic calculations to evaluate the feasibility of reference disposal concepts. A full compendium of literature data is beyond the scope of this report. The term “uncertainty” is used here to represent both measurement uncertainty and spatial variability, or variability across host geologic units. For the most important parameters (e.g., buffer thermal conductivity) the extent of literature data surveyed samples these different forms of uncertainty and variability. Finally, this report is intended to be one chapter or section of a larger FY12 deliverable summarizing all the work on design concepts and thermal load management for geologic disposal (M3FT-12SN0804032, due 15Aug2012).

2. Analytical Sensitivity

The purpose of this analysis is to determine the relative contribution of variance in each key parameter to overall variance in temperature, as calculated with the analytical method from the FY11 report (Hardin et al. 2011a, Section 5). A classical analysis-of-variance approach is used for thermal conductivity, heat capacity, and buffer radius ratio parameters, while a direct approach is used for sensitivity to initial waste heat output. In the classical approach, variance in key parameters and in overall temperature, is evaluated for parameter values in the local vicinity of solutions used to represent each reference disposal concept (i.e., this is not a global variance analysis). This limitation is appropriate because the purpose of this analysis is to gain insight on generic disposal concepts, where each input parameter can be considered separately and the parameters are uncorrelated. For a particular site, other approaches such as Monte Carlo sampling could be used with more definitive parameter support (e.g., separately quantified spatial variability).

The direct approach is described in Section 5, and is used to show the correlation between maximum temperature and waste package power at emplacement (taking into account the form of the thermal decay function). Such correlations for SNF disposal in each host medium are developed for use in system studies that impose thermal power limits on SNF packaging, storage, transport, or disposal.

2.1 Analytical Derivation of Temperature Sensitivity

A simplified model is used for uncertainty analysis, that represents both the transient and steady-state parts of the analytical model from the FY11 report. The transient part is represented using an analytical line-source solution (Hardin et al. 2011a, Section G.3) and the steady-state part is represented by adding the same axisymmetric function (Section G.4). This approach departs from the full solution documented in the FY11 report, only with respect to the difference between an infinite line source, and a finite line source plus an array of point sources. For this analysis heating from adjacent drifts is less important for peak near-field temperatures that occur in the first few years after waste emplacement (Hardin et al. 2011a; comparing the sum of the central package and adjacent package contributions, to the adjacent drift contributions in Figures 5.3-3 and 5.3-4). Whereas the model developed in the FY11 report used multiple annular layers to represent the EBS (Hardin et al. 2011a, Figures 5.1-1, and 5.1-3 through 5.1-6), the simplified model used here uses a single annular layer to address the impact of an uncertain thermal resistance (e.g., dominated by a clay buffer) on the total variance for temperature. The simplified model for temperature T as a function of radius r (with $r = r_2$) and time t, to be used for parameter uncertainty analysis, has the form:

$$T(t) = T_{amb} + \frac{Q(t)}{2\pi K_{buf}} \ln\left(\frac{r_2}{r_1}\right) + \int_0^t \frac{Q(\tau)}{4\pi K_{rock}(t-\tau)} e^{\frac{-r_2^2 \rho C_p}{4K_{rock}(t-\tau)}} d\tau \qquad \text{Eqn. 1}$$

where K_{rock} = rock thermal conductivity (W/m-K)
ρC_p = rock heat capacitance (volumetric heat capacity; J/m^3-K)
K_{buf} = buffer thermal conductivity (W/m-K)
$Q(t)$ = the line source strength (W/m)
r_1 = waste package radius (m)
r_2 = buffer radius (m)
T_{amb} = the ambient (far-field) rock temperature (°C)

The line-source temperature at radius r_2 (outer radius of the buffer, or alternatively, the interface between the EBS and the host rock) represented by the third term on the right-hand side of Equation 1, is increased by the second term to account for heat conductance across a simple single-layer annular buffer. Additional layers could be added to the engineered barriers between the waste package and the rock, such as a metallic liner or envelope, but metallic layers have little effect on peak waste package surface temperature because they are thin and have high thermal conductivity. The overall variance of *T(t)* is given by (Hahn and Shapiro (1967, p. 231):

$$Var\{T(t)\} = \sum_{i=1}^{n} \left(\frac{\partial T}{\partial z_i}\right)^2 Var\{z_i\} \qquad \text{Eqn. 2}$$

where there are n parameters z_i. Analytical expressions for $\frac{\partial T}{\partial z_i}$ were symbolically calculated using MathCad14®, with respect to parameters K_{rock}, K_{buf}, ρC_p, and r_2/r_1. The calculation point for maximum temperature is selected as the waste package wall, as it was for the FY11 analysis, because package contents can withstand higher temperatures than the ex-container engineered materials, particularly clay buffers. Spent fuel zirconium alloy cladding can withstand 350°C for indefinite (postclosure) duration (BSC 2008a, Section 11.2). Following the methodology outlined by BSC (2008b, Section 6.1.6) for 21-PWR transport-aging-disposal (TAD) canisters, fuel cladding will not exceed 350°C even for waste package surface temperatures up to approximately 300°C. The highest waste package surface temperature considered in this body of work is 250°C as discussed for the salt repository (Hardin et al. 2011a, Section 4.1.1.2).

Materials outside the waste package (clay-based buffer, intact clay/shale, crushed salt backfill, intact salt, etc.) have maximum allowable temperatures (e.g., 100°C or possibly higher for clay buffers, 200°C for crushed salt; see Hardin et al. 2011a) that are less than the limit on waste package wall temperature associated with package contents. These materials are therefore limiting for management of waste heat after emplacement.

Framing parameter uncertainty as a variance analysis for this model, incorporates not only the functional dependence $\frac{\partial T}{\partial z_i}$ but also the range of variability for key parameters, expressed in $Var\{z_i\}$. Values for $Var\{z_i\}$ are estimated in the next section using ranges reported in the literature for similar materials.

With the addition of open modes to the portfolio of reference disposal options, thermal analysis must account for the heat removed by preclosure ventilation, and radiative heat transfer across gaps whenever ventilation is not effective. During ventilation, heat removal decreases the power dissipated to the waste package surroundings by as much as a factor of 6 (BSC 2004) so there is no possibility of exceeding near-field temperature limits for normal operation. (Off-normal operations are beyond the scope of this report.) For heat transfer across gaps, the effect is similar to a high effective thermal conductivity (r.g., see BSC 2004, Equation 6-53).

Selection of the ratio r_2/r_1 is based on the idea that buffer size (r_2) would be selected after waste package size (r_1). For the four key parameters K_{rock}, K_{buf}, ρC_p, and r_2/r_1 of the model (Equation 1) the derivatives comprising the right-hand side of Equation 2 are represented by:

$$\frac{d}{dKrock}T(t) = \int_0^t \frac{e^{\frac{\rho Cp\cdot(r_2)^2}{4\cdot Krock\cdot(\tau-t)}}\cdot Q(\tau)}{4\cdot\pi\cdot Krock^2\cdot(\tau-t)} + \frac{\rho Cp\cdot(r_2)^2\cdot e^{\frac{\rho Cp\cdot(r_2)^2}{4\cdot Krock\cdot(\tau-t)}}\cdot Q(\tau)}{16\cdot\pi\cdot Krock^3\cdot(\tau-t)^2}\,d\tau \qquad \text{Eqn. 3}$$

$$\frac{d}{dKbuff}T(t) = \cdot -\frac{\ln\left(\frac{r_2}{r_1}\right)\cdot Q(\tau)}{2\cdot\pi\cdot Kbuff^2} \qquad \text{Eqn. 4}$$

$$\frac{d}{d\rho Cp}T(t) = \int_0^t -\frac{\left(r_2\right)^2\cdot e^{\frac{\rho Cp\cdot\left(r_2\right)^2}{4\cdot Krock\cdot(\tau-t)}}\cdot Q(\tau)}{16\cdot\pi\cdot Krock^2\cdot(\tau-t)^2}\,d\tau \qquad \text{Eqn. 5}$$

$$\frac{d}{dr2r1}T(t) = \cdot\frac{Q(\tau)}{2\cdot\pi\cdot Kbuf\cdot r2r1} + \int_0^t -\frac{\left(r_2\right)^2\cdot\rho Cp\cdot e^{\frac{\left(r_2\right)^2\cdot\rho Cp}{4\cdot Krock\cdot(\tau-t)}}\cdot Q(\tau)}{8\cdot\pi\cdot Krock^2\cdot(\tau-t)^2}\,d\tau \qquad \text{Eqn. 6}$$

