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**THERMAL ANALYSIS OF YUCCA MOUNTAIN
COMMERCIAL HIGH-LEVEL WASTE PACKAGES**

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SUMMARY

The thermal performance of commercial high-level waste packages was evaluated on a preliminary basis for the candidate Yucca Mountain repository site. The purpose of this study is to provide an estimate for waste package component temperatures as a function of isolation time in tuff. Several recommendations are made concerning the additional information and modeling needed to evaluate the thermal performance of the Yucca Mountain repository system.

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1.0 INTRODUCTION

The U.S. Department of Energy's (DOE) Office of Civilian Radioactive Waste Management (OCRWM) is studying the option of reprocessing commercial spent fuel to reduce the long-term risks associated with geologic waste disposal. A study of actinide partitioning and transmutation is being performed by the Performance Assessment Scientific Support Program at Pacific Northwest Laboratory (PNL)^(a) for the DOE Yucca Mountain Repository Site Characterization Project.

One objective of this performance assessment study is to evaluate the near-field thermal conditions for a commercial high-level waste (CHLW) package. A literature survey provided the reference CHLW form characteristics and conceptual design information needed for this study. A preliminary thermal analysis was performed using a heat-conduction model to estimate the CHLW package temperatures in tuff. Several recommendations are made to further evaluate the thermal performance of the Yucca Mountain repository system.

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2.0 COMMERCIAL HIGH-LEVEL WASTE FORM DESCRIPTION

The spent nuclear fuel discharged from commercial light water reactors (LWRs) is highly radioactive and generates a significant amount of heat due primarily to the radioactive decay of fission products and actinides that are formed in the reactor. Following a cooling period, the spent fuel may be shipped to a commercial reprocessing facility for actinide partitioning prior to geologic disposal. It is being proposed that the partitioned actinides be transmuted into stable elements by neutron irradiation in advanced liquid-metal reactors (LMRs). This section describes the baseline CHLW form and canister from a future spent fuel reprocessing facility.

The Plutonium-Uranium Extraction (PUREX) process is likely to be the future reprocessing technique for LWR spent fuels, although a pyrochemical process is being investigated for both LWR and LMR spent fuels (Wilems and Danna 1991). The baseline composition ranges of high-level liquid waste resulting from PUREX reprocessing of commercial LWR spent fuels have been reported by Swanson (1986). The reference CHLW glass and canister definition reported by Slate et al. (1981) provided the basis for the waste package conceptual designs in tuff (Schornhorst et al. 1983).

The reference CHLW glass and canister design specifications are given in Table 1. The radioactive decay characteristics of reference CHLW were evaluated with the ORIGEN-II code by partitioning 99% of the U, Pu, and I, and 100% of the He, C, N, Ne, Ar, Kr, Xe, Rn, and H from spent fuel at 5 years after reactor discharge. The thermal properties of the borosilicate glass and physical dimensions of the canister are the most significant parameters for this study. The information in Table 1 is based on a typical pressurized water reactor (PWR) spent fuel type and the "once-through" nuclear fuel cycle (i.e., the partitioned uranium and plutonium is not used in fabricating additional LWR fuel elements). The decay characteristics of several LWR spent fuel types and high-level wastes have been reported by Croff and Alexander (1980). Recent studies have investigated the thermal impacts associated with several nuclear fuel cycle options (Wang et al. 1983; McKee et al. 1983). However, little site specific information is available on partitioning and transmutation concepts, which allows for the removal of less abundant transuranics (Np, Am, and Cm) and heat producing fission products (Cs and Sr) from spent fuel reprocessing wastes.

