225

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Abstract

Lawrence Livermore National Laboratory is involved in the design and testing of high level nuclear waste packages. Many of the aspects of waste package design and testing (e.g., corrosion and leaching) depend in part on the temperature history of the emplaced packages. This paper discusses thermal modeling and analysis of various emplaced waste package conceptual designs including the models used, the assumptions and approximations made, and the results obtained.

Introduction

The Nevada Nuclear Waste Storage Investigations (NNWSI) Project is part of the U.S. Department of Energy's Civilian Radioactive Waste Management (CRWM) Program. The Waste Package task of the NNWSI Project is working towards the development of multibarriered packages for the disposal of spent fuel and high-level waste in tuff in the unsaturated zone at Yucca Mountain located at the Nevada Test Site (NTS). Lawrence Livermore National Laboratory (LLNL) is responsible for the design, modeling and testing of the waste forms and barriers leading to the final waste package designs and specifications. The final engineered barrier system design may be composed of a waste form, canister, overpack, borehole liner, packing and the near field host rock, or some combination thereof. This paper addresses the thermal analysis of waste packages in the repository host rock.

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Need for Thermal Analysis

Many aspects of waste package design and testing depend in part on the temperature environment to which the emplaced packages will be exposed. Information produced by thermal analysis is needed for the following reasons.

- To demonstrate that designs will not exceed maximum temperature criteria for the various waste forms: 773 K (500°C) for Defense High Level Waste (DHLW) glass, 673 K (400°C) for Commercial High Level Waste (CHLW) glass, and 623 K (350°C) for Spent Fuel (SF);
- To provide projected temperature histories for materials selection;
- To assist in the verification of the performance analysis code, WAPPA [1];*
- To provide temperature boundary conditions for the performance analysis code;
- To provide the temperature environment for transportation, handling, storage and retrieval analyses;
- To calculate approximate time periods of steam/water contact with waste package;
- To provide temperature histories for corrosion testing;
- To provide temperature histories for waste form leach testing;
- To provide temperature histories and boundary conditions for very near field steam/air/water porous flow calculations;

* (WAPPA is a one-dimensional code designed to calculate the corrosion and leaching of the various waste package components and to calculate the eventual breaching and the release rate to the repository. WAPPA consists of five process submodels including the radiation, thermal, mechanical, corrosion and leach submodels).

- To provide the temperature field for thermal stress analysis of waste packages and very near field host rock;

- To predict temperatures which would occur in canister fire tests.

Model

We have completed thermal analyses of a number of conceptual designs to determine temperature-limited waste package dimensions. Figure 1 shows the reference vertically emplaced PWR spent fuel canister. This particular design employs a heat conducting space frame separating the consolidated spent fuel rods into 14 distinct compartments. The radial portions of the space frame serve as heat conducting fins which act to lower the peak fuel temperature.

We are using TACO2D [2], a two-dimensional implicit finite element code to analyze this and other conceptual designs. TACO2D requires temperature dependent material properties data, a mesh representing the physical geometry and the time dependent thermal loading of the waste form as input. Code output consists of temperature histories at all nodes of the mesh. Results obtained with TACO2D have shown good agreement with the results from other one- and two-dimensional codes (e.g., WAPPA).

Two different emplacement schemes (horizontal and vertical) have been analyzed. In the horizontal emplacement mode, horizontal boreholes of lengths near 180 m would be bored at predetermined spacings perpendicular to the access drifts. A 2D model oriented perpendicular to the axis of a borehole of infinite length was used to model this emplacement mode. This is a reasonable approximation since the ratio of borehole length to borehole diameter is about 200. The accuracy of results produced by this model are better for packages emplaced near the center of the borehole where end effects do not play a significant role until very late times. For conservatism, final designs will be based on the "hottest" package. Figure 2 shows the finite element mesh and model used for a typical thermal analysis of a horizontally emplaced PWR spent fuel package with twenty-four internal heat conducting fins.