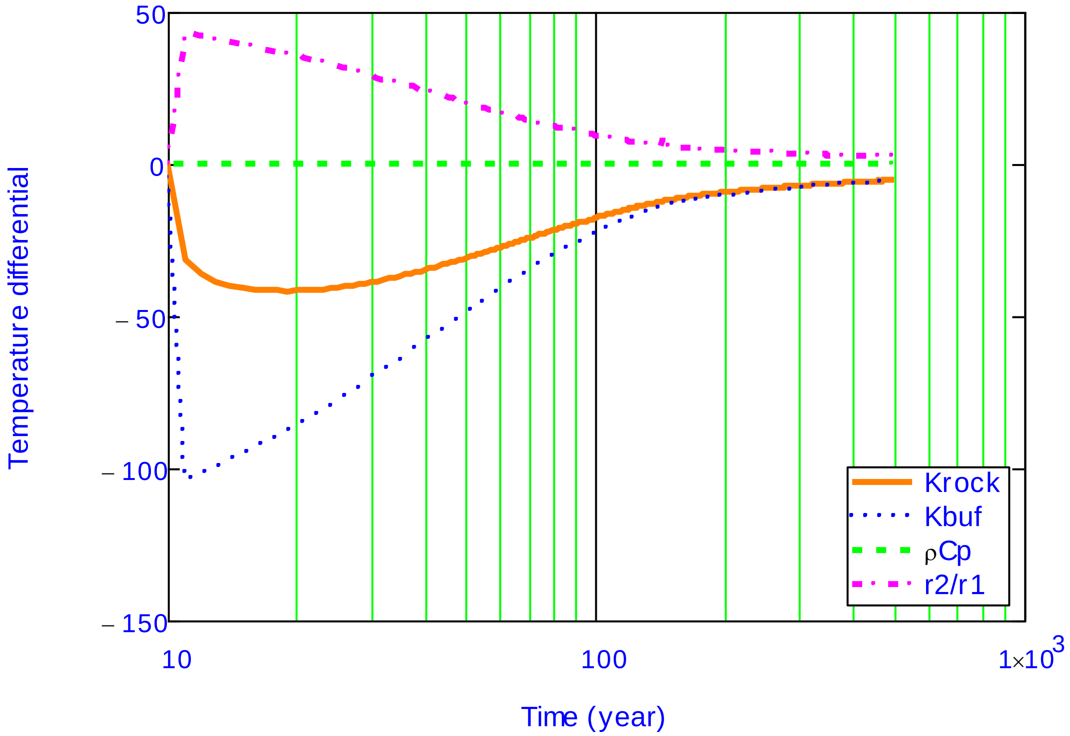
where parameter r2r1 represents r_2/r_1. Note that the derivative expressions above are presented in MathCad® syntax as total derivatives, whereas Equation 2 is written with partials. The distinction is not meaningful here because the parameters of interest as applied here are essentially independent, uniform (within the domains where they apply), and not time-varying (e.g., K_{buf} is an effective value). Thus, the two types of derivatives are equivalent for this analysis.

Each of the expressions above (Equations 3 through 6) contains an integral which is the convolution of the thermal decay function and must be evaluated numerically. The results from applying these derivatives are presented below as the unnormalized magnitudes of the differentials $\frac{\partial T}{\partial z_i}$ (Figure 1). The differentials with respect to thermal conductivities of the rock and buffer are negative, as expected, while the differential with respect to r_2/r_1 is positive, and that with respect to ρC_p is close to zero. Because these curves are unnormalized and therefore have different dimensions, they cannot be compared directly in magnitude. The variance approach outlined above is used in Section 4 below to facilitate direct comparison.

The above discussion does not consider uncertainty on the heat input, i.e., the line source strength *Q(t)*. Uncertainty in heat output from SNF or HLW is related to uncertainty in composition, particularly the major heat-producing fission products (Cs-137 and Sr-90) and actinides such as Am-241. Whereas uncertainty in heat output of SNF assemblies is possible, it is not treated as parametric uncertainty here because it is relatively small compared to that associated with other parameters such as clay buffer characteristics and host rock thermal conductivity. Also, the uncertainty for a waste package containing multiple assemblies decreases statistically, to the extent that the variability among assemblies is uncorrelated. The potential effects of uncertainty in waste package heat output on maximum temperature can be readily visualized using the correlations developed in Section 5.2.

3. Parameter Uncertainty Ranges

This section presents a limited survey of literature data for Krock and ρCp, specific to crystalline rock, clay/shale media, salt, and alluvium. It also reviews literature data for Kbuf, for clay buffer materials and other engineered materials. The important result of these reviews is a set of low-high ranges for each parameter, for each host medium. Treating the reported literature data as samples from populations of independent data, the sample mean and sample standard deviation were calculated (Tables 1 though 4).



Note: For the case of crystalline host rock, 4-PWR waste packages (0.66 m diameter), 0.35 m buffer thickness, and SNF with 40 GW-d/MT burnup (10 yr out-of-reactor). For buffer thermal conductivity the average of dry and hydrated values was used.

Figure 1. Unnormalized (dimensional) Partial Derivatives of Temperature at the Waste Package Surface with Respect to Key Model Parameters (K_{rock}, K_{buf}, ρC_p, and r_2/r_1), for the Crystalline Rock SNF Disposal Reference Case.

The estimated sample statistics are useful to describe the uncertainty in these key parameters, subject to limitations because the literature data were not all produced the same way, have associated measurement errors or biases, and in some instances the data are sparse. Accordingly, a range selection is also provided, rounding the estimates (mean ± standard deviation) up or down, consistent with qualitative indications of the reproducibility and stability in reported data of each type. The adjusted estimate of the standard deviation is then half the selected range, and the estimated parameter variance for use in this study is the square of the standard deviation.

3.1 Host Rock Thermal Conductivity

Thermal conductivity for the different host geologic media are shown in Table 1, derived from a collection of literature (much of which is related to geologic disposal of heat-generating waste). Some of the sources have provided ranges, and the endpoints are treated as separate estimates thereby assigning twice the weight to these sources.

Granite and other crystalline rocks (metamorphic or igneous) have small porosity, and thermal conductivity is not sensitive to the state of moisture saturation. Hence, the values used here do not distinguish saturation state. The calculated standard deviation of K_{rock} is 0.37, but the selected range (representing $\pm 1\sigma$) has a width of 0.8 allowing for some unknown variations in porosity, saturation, measurement method, spatial variability, etc. The variance $Var\{K_{rock}\}$is estimated from the square of the estimated standard deviation ($0.37^2 = 0.14$, units of $(\text{W/m-K})^2$).

For clay and shale media the range is broader reflecting the incorporation of indurated shales and non-indurated plastic clays. Also, the parallel and perpendicular orientations are lumped together, which is appropriate for a temperature solution for isotropic media (the estimates could be split for anistropy calculations). For in situ or intact measurements on these materials, the moisture content is assumed to be close to undisturbed conditions, so the values here do not distinguish saturation state. The excavation damage zone (EDZ) measurement of Johnson et al. (2002) is included, but falls near the middle of the selected range.

For salt two thermal conductivity ranges are selected, for 100°C and 200°C. Only one value for 200°C is presented here (model based, supported by experimental data) so the standard deviation from the 100°C data is used for the 200°C case. Salt has low porosity and moisture content so thermal conductivity is not sensitive to the state of moisture saturation.

Alluvium has high porosity (on the order of 30% or greater) and volumetric (total) moisture content from approximately 5% to 20% (i.e., moisture saturation up to 70% or greater). Accordingly, two ranges are presented for in situ or unsaturated conditions, and for wet or saturated conditions. Only data for naturally consolidated (not re-consolidated) samples or in situ measurements are presented. The unsaturated data are recommended for use with the unsaturated, sedimentary disposal concept, although the “wet” or saturated data could be used with justification.

Finally, no literature data survey is provided for the crystalline basement host medium. This is a somewhat generic category of rock types so a wide range of igneous and metamorphic rock types is possible. Importantly, the FY11 analysis (Hardin et al. 2011a, Section 5) showed that maximum temperatures for the deep borehole concept would be relatively low because of the small diameter and limited waste content of the canisters. Further, no temperature limits were identified, so the uncertainty in basement rock thermal conductivity does not appear to be a significant factor, and no analysis is provided here.

3.2 Engineered Material Thermal Conductivity

Thermal conductivity for clay buffer materials described in the geologic disposal literature, and for metals and alloys used in waste packages, are presented in Table 2. Thermal properties of dry and hydrated bentonite clay-based buffer materials are well studied. Dry and hydrated data are separated in Table 2, and the modeling strategy should determine the state of the buffer for which maximum temperatures are calculated. An intermediate value was used in previous analysis (Hardin et al. 2011a, Section 5.3.2) subject to verification by modeling or experiment.

The results for metals and alloys show that the range of uncertainty is small for all materials except stainless steels, which exhibit variation with differences in type and composition. Regardless, thermal conductivities for all these materials are great enough, and thickness small enough, that they have no significant impact on maximum temperatures (even if used in the engineered barrier system outside of the waste package, such as for liners).