TABLE 1. Reference Commercial High-Level Waste Glass and Canister Design Specifications (Slate et al. 1981)

<u>High-Level Waste Glass</u>	<u>Description</u>																										
PNL identification	The reference glass is very similar to high-level waste glass 77-260 developed for the Allied General Nuclear Services Fuel Reprocessing Plant flowsheet																										
Composition	<table border="1"> <thead> <tr> <th>Constituents</th> <th>wt%</th> </tr> </thead> <tbody> <tr> <td>SiO₂</td> <td>36</td> </tr> <tr> <td>B₂O₃</td> <td>9</td> </tr> <tr> <td>P₂O₅</td> <td>2</td> </tr> <tr> <td>Alkali metal oxides</td> <td>13</td> </tr> <tr> <td>Alkaline earth oxides</td> <td>1</td> </tr> <tr> <td>Fe₂O₃, Cr₂O₃, NiO</td> <td>1</td> </tr> <tr> <td>Al₂O₃</td> <td>2</td> </tr> <tr> <td>TiO₂</td> <td>6</td> </tr> <tr> <td>CuO</td> <td>3</td> </tr> <tr> <td>Gd₂O₃</td> <td>10</td> </tr> <tr> <td>Fission product oxides</td> <td>12</td> </tr> <tr> <td>Actinide oxides</td> <td>5</td> </tr> </tbody> </table>	Constituents	wt%	SiO ₂	36	B ₂ O ₃	9	P ₂ O ₅	2	Alkali metal oxides	13	Alkaline earth oxides	1	Fe ₂ O ₃ , Cr ₂ O ₃ , NiO	1	Al ₂ O ₃	2	TiO ₂	6	CuO	3	Gd ₂ O ₃	10	Fission product oxides	12	Actinide oxides	5
Constituents	wt%																										
SiO ₂	36																										
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Al ₂ O ₃	2																										
TiO ₂	6																										
CuO	3																										
Gd ₂ O ₃	10																										
Fission product oxides	12																										
Actinide oxides	5																										
Waste loading	The oxides from the high liquid constitute 31 wt% of the glass																										
Quantity	277 kg/MTU (89 L/MTU)																										
Activity	1616 Ci/kg (5029 Ci/L) (at 5 years after reactor discharge)																										
Decay heat	5.9 W/kg; 18.3 W/L (at 5 years after reactor discharge)																										
Density	3.1 g/cm ³																										
Process melting temperature	10,500 to 11,500°C																										
Softening temperature	5750 to 650°C (viscosity = 4 x 10 ⁷ poise)																										
Transition temperature	5000 to 5500°C (viscosity = 1013 poise)																										
Temperature limit to prevent devitrification	500°C																										
Leach rate	1.0-2.0 x 10 ⁻⁶ g/cm ² -d (250°C water)																										

TABLE 1. (contd)

<u>High-Level Waste Glass</u>	<u>Description</u>
Thermal conductivity	0.8-1.3 W/m-°C from 0 to 500°C
Heat capacity	700 to 800 J/kg-°C (estimated)
Thermal expansion	1 x 10 ⁻⁵ /°C
Compressive tensile strength	4 x 10 ⁷ Pa
Young's Modulus	7 x 10 ¹⁰ Pa (estimated)
<u>HLW Canister</u>	
Material	Stainless Steel 304L
Dimensions	3-m high by 31.1-cm-ID cylinder; 6.35-mm wall thickness (12-in. Schedule 20 Pipe)
Bottom	Slightly reversed dished/flanged tank end
Top	Flanged only tank head
Closure	PNL "twist-lock"
Fins (internal)	Required for in-can melting process but not for joule heating process. Capacities given below assume no fins.
Empty weight	160 kg ± 5%
Fill height	90%
Glass content	200 L; 630 kg; 2.28 MTU high-level waste (± 5%)
Weight when filled	790 kg ± 5%
Activity	1.02 x 10 ⁶ Ci (5 years from reactor discharge) 6.58 x 10 ⁵ Ci (10 years from reactor discharge)
Decay heat	3.71 kW (5 years from reactor discharge) 2.21 kW (10 years from reactor discharge)

3.0 WASTE PACKAGE THERMAL MODEL DESCRIPTION

The TEMPEST (Transient Energy, Momentum, and Pressure Equation Solution in Three Dimensions) finite-difference code was used to evaluate near-field host rock and waste package component temperatures for the geologic repository system. The TEMPEST code, Version N, Mod 32, was developed at PNL (Trent and Eyler 1990) to provide a numerical modeling capability for analyzing coupled fluid dynamic, heat transfer, and mass transport processes. The TEMPEST code has been constructed with reasonable generality and many useful features, which support a broad range of engineering and scientific applications. The transient heat conduction capabilities of the TEMPEST code were utilized in this heat transfer study.