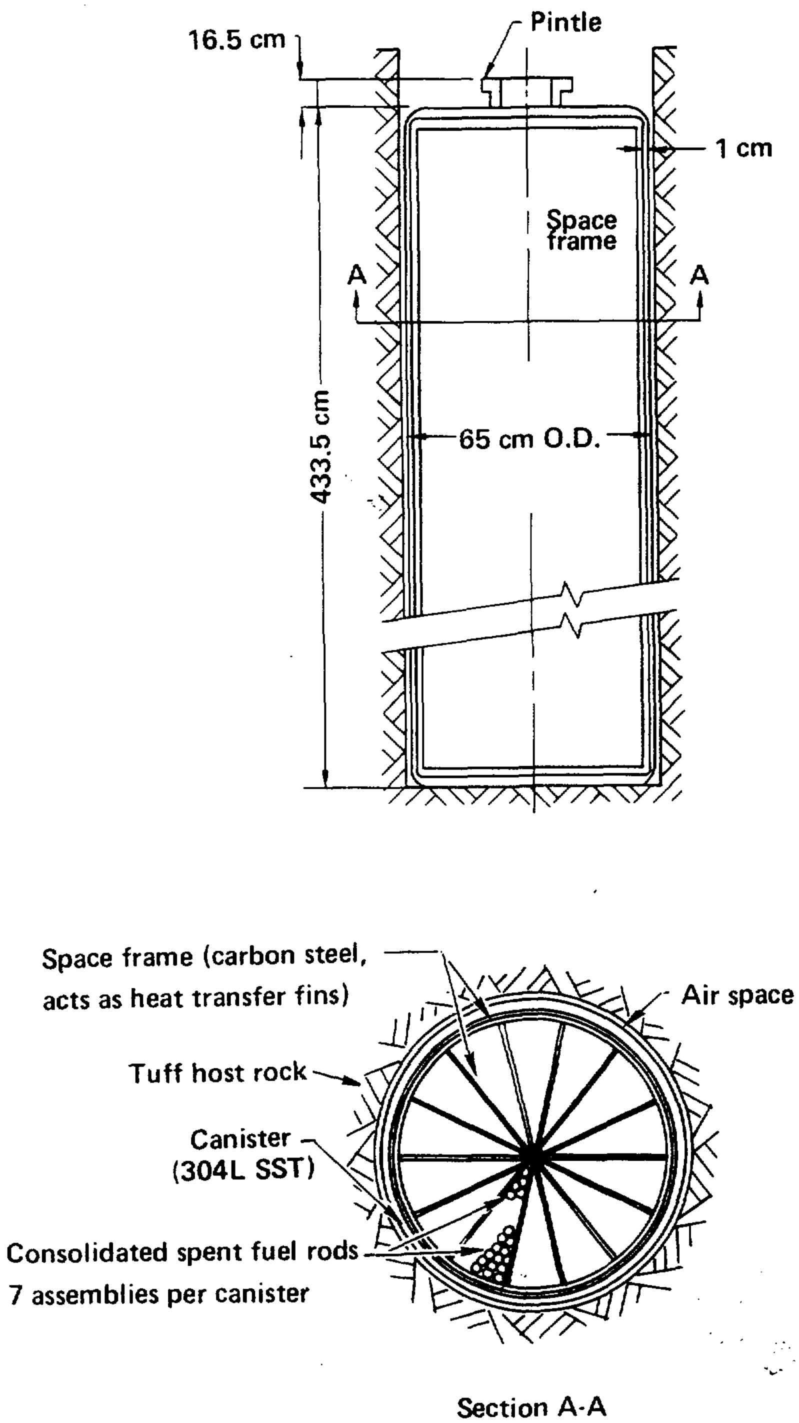


Figure 1. Reference vertically emplaced PWR spent fuel canister with fourteen radial heat conducting fins separating the consolidated rods.