3.3 Host Rock Heat Capacity

Heat capacitance (volumetric heat capacity) for the different host geologic media are shown in Table 3. A somewhat different approach was used for range selection, to allow for additional uncertainty due to saturation and compositional differences, and more direct comparison of the different media. The ranges use the estimated sample mean as the midpoint, and are guided by the calculated standard deviations. For low porosity salt and granite, a ±5% range is selected, while for clay/shale and alluvium, ranges of ±15% and ±20% are selected, respectively. For the crystalline basement (deep borehole) a range of ±10% is assumed.

3.4 Waste Package and Buffer Size

The buffer size ratio parameter r_2/r_1 is an engineering detail and not a material physical property. However, it is shown by this report to be an important parameter in the uncertainty of maximum temperature predictions, and a “variance” is estimated to reflect the need for flexibility in the engineering details of disposal concepts. As shown in Table 4, the variance is approximated using a ±50% range about a nominal buffer thickness ($r_2 - r_1$), for a range of waste package sizes (r_1).

The open-mode data in Table 4 are suitable for use in calculations that involve pre-closure ventilation (reducing $Q(t)$) followed by cessation of forced ventilation at or before repository closure, and either: 1) installation of a backfill around the waste packages, or 2) leaving the air space open around the waste packages. In the first instance, the temperatures after backfilling can be calculated using a model that includes the backfill even during preclosure ventilation, but adjusts $Q(t)$ to account for ventilation heat removal (this is consistent with the model in Equation 1 because the annular EBS term is steady-state). The point of temperature calculation may be chosen at the waste package surface, to limit the maximum temperature of the engineered backfill. In the second instance, the backfill is replaced by an effective thermal conductivity for the air space throughout the calculation. This is a good approximation because the thermal resistance of an air gap is much lower than backfill or buffer material (effective K_{th} much greater than buffer conductivity K_{buf}). In this second instance the point of temperature calculation may be selected at the rock wall or the waste package depending on which is limiting.

3.5 Summary

Key parameters (K_{rock}, K_{buf}, ρC_p, and r_2/r_1) were identified for an analytical solution for repository temperatures, that represents the analysis approach used in the FY11 report (Hardin et al. 2011a). Literature data were compiled (Tables 1 through 3) and uncertainty ranges selected for different host geologic media and for clay-based buffers. The buffer radius ratio (expressed as r_2/r_1) was similarly described using ±50% variation around the reference values (Table 4; reference values from Hardin et al. 2011a). The results consisting of average and low, high ($\pm 1\sigma$) values for each parameter, are intended for use in temperature uncertainty analyses using calculation approaches based on Equation 1.

Parameter ranges for K_{rock}, K_{buf}, ρC_p, and r_2/r_1 from Section 2 are converted to estimates of variance representing for host media, and clay-based buffers, using the range endpoints as estimates of $\pm 1\sigma$ values. The sample variance is then estimated from

$$Var\{z_i\} \approx \left[\frac{\left(Range_{high} - Range_{low} \right)_i}{2} \right]^2 \qquad \text{Eqn. 7}$$

The resulting sample variance estimates for the key parameters K_{rock}, K_{buf}, ρC_p, and r_2/r_1, along with the nominal values of these parameters for reference disposal concepts, are summarized in Table 5.

Table 1. Host Rock Thermal Conductivity Ranges and Parameter Variance

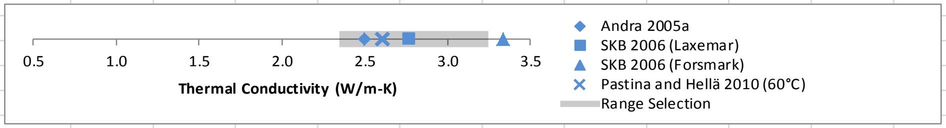
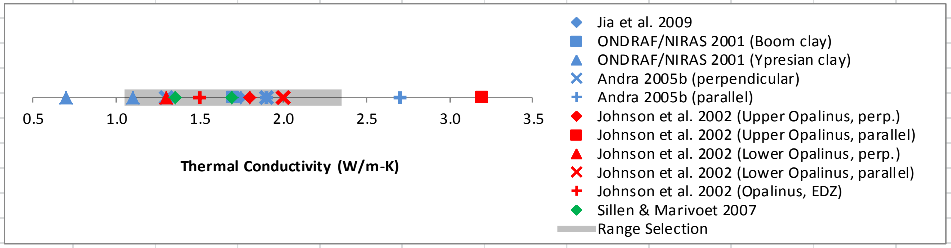
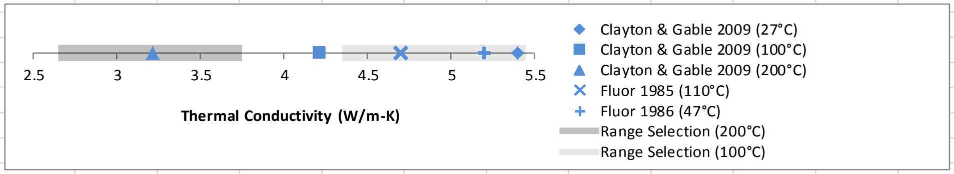
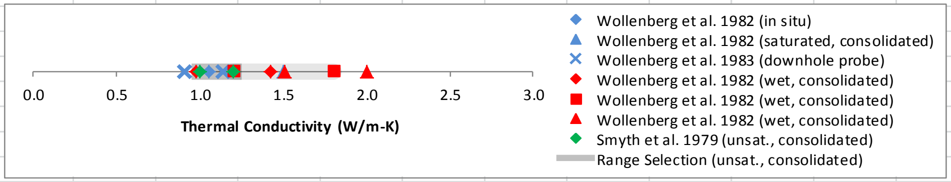
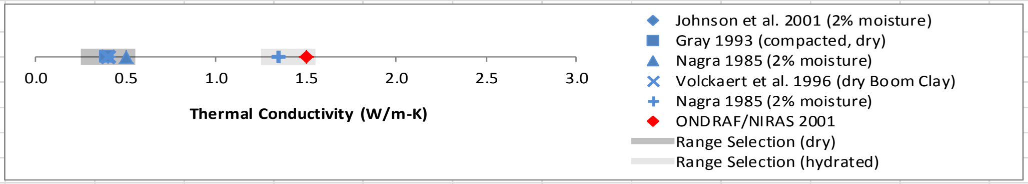
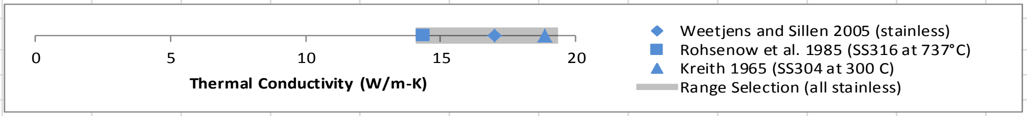
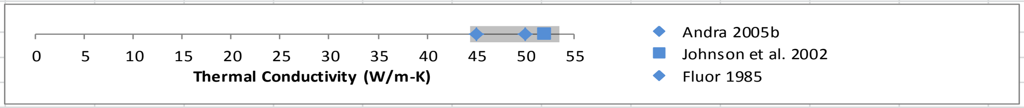
Host Rock Thermal Conductivity					
Low	**High**	**Source**	**Average**	**Std. Dev.**	
Granite					
2.50		Andra 2005a	2.81	0.37	
2.77		SKB 2006 (Laxemar)			
3.34		SKB 2006 (Forsmark)			
2.61		Pastina and Hellä 2010 (60°C)			
2.4	3.2	Range Selection			
Clay/Shale					
1.75		Jia et al. 2009	1.73	0.61	
1.70		ONDRAF/NIRAS 2001 (Boom clay)			
0.70	1.1	ONDRAF/NIRAS 2001 (Ypresian clay)			
1.3	1.9	Andra 2005b (perpendicular)			
1.9	2.7	Andra 2005b (parallel)			
1.8		Johnson et al. 2002 (Upper Opalinus, perp.)			
3.2		Johnson et al. 2002 (Upper Opalinus, parallel)			
1.3		Johnson et al. 2002 (Lower Opalinus, perp.)			
2.0		Johnson et al. 2002 (Lower Opalinus, parallel)			
1.5		Johnson et al. 2002 (Opalinus, EDZ)			
1.35	1.69	Sillen & Marivoet 2007			
1.1	2.3	Range Selection			
Salt					
5.4		Clayton & Gable 2009 (27°C)	4.88	0.53	
4.2		Clayton & Gable 2009 (100°C)			
4.7		Fluor 1985 (110°C)			
5.2		Fluor 1986 (47°C)			
3.2		Clayton & Gable 2009 (200°C)	3.21	0.53	
4.4	5.4	Range Selection (100°C)			
2.7	3.7	Range Selection (200°C)			
Alluvium					
1.05		Wollenberg et al. 1982 (in situ)	1.06	0.11	
0.91	1.14	Wollenberg et al. 1983 (downhole probe)			
1.0	1.2	Smyth et al. 1979 (unsat., consolidated)			
1.0	1.2	Range Selection (unsat., consolidated)			
0.98	1.42	Wollenberg et al. 1982 (wet, consolidated)	1.49	0.34	
1.21	1.81	Wollenberg et al. 1982 (wet, consolidated)			
1.51	2	Wollenberg et al. 1982 (wet, consolidated)			
1.5		Wollenberg et al. 1982 (saturated, consolidated)			
1.2	1.8	Range Selection (saturated, consolidated)			
Crystalline Basement					
3.0		Brady et al. 2009			No temperature limits identified for deep borehole disposal concept (Hardin et al. 2011).