The Yucca Mountain Site Characterization Plan (SCP) Conceptual Design (MacDougal et al. 1987) provides information for only commercial spent fuel and defense high-level waste (DHLW). As a result, the waste package thermal model developed for this study is based on the pre-SCP conceptual waste package design reported by Schornhorst et al. (1983) and evaluated by Stein et al. (1984). As shown in Figure 1, the CHLW form canister is emplaced in a vertical borehole and surrounded by a crushed tuff packing. The SCP conceptual design waste emplacement concept is also characterized by single rows of equally spaced boreholes drilled into the drift floor. The SCP conceptual design for DHLW, however, includes a container (i.e., overpack) which is surrounded by a thin air gap (i.e. no packing). A packing layer was assumed in this study to avoid the non-conductive heat transfer modes and issues associated with modeling a thin air gap layer (Lowry et al. 1980). Crushed tuff is currently being investigated for the emplacement room back-fill material and has been shown to be potentially effective as a radionuclide diffusion barrier (Conca and Wright 1990).

For this study, an axisymmetric model of the pre-SCP conceptual waste package design and emplacement configuration was constructed. The two-dimensional waste package scale thermal model is shown in Figure 2. The model extends along the Z-axis to a horizontal boundary located 500 m above the canister midplane with a constant temperature condition of 29°C. This distance is sufficiently large enough not to influence the near-field temperatures and does not simulate surface conditions at the Yucca Mountain site. An adiabatic (e.g., zero flux) condition was specified at the vertical boundary of the model to simulate the repository area thermal loading and at the horizontal canister midplane due to symmetry.