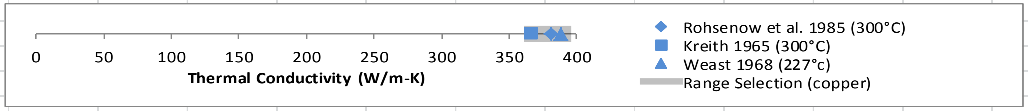
Table 2. Engineered Material Thermal Conductivity Ranges and Parameter Variance

Engineered Material Thermal Conductivity				
Low	**High**	**Source**	**Average**	**Std. Dev.**
Clay Buffer (compacted)				
0.4		Johnson et al. 2001 (2% moisture)	0.42	0.05
0.39		Gray 1993 (compacted, dry)		
0.5		Nagra 1985 (2% moisture)		
0.4		Volckaert et al. 1996 (dry Boom Clay)		
0.3	**0.5**	Range Selection (dry)		
1.35		Nagra 1985 (2% moisture)	1.43	0.11
1.5		ONDRAF/NIRAS 2001		
1.3	**1.5**	Range Selection (hydrated)		
Stainless Steel				
17.0		Weetjens and Sillen 2005 (stainless)	16.7	2.26
14.4		Rohsenow et al. 1985 (SS316 at 737°C)		
18.9		Kreith 1965 (SS304 at 300 C)		
14.4	**19**	Range Selection (all stainless)		
Carbon Steel				
50.0		Andra 2005b	49.0	3.61
52.0		Johnson et al. 2002		
45.0		Fluor 1985		
45.4	**52.6**	Range Selection (carbon steel)		
Copper				
380.9		Rohsenow et al. 1985 (300°C)	378.6	10.73
366.9		Kreith 1965 (300°C)		
388.0		Weast 1968 (227°c)		
367.9	**389.3**	Range Selection (copper)		
Crushed Salt (partially consolidated)				
0.46		Fluor 1985	0.47	0.01
0.47		Bechtold et al. 2004 (30% porosity, 100°C)		
0.4	**0.6**	Range Selection (30% porosity, 100°C)		
1.34		Bechtold et al. 2004 (20% porosity, 200°C)	1.34	0.01
1.2	**1.4**	Range Selection (20% porosity, 200°C)		









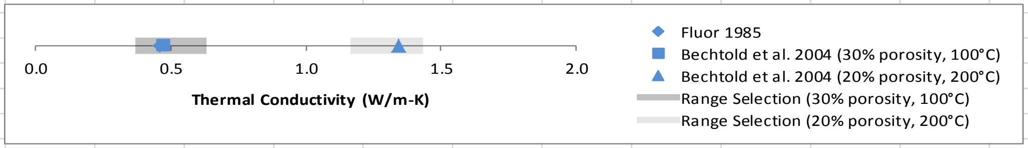
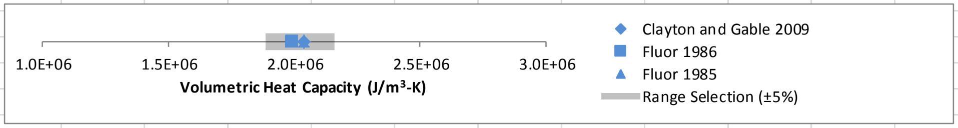
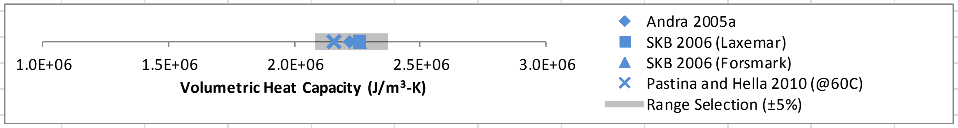
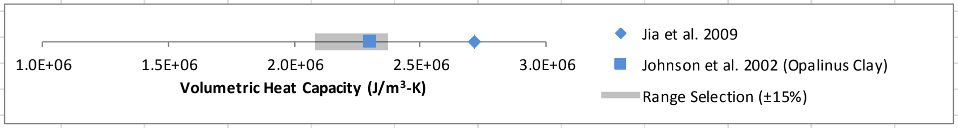


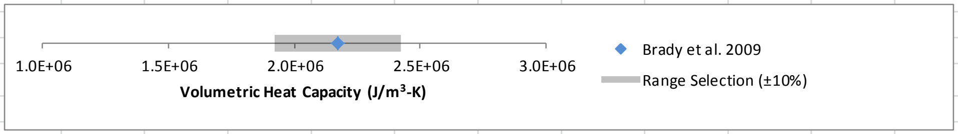
Table 3. Host Rock Heat Capacitance (Volumetric Heat Capacity) Ranges and Parameter Variance

Gravim. Heat Cap. (J/kg-K)	Dry Bulk Density (kg/m^3)	Volum. Heat Cap. (J/m^3-K)	Host Rock Heat Capacitance	Avg.	Std. Dev.
Salt					
931	2190	2.04E+06	Clayton and Gable 2009	2.02E+06	2.88E+04
920	2162	1.99E+06	Fluor 1986		
931	2190	2.04E+06	Fluor 1985		
			Range Selection (±5%): 1.92E+06 to 2.12E+06		
Granite					
837.5	2650	2.22E+06	Andra 2005a	2.22E+06	5.01E+04
837.5	2700	2.26E+06	SKB 2006 (Laxemar)		
837.5	2700	2.26E+06	SKB 2006 (Forsmark)		
784	2749	2.16E+06	Pastina and Hella 2010 (@60C)		
			Range Selection (±5%): 2.11E+06 to 2.34E+06		
Clay/Shale					
1005	2700	2.71E+06	Jia et al. 2009	2.51E+06	2.92E+05
	2400	2.30E+06	Johnson et al. 2002 (Opalinus Clay)		
			Range Selection (±15%): 2.13E+06 to 2.88E+06		
Deep Borehole (Crystalline Basement)					
790	2750	2.17E+06	Brady et al. 2009	2.17E+06	NA
			Range Selection (±10%): 1.96E+06 to 2.39E+06		
Alluvium					
1000	1700	1.70E+06	Smyth et al. 1979	1.46E+06	2.31E+05
1000	1200	1.20E+06	Smyth et al. 1979		
836	1600	1.34E+06	Wollenberg et al. 1983		
1000	1600	1.60E+06	Wollenberg et al. 1983		
			Range Selection (±20%): 1.17E+06 to 1.75E+06		









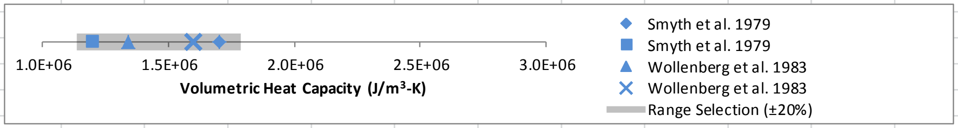


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Table 4. Buffer:Waste Package Radius Ratio Ranges and Parameter Variance

Buffer:Waste Package Radius Ratio								
			Thickness Range Selection		**Ratio Range Selection**		**Std. Dev.**	**Variance**
Waste Package	**Radius (m)**	**Buffer Thickness (m)**	**-50%**	**+50%**	**r2/r1 (-50%)**	**r2/r1 (+50%)**	**r2/r1**	**r2/21**
Crystalline Rock (Clay buffer)								
1-PWR	0.17	0.35	0.175	0.525	2.06	4.18	1.06	1.12
4-PWR	0.33	0.35	0.175	0.525	1.53	2.59	0.53	0.28
1-HLW	0.30	0.35	0.175	0.525	1.57	2.72	0.57	0.33
Clay/Shale (Enclosed Mode)								
1-PWR	0.17	0.7	0.35	1.05	3.12	7.36	2.12	4.50
4-PWR	0.33	0.7	0.35	1.05	2.06	4.18	1.06	1.12
1-HLW - no buffer								
Salt (Enclosed Mode) - no buffer								
Deep Borehole - negligible buffer thermal resistance								
Shale Open Mode (backfilled or open at closure)								
4-PWR	0.33	1.82	0.91	2.73	3.76	9.27	2.76	7.60
12-PWR	0.62	1.53	0.765	2.295	2.23	4.70	1.23	1.52
21-PWR	0.90	1.25	0.625	1.875	1.69	3.08	0.69	0.48
32-PWR	1.00	1.15	0.575	1.725	1.58	2.73	0.58	0.33
Sedimentary Open Mode (alluvium, backfilled at closure)								
4-PWR	0.33	1.82	0.91	2.73	3.76	9.27	2.76	7.60
12-PWR	0.62	1.53	0.765	2.295	2.23	4.70	1.23	1.52
21-PWR	0.90	1.25	0.625	1.875	1.69	3.08	0.69	0.48
32-PWR	1.00	1.15	0.575	1.725	1.58	2.73	0.58	0.33