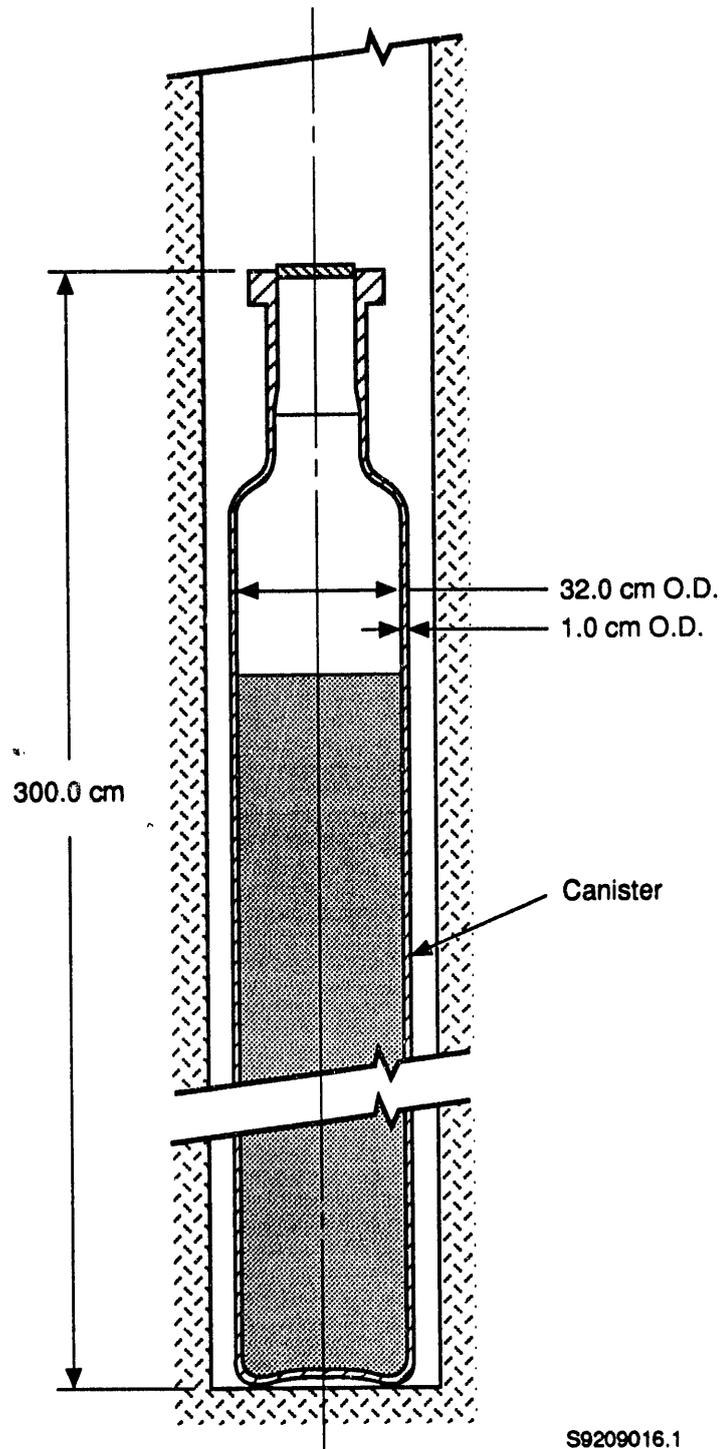


FIGURE 1. Pre-Site Characterization Plan Commercial High-Level Waste Package Conceptual Design (Stein et al. 1984)

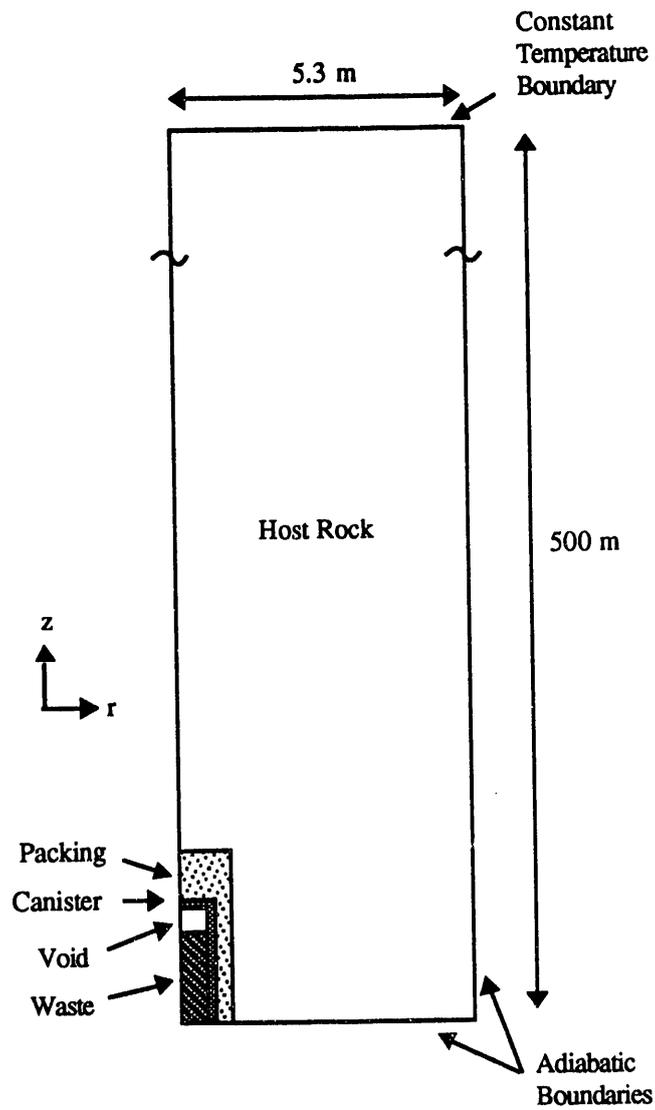


FIGURE 2. Waste Package Thermal Model Description

An initial waste package thermal load value of 2.21 kW was used based on the CHLW form glass and canister specifications given in Table 2. Table 3 provides the decay heat generation rate data normalized to the time of initial waste emplacement, assumed to be 10 years after discharge from reactor. A repository area thermal load value of 25 W/m² was assumed based on established thermal criteria for commercial high-level waste disposal (DOE 1980, WEC 1983).

The repository and waste package thermal load values are major factors in the design of the underground facility because of the constraints imposed by near-field temperature limits. A waste form temperature limit of 375°C has been proposed to reduce the devitrification rate of borosilicate glass (Scott 1983). The Yucca Mountain SCP conceptual design specifies a near-field host rock temperature limit of 200°C to maintain borehole stability and a minimum container temperature goal of 100°C to limit aqueous corrosion during the waste containment period (DOE 1988).

Table 3 provides the thermal properties for the tuff host rock and waste package materials used in this study. Thermal properties of the intact tuff host rock are reduced at temperatures above 100°C to account for the effect of dehydration in the local rock mass^(a). The packing thermal conductivity was varied over a range of 0.15 to 0.97 W/m°C to account for the higher degree of

TABLE 2. Relative Decay Heat Generation Rate Data

<u>Year</u>	<u>Fraction</u>	<u>Year</u>	<u>Fraction</u>
0	1.0000	80	0.148
1	0.963	100	0.125
3	0.893	125	0.116
5	0.830	150	0.102
8	0.760	175	0.091
10	0.724	200	0.081
15	0.660	250	0.066
20	0.600	300	0.055
25	0.536	400	0.040
30	0.475	500	0.030
40	0.358	600	0.023
50	0.270	800	0.015
60	0.213	1000	0.010
70	0.170		

(a) Yucca Mountain Project Office. 1988. Yucca Mountain Project Reference Information Base (RIB). Version 4, Revision 0. U.S. Department of Energy, Las Vegas, Nevada.

TABLE 3. Waste Package Material Thermal Properties

<u>Material</u>	<u>Density, kg/m³</u>	<u>Heat Capacity, J/kg°C</u>	<u>Thermal Conductivity, W/m°C</u>
Intact Tuff Rock			
Below 100°C	2297.0	1019.0	1.91
Above 100°C	2297.0	807.9	1.84
Crushed Tuff Packing			
Thickness = 2 cm	1400.0	900.0	0.15
Thickness = 5 cm	1600.0	900.0	0.65
Thickness = 10 cm	1700.0	900.0	0.97
Stainless Steel Canister	7861.0	485.7	51.0
Glass Waste Form			
At 0°C	3100.0	750.0	0.83
At 500°C	3100.0	750.0	1.33

compaction anticipated with increasing packing layer thickness from 2.0 to 10.0 cm. The thermal conductivity of the packing materials are based on a thermal analysis of Yucca Mountain conceptual waste package designs (Stein et al. 1984). The thermal conductivity of glass is assumed to vary linearly with temperature from 0°C to 500°C. The thermal properties of dry air were used for the void region in the canister and radiation heat transfer across the void was neglected.

There are some important limitations with the thermal modeling approach used in this study. Recent studies have indicated that the near-field temperatures can be influenced by the multiphase groundwater flow conditions, depending on the local permeability and initial saturation of the host rock (White and Altenhofen 1989). Other studies have shown that larger repository-scale thermal models are needed to simulate the underground facility layout design and variable heat generation rate characteristics (Altenhofen and Eslinger 1990).

4.0 WASTE PACKAGE TEMPERATURE RESULTS

The results of the waste package scale thermal model are shown in Figures 3 through 5. As indicated, three separate cases were evaluated to address the impact of increasing packing layer thickness and thermal conductivity. For the assumed parameters, the effect of increasing packing