4. Variance Estimates for Temperature

Variance estimates from Table 5 are then used with Equation 2, to calculate contributions to the overall temperature variance from the variance assigned to each parameter. Figures 2 through 4 contributions from key parameters, with and without a buffer. For Figure 3 the temperature is normalized to temperature using Equations 1 and 2:

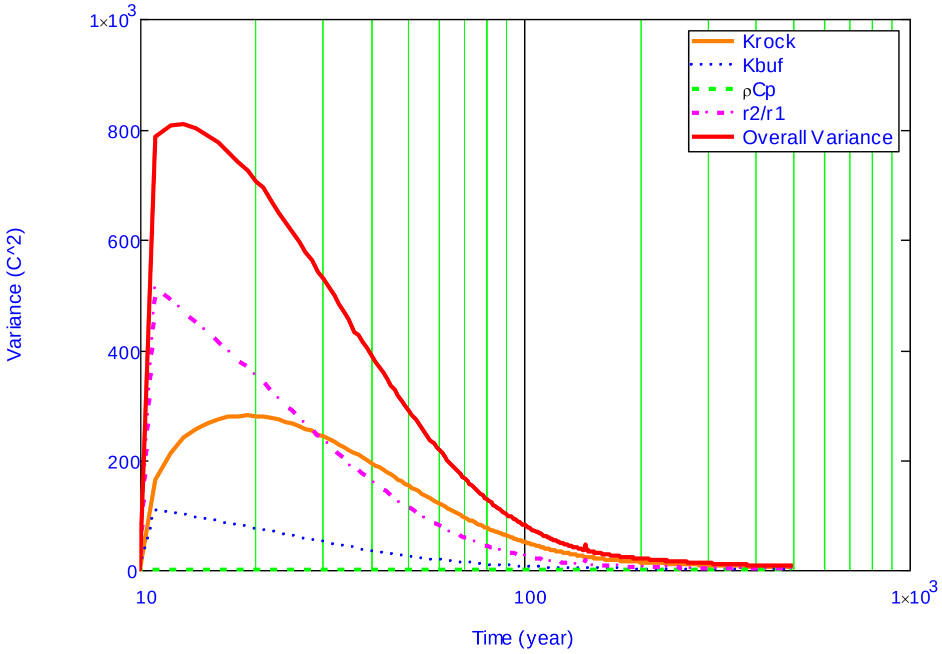
$$Normalized\ temperature\ variance = \frac{Var\{T(t)\}}{T^2(t)} \qquad \text{Eqn. 8}$$

The discussion below focuses on the un-normalized, time-varying temperature variance (Figures 2 and 4) which applies directly to temperature histories calculated for these cases. (The standard deviation of temperature uncertainty can be estimated by taking the square root of variance in Figures 2 and 4.)

Figure 2 summarizes the results of the analytical sensitivity analysis. The components of variance are summed to generate the overall variance on temperature. The K_{buf} (buffer) curve can be neglected and the overall variance adjusted accordingly, for concepts with no buffer (e.g., Figure 4). Similarly, the r_2/r_1 curve can be ignored for applications where the waste package and buffer diameters are known.

Table 5. Parameter Variance Values Used in Analysis

Medium	Range Selection [Low High]	Nominal Value	Std. Deviation	Variance
Host Rock Thermal Conductivity (W/m-K)				
Granite	[2.4 3.2]	2.8	0.37	0.16
Clay/Shale	[1.1 2.3]	1.7	0.61	0.36
Salt (100°C)	[4.4 5.4]	4.9	0.53	0.25
Salt (200°C)	[2.7 3.7]	3.2	0.53	0.25
Alluvium (unsaturated)	[1.0 1.2]	1.1	0.11	0.01
Alluvium (saturated)	[1.2 1.8]	1.5	0.34	0.09
Crystalline Basement	NA	3.0	NA	NA
Engineered Material Thermal Conductivity (W/m-K)				
Clay Buffer (dry)	[0.3 0.5]	0.4	0.05	0.01
Clay Buffer (hydrated)	[1.3 1.5]	1.4	0.11	0.01
Stainless Steel	[14.4 19]	16.7	2.26	5.3
Carbon Steel	[45.4 52.6]	49.0	3.6	13.0
Copper	[367.9 389.3]	378.6	10.7	114.5
Crushed Salt (100°C)	[0.4 0.6]	0.5	0.01	0.01
Crushed salt (200°C)	[1.2 1.4]	1.3	0.01	0.01
Host Rock Heat Capacitance (J/m3-K)				
Granite	[2.11E6 2.34E6]	2.23E6	5.0E4	3.3E9
Clay/Shale	[2.13E6 2.88E6]	2.5E6	2.9E5	1.4E11
Salt	[1.92E6 2.12E6]	2.0E6	2.9E4	1.0E10
Alluvium	[1.17E6 1.75E6]	1.46E6	2.3E5	8.4E10
Crystalline Basement	[1.96E6 2.39E6]	1.18E6	NA	4.6E10
Buffer:Waste Package Radius Ratio				
Granite (enclosed 4-PWR)	[1.53 2.59]	2.06	0.53	0.28
Clay/Shale (enclosed 4-PWR)	[2.06 4.18]	3.12	1.06	1.12
Salt (enclosed all packages)	no buffer			
Alluvium (enclosed 21-PWR)	[1.69 3.08]	2.39	0.69	0.48
Crystalline Basement (enclosed 1-PWR)	negligible thermal resistance			



Note: For the case of crystalline host rock, 4-PWR waste packages (0.66 m diameter), 0.35 m buffer thickness, and SNF with 40 GW-d/MT burnup (10 yr out-of-reactor). For buffer thermal conductivity the average of dry and hydrated values was used. Units of y-axis are (°C)^2.

Figure 2. Contributions to Overall Un-normalized Variance of Temperature (Equation 2) at the Waste Package Surface, from Parameters (K_{rock}, K_{buf}, ρC_p, and r_2/r_1) for the Crystalline Rock SNF Disposal Reference Case from Figure 1.