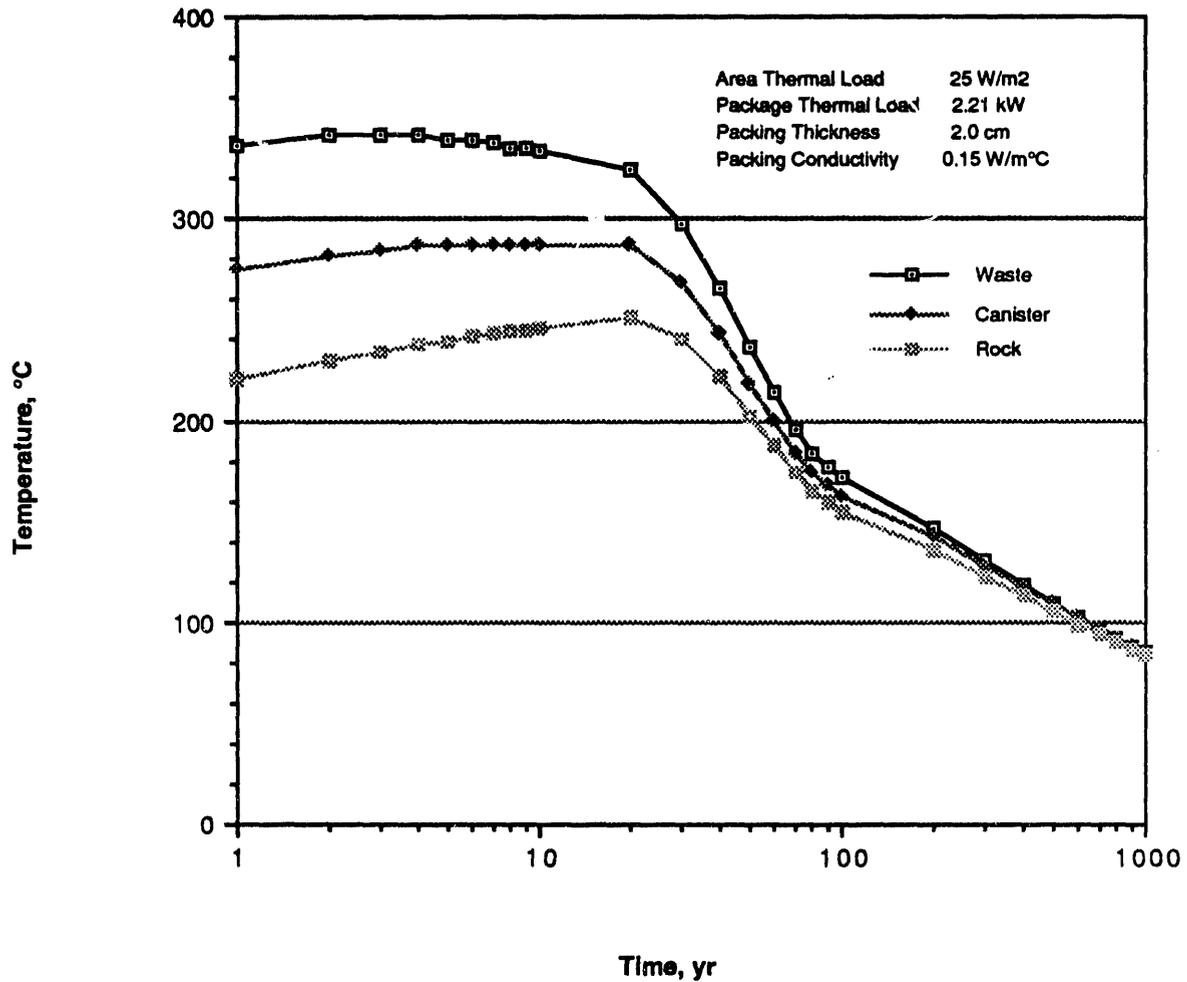


FIGURE 3. Commercial High-Level Waste Package Temperatures: Packing Thickness = 2 cm, Thermal Conductivity = 0.15 W/m°C

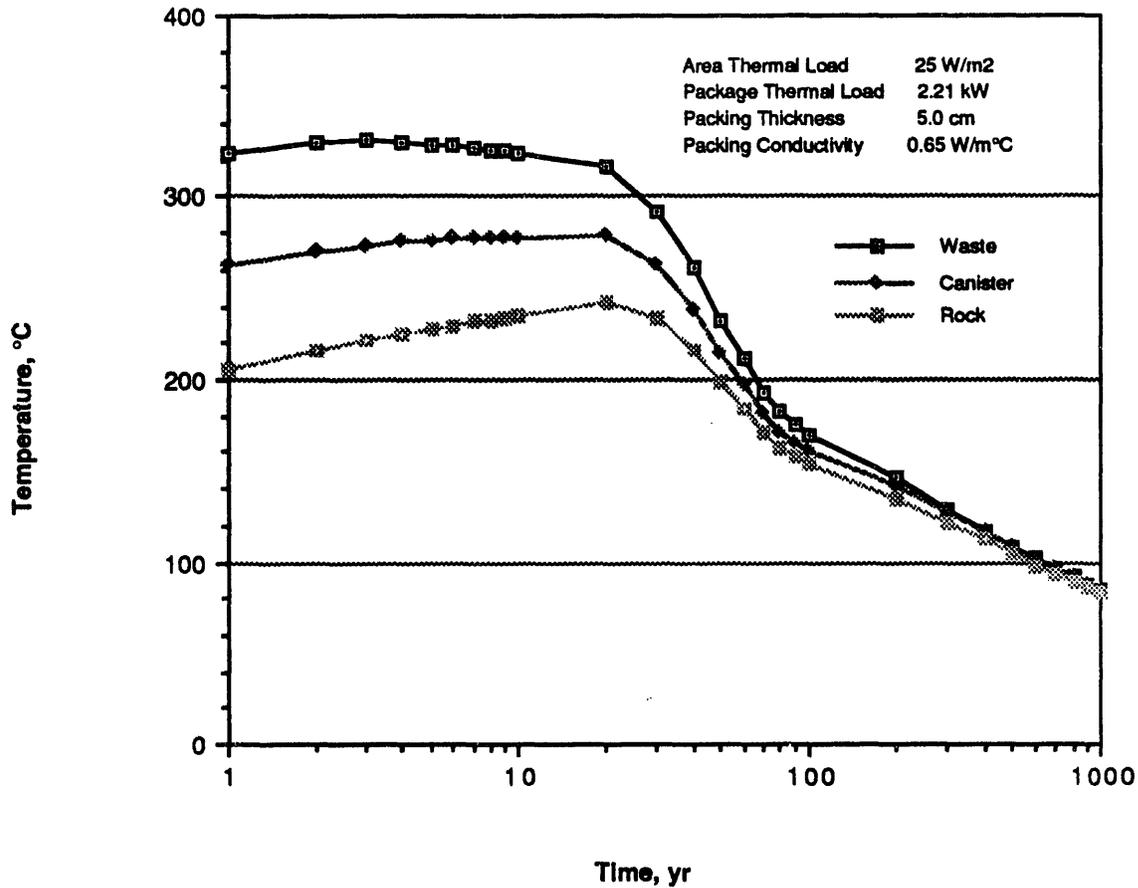


FIGURE 4. Commercial High-Level Waste Package Temperatures: Packing Thickness = 5 cm, Thermal Conductivity = 0.65 W/m°C

thickness and conductivity values is a slight reduction in the maximum waste package component temperatures (i.e., the impact of increasing thermal conductivity compensates for increasing layer thickness). Overall, the maximum glass temperatures are estimated to be between 327°C and 342°C at 3 years after waste emplacement. The maximum canister temperatures are estimated to be between 277°C and 287°C at 20 years after emplacement, with the peak rock temperatures estimated to be between 231°C and 252°C.