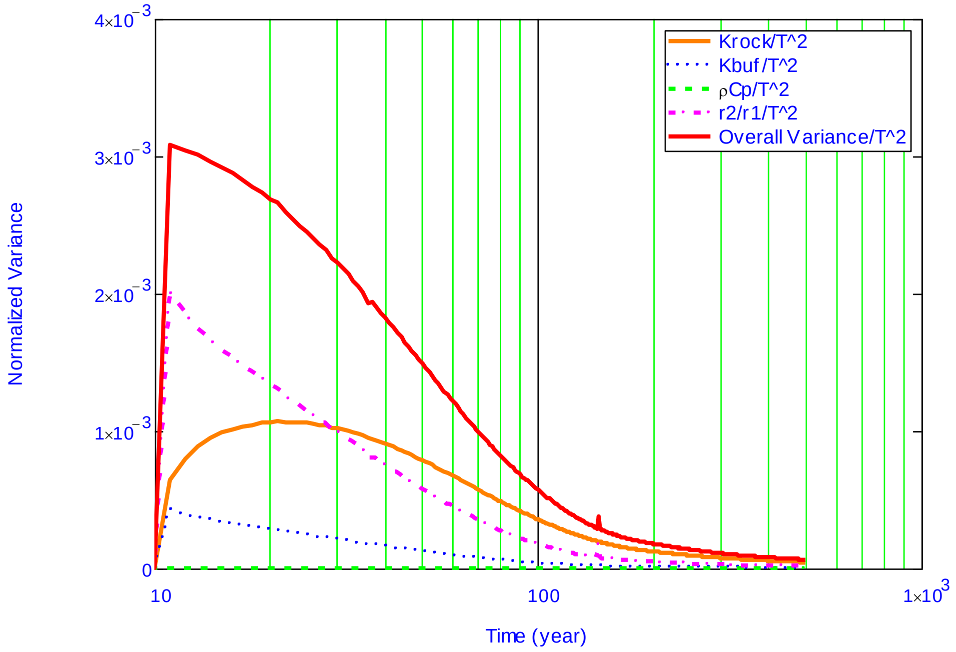
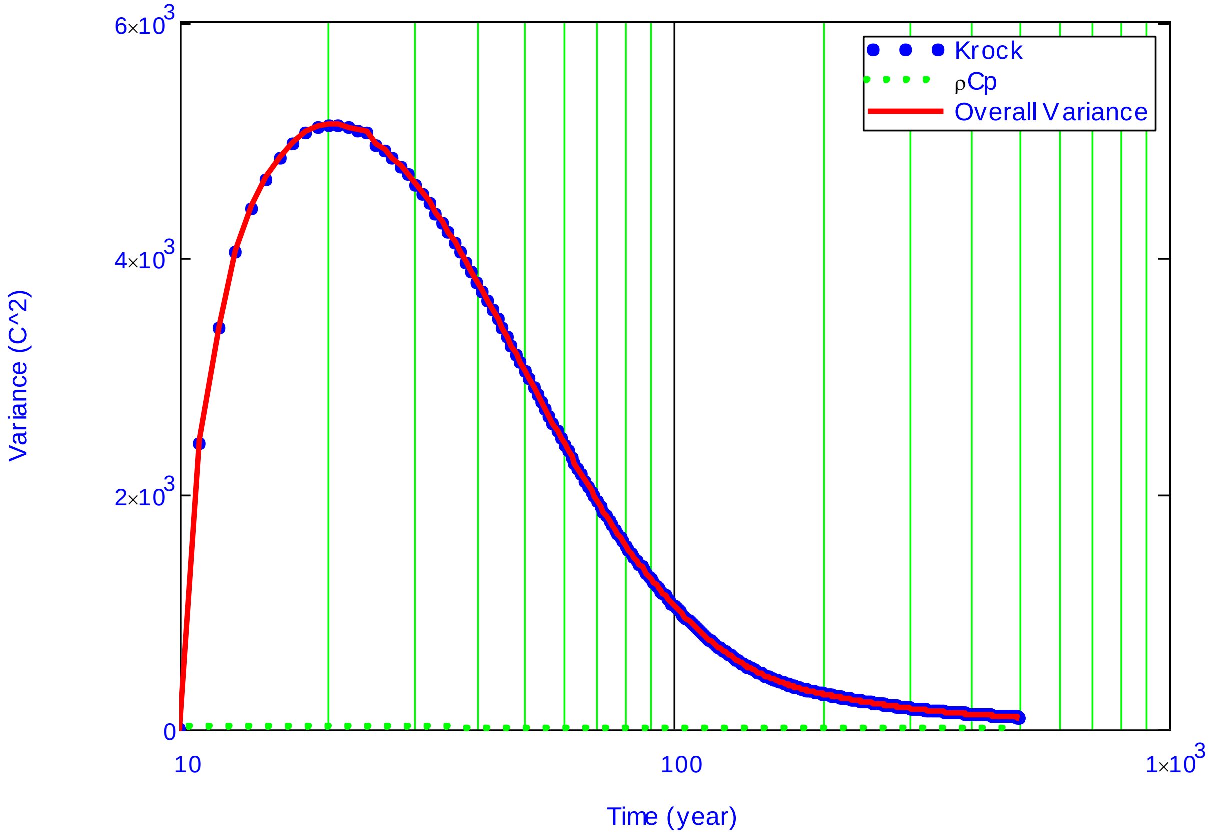


Figure 3. Normalized Variance of Temperature (Equation 8) at the Waste Package Surface, for the Crystalline Rock SNF Disposal Reference Case from Figures 1 and 2.

Uncertainty in heat capacitance (ρC_p) has little or no influence on overall temperature uncertainty at all times (Figures 2 through 4) which is expected and consistent with the limited effect and narrow uncertainty ranges for this parameter. Uncertainty in buffer thermal conductivity is less important than the uncertainty in the buffer radius ratio parameter, given the uncertainty ranges assigned to each parameter (Table 5). Uncertainty in rock thermal conductivity (K_{rock}) becomes most important (Figures 2 and 4) after an initial heating period. Similar figures can be generated for other disposal concepts using different waste types and package sizes, but the results are similar to those presented here.

A clay buffer can be a large thermal resistance (combining the effects of K_{buf} and r_2/r_1), and potentially dominate the maximum temperature as shown by the unnormalized derivatives (Figure 1). Note that the partial derivatives are squared in Equation 2, so that differences in sign, e.g., between $\partial T/\partial K_{buf}$ and $\partial T/\partial(r_2/r_1)$, do not appear in the overall variance (Figure 2). Only when the state of knowledge about K_{buf} as represented by $Var\{K_{buf}\}$ is incorporated, is the variance contribution less than for the host rock (K_{rock}) or buffer radius ratio (r_2/r_1).



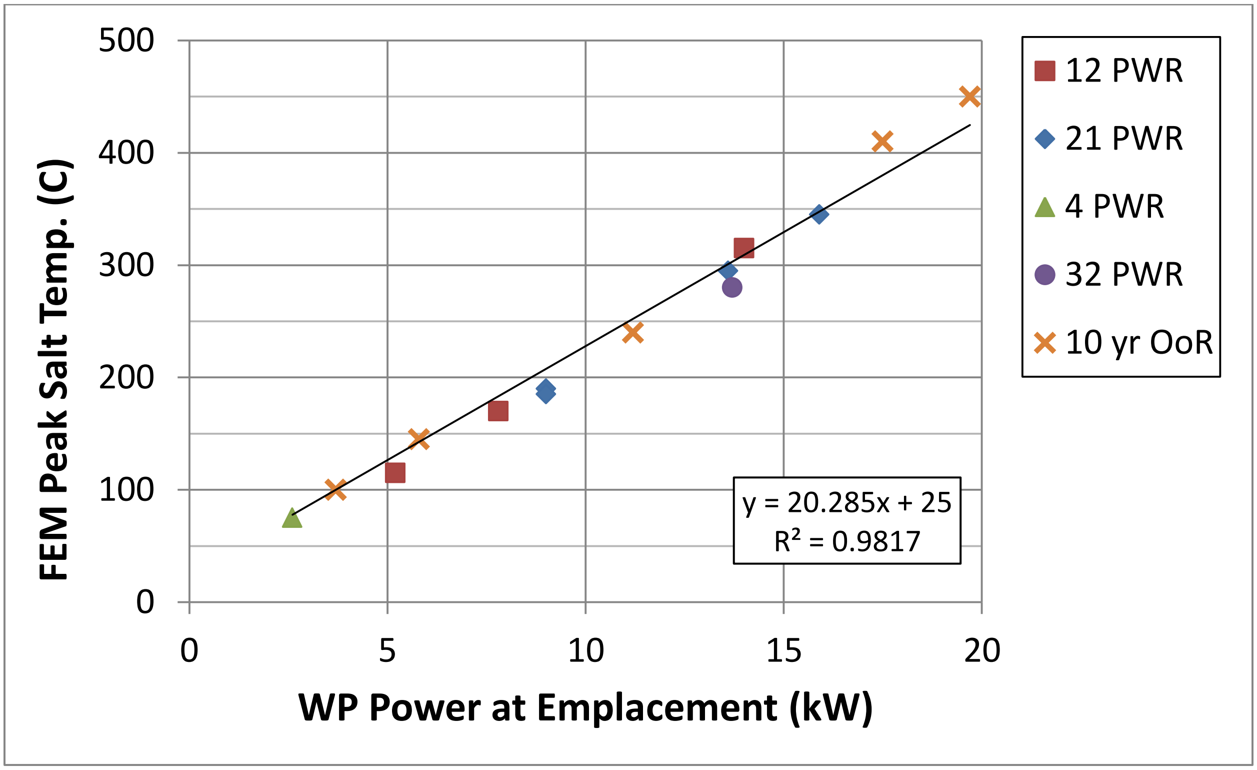
Note: For the case of salt host rock, 21-PWR waste packages (1.80 m diameter), and SNF with 40 GW-d/MT burnup (10 yr out-of-reactor). Thermal conductivity of intact salt at 200 °C was used. The concept does not involve a buffer, so this solution is based on a simple line-source calculation. Units of y-axis are (°C)^2.

Figure 4. Contributions to Overall Un-normalized Variance of Temperature (Equation 2) at the Waste Package Surface, from Parameters (K_{rock} and ρC_p).

5. Maximum Temperature Sensitivity

5.1 Finite Element Based Correlation for Generic Salt Repository

An earlier study using finite-element (FEM) simulation of the generic salt repository (Clayton et al., 2012; Hardin et al. 2011b) showed that maximum salt temperature (peak temperature at the waste package surface) is correlated with the initial thermal power of the package at emplacement. The correlation applies over a wide range of package sizes, for a range of SNF burnup (Figure 5). This result is potentially useful as a thermal-power acceptance criterion for when SNF can be emplaced in a repository, in fuel management system studies. The correlation is further explored in the following section using the analytical solution (Equation 1) for different geologic host media, waste package sizes, SNF burnup, and decay storage periods.



Note: Calculations combine waste package sizes from Hardin et al. (2011a), SNF inventory from Carter and Luptak (2009), with the generic salt disposal concept (Carter et al. 2011), in a series of thermal and thermal-mechanical coupled calculations.