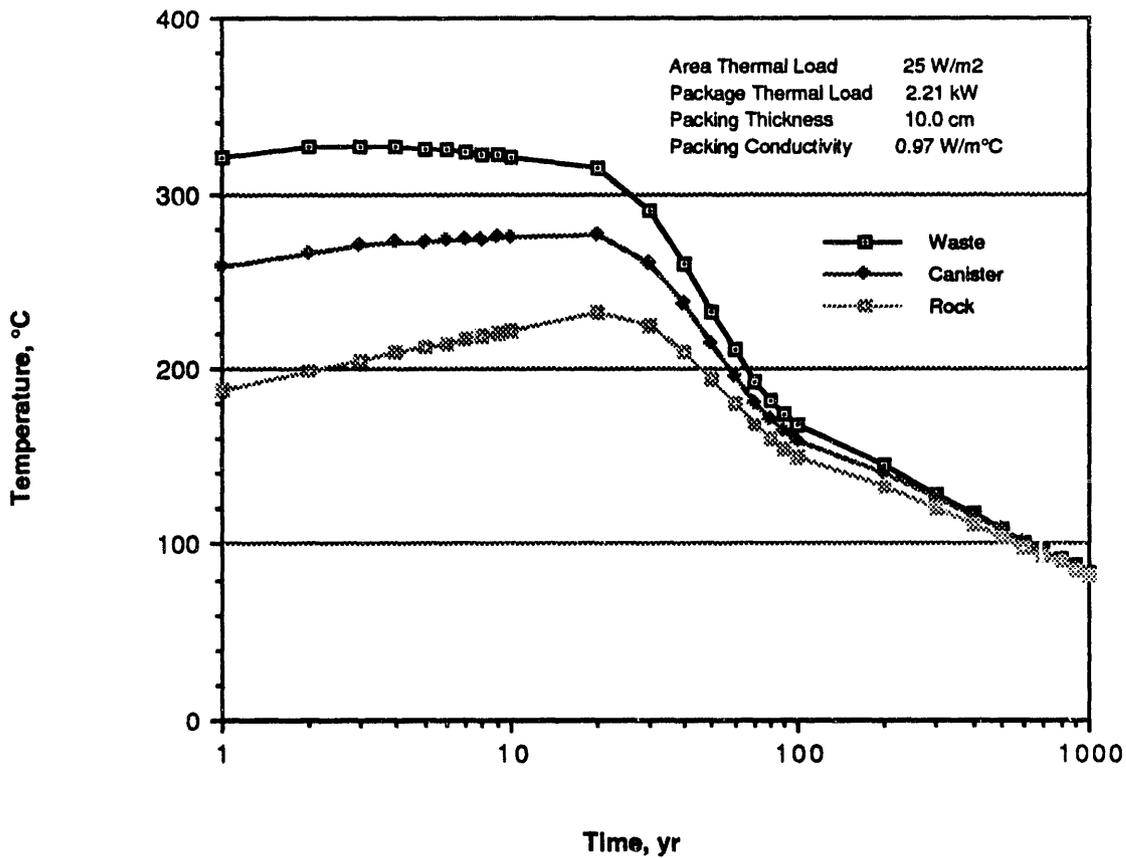


FIGURE 5. Commercial High-Level Waste Package Temperatures: Packing Thickness = 10 cm, Thermal Conductivity = 0.97 W/m°C

After 20 years, the waste package temperatures decrease as a result of the decay of heat-producing isotopes in the high-level waste and conduction of heat into the surrounding host rock. Assuming a conduction dominated system, waste package container surface temperatures are estimated to stay above the boiling point (100°C) of groundwater for approximately 600 years after waste emplacement. At 1000 years, the waste package temperatures reduced to 84°C, well above the ambient temperature (29°C).

5.0 RECOMMENDATIONS

The preliminary results of this thermal analysis can be used in repository source-term model evaluations of waste package containment time and release rate performance. It is important to note the key assumptions that were made concerning the thermal properties and modeling approach used in this study. The following recommendations are made based on the additional information and modeling needed to evaluate the thermal performance of CHLW in the Yucca Mountain repository system.

As indicated in Section 2.0, little information is available on the characteristics of high-level waste forms resulting from actinide partitioning and transmutation. Therefore, a nuclide depletion analysis is needed to determine the radiological decay heat characteristics of high-level wastes from aqueous and pyro-chemical reprocessing operations.

As described in Section 3.0, a two-dimensional cylindrical model was used to simulate the CHLW waste package emplacement concept. This assumes that the area thermal and mass loading are uniform throughout the repository. Three-dimensional models of the repository underground facility are needed to simulate the actual waste emplacement configuration and the commingling of high-level wastes with variable heat characteristics.

A key assumption of this study is that near-field heat transfer is dominated by conduction, although temperature-dependent thermal properties were used to simulate local dehydration in the partially saturated host rock. It is important to emphasize that ignoring multi-phase groundwater processes in the near-field tends to over-predict the period of dehydrated conditions, which may be non-conservative with respect to waste package containment time performance.

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