Figure 5. Correlation of Maximum Salt Temperature (Peak Package Surface Temperature) from a Set of Finite Element Simulations of the Generic Salt Repository (Clayton et al. 2012; Hardin et al. 2011a).

5.2 Analytical Line Source Correlations

To corroborate the FEM results for salt, maximum temperatures are calculated for the FY11 reference disposal concepts for SNF using Equation 1, implemented in MathCad14®. For the salt and deep borehole cases, no buffer is included (i.e., the second term on the right-hand side of Equation 1 was zero). Input parameters for these calculations include:

- Geologic host media: crystalline (granite), clay/shale, salt, crystalline basement (deep borehole)
- Waste package sizes: 4-, 12- and 21-PWR packages (0.33, 0.6 and 0.9 m diameter; Hardin et al. 2011a)
- Decay heat based on 40 and 60 GW-d/MTHM burnup (Carter and Luptak 2009)
- Surface storage times: 10, 20, 50, 100 years

The calculations are based on a surface temperature of 15°C, a geothermal gradient of 25°C/km, and a depth of 500 m (giving in situ temperature for the disposal depths described by Hardin et al. 2011a) except for the deep borehole calculation which is for a depth of 4 km. For this analysis only PWR assemblies (UOX) are considered, and waste package length is 5 m. Figure 6 shows decay heat for single SNF assemblies with burnup of 40 and 60 GW-d/MTHM.

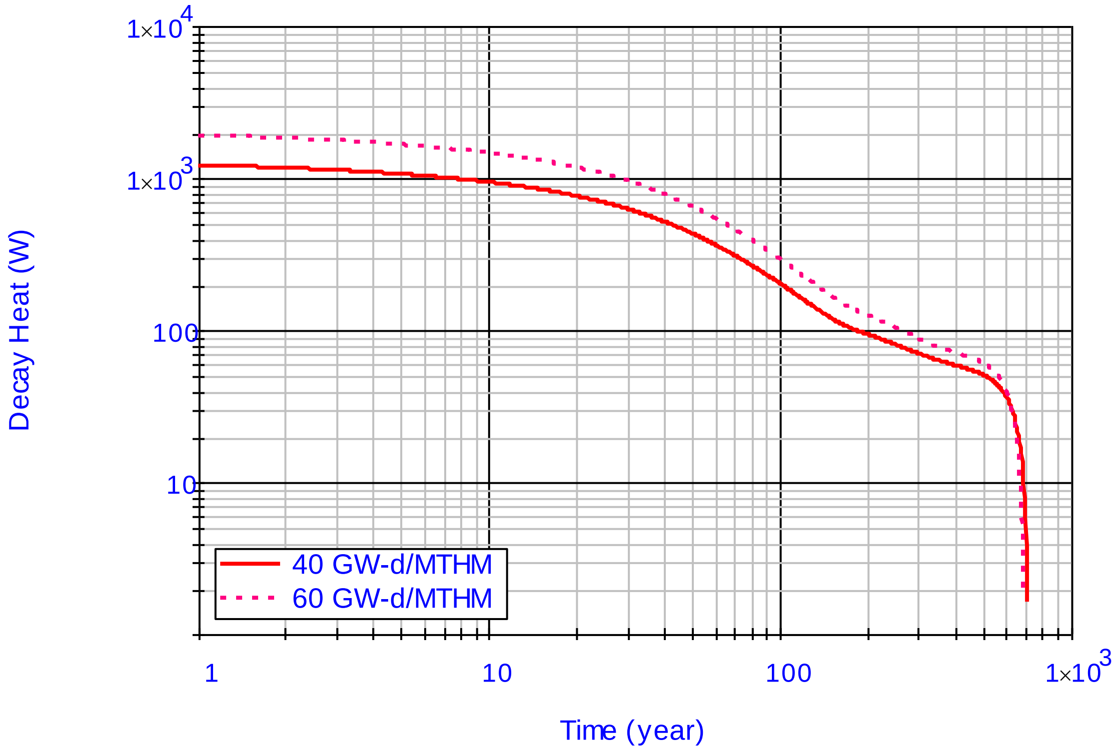


Figure 6. Decay Heat vs. Time Out of Reactor for Individual SNF Assemblies with Burnup of 40 and 60 GW-d/MTHM.

The results (Figures 7 to 10) show calculated maximum temperatures (peak waste package surface temperatures) for the different disposal concepts, as functions of initial power, waste package size, SNF burnup, and fuel age prior to disposal. The figures show strong correlation between maximum temperature and initial power, with slight shifts due to burnup and age.

For the salt calculation heat dissipation through the crushed salt backfill (comprising 1/4 of the package circumference) is ignored, i.e., the waste heat output is increased by 4/3, and the heat dissipates directly into intact salt. A similar approach was taken for salt in the original calculation (Hardin et al. 2001a, Section 5). The calculated maximum temperatures in salt (Figure 8) are greater than calculated using the FEM (Figure 4) because of this approximation. Thus, because of the more complex emplacement geometry of the generic salt repository, numerical analysis that includes backfill consolidation should be used (Clayton et al. 2012).

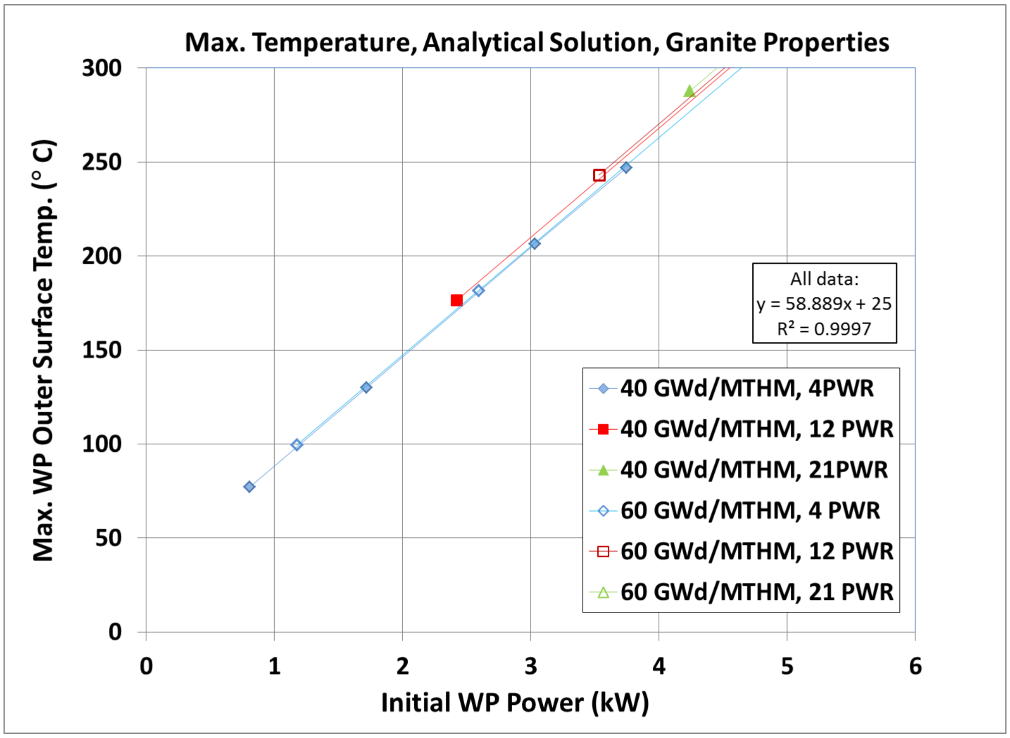


Figure 7. Maximum Temperature vs. Initial Power for Disposal in Crystalline Rock (with buffer) for Combinations of Waste Package Size, SNF Burnup, and Age

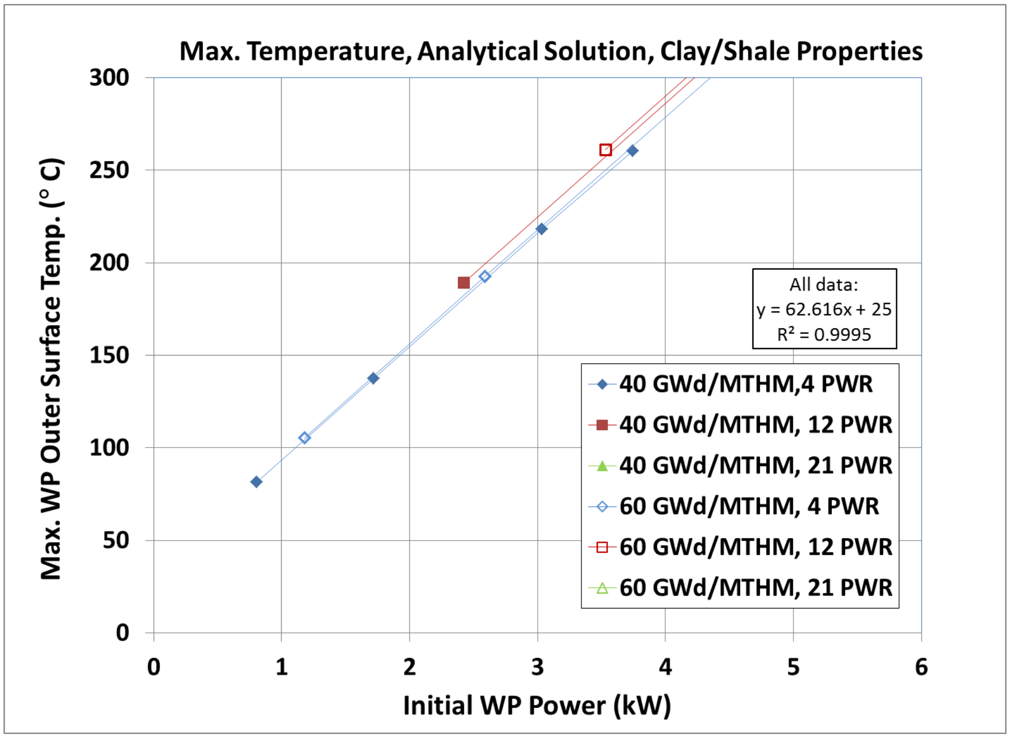


Figure 8. Maximum Temperature vs. Initial Power for Disposal in Clay/Shale (with buffer) for Combinations of Waste Package Size, SNF Burnup, and Age

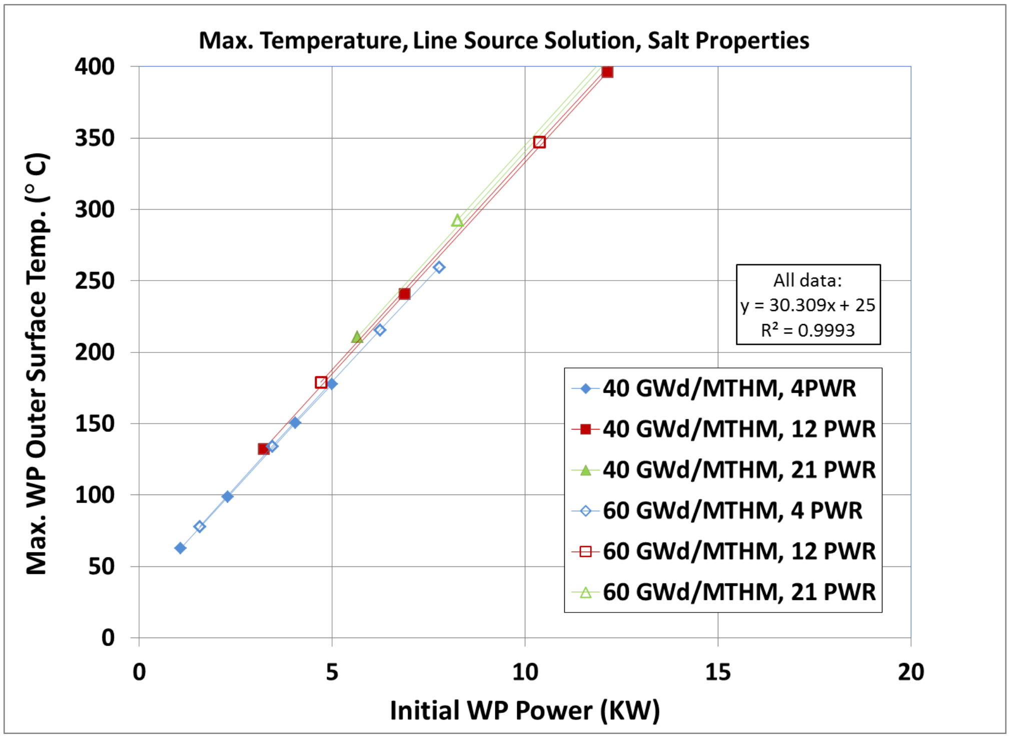


Figure 9. Maximum Temperature vs. Initial Power for Disposal in Salt (no buffer) for Combinations of Waste Package Size, SNF Burnup, and Age

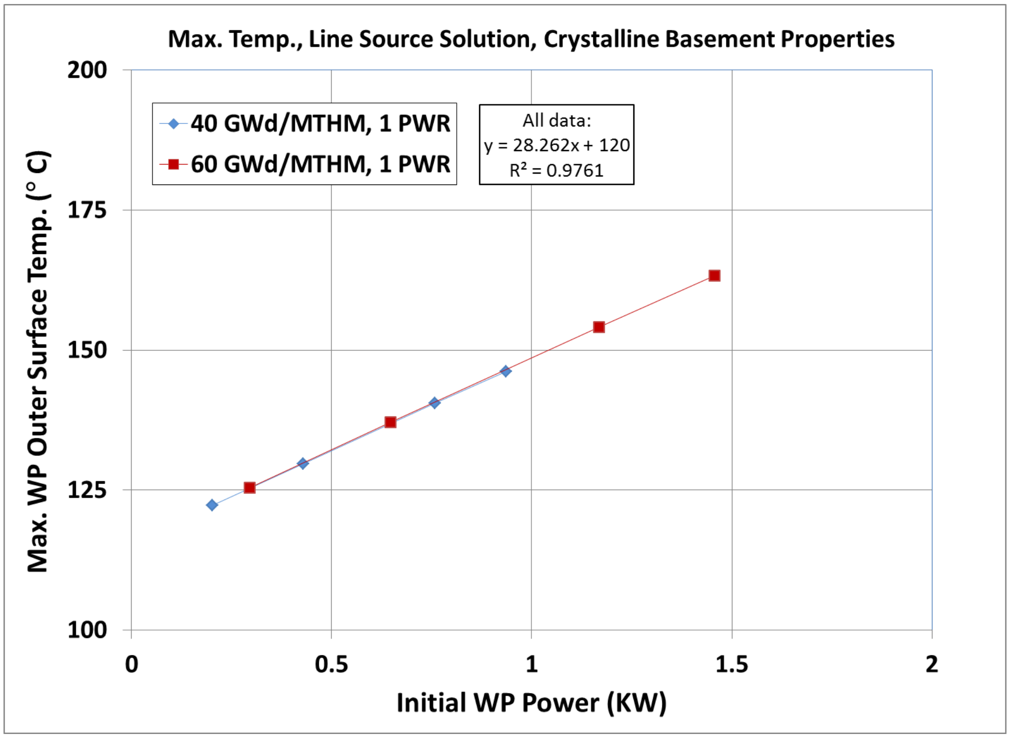


Figure 10. Maximum Temperature vs. Initial Power for Disposal in the Crystalline Basement (deep borehole concept; no buffer) for Combinations of Package Size, SNF Burnup, and Age

6. Summary and Conclusions

This report describes three contributions to analysis of uncertainty in maximum repository (peak waste package surface) temperatures:

- Analytical description of overall variance in temperature, as a function of contributions from key parameters of the analytical solution used in previous temperature analyses (Hardin et al. 2011a).
- Compilation of literature data on key parameter values, for various geologic host media and clay-based buffer materials, drawing on international work to develop geologic disposal solutions for heat-generating waste.
- Correlation between maximum repository temperature and waste package power at emplacement, without explicit adjustment for waste package size, SNF burnup, or fuel age.

The analytical treatment of temperature variance (Sections 3 and 4) uses partial derivatives of temperature with respect to each key parameter (K_{rock}, K_{buf}, ρC_p, and r_2/r_1), and separate variance estimates for the parameters, in a classical approach. The results include the following:

- Temperature at all times is relatively insensitive to heat capacitance (volumetric heat capacity) given the state of knowledge represented by the assigned parameter variance.
- Buffer thermal conductivity is an important parameter in early time (except for disposal concepts that have no buffer), but reported properties for dry and hydrated, clay-based buffer materials are relatively tightly grouped. Hence, the buffer radius ratio (expressed as r_2/r_1) may be a more important parameter depending on how much it is allowed to vary in developing a disposal concept. This implies that disposal concepts that allow partial buffer hydration during the thermal period, are potentially increasing the greatest source of uncertainty in maximum temperature.
- Host rock thermal conductivity is the most important input parameter, especially at later time (e.g., greater than 10 years after emplacement) and where buffers are not used.

Compilation of literature data and selection of uncertainty ranges (Tables 1 through 5) are intended to provide mean and $\pm 1\sigma$ property values for temperature uncertainty analysis based on the analytical solution (Equation 1).

Finally, the study of maximum (peak waste package surface) temperature (Section 5.2) corroborates the earlier finding from FEM simulations of the generic salt repository (Section 5.1). Thus the waste package heat output at emplacement can be used to predict maximum temperature, to a good approximation evident from the linearity in Figures 7 through 10, for all host media, waste package sizes, SNF burnup, and decay storage duration cases considered.

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