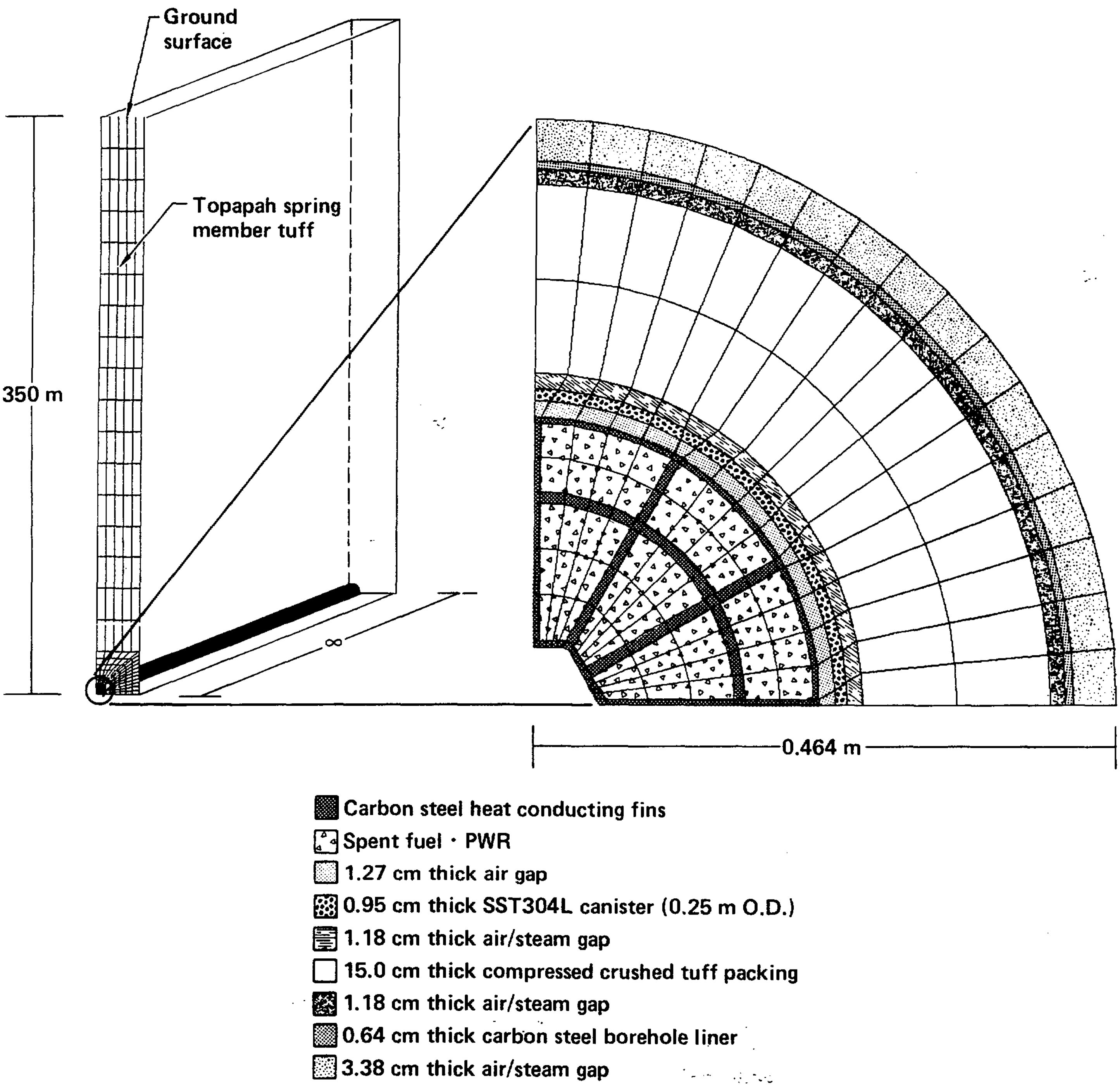


Figure 2. The finite element mesh of the infinite cylinder model used for the thermal analysis of horizontally emplaced PWR spent fuel with 24 fins, packing and a borehole liner.

In the horizontal configuration, packages are placed end to end in the boreholes. However, even when canisters are touching, space does exist in the borehole volume that does not contain waste (e.g., pintles, partially filled canisters). To account for this in the 2D infinite cylinder model, a combination of two computer runs were used. The first run assumed an infinite cylinder of fully loaded waste with no allowance for gaps and partially filled canisters. The second run allowed for gaps by means of a lower loading density, with the total heat load per package spread evenly over the volume bounded by the waste form diameter and waste package pitch in the borehole. The temperature drop across the waste form and canister from the first run was then superimposed onto the temperature history of the borehole wall from the second run. This super position technique is necessary to approach 3D accuracy using the more efficient 2D code.

The vertical emplacement scheme allows for packages to be emplaced in boreholes drilled vertically in the access drift floor. It is difficult to accurately model vertically emplaced waste in two dimensions but even more time consuming to model the packages in three dimensions. For analyses of conceptual designs, we elected to use a 2D axisymmetric model modified from the standard cylindrical shape to an hour-glass shaped model. Figure 3 shows a portion of the mesh used for the analysis of a CHLW canister vertically emplaced in a repository. The smaller of the two radii shown represents the distance defined by one-half the package pitch. The larger radius represents the radius of a circle whose area is the same as that of the rectangle defined by the drift pitch and the package pitch.

This allows a package to see the thermal effects of adjacent packages at a time much sooner (and more realistically) than would be experienced had the more conventional cylindrical axisymmetric model been used. Similarly, far field effects are preserved since the same amount of rock is available as a heat sink. The heat flux which would in reality discharge into the host rock between drifts in a horizontal direction is forced by the model to flow in a vertical path with the total volume of tuff available as a heat sink being identical in either case. It should be noted that LLNL is mainly concerned with the waste package so that accuracy in temperature distributions within the near-field is the first priority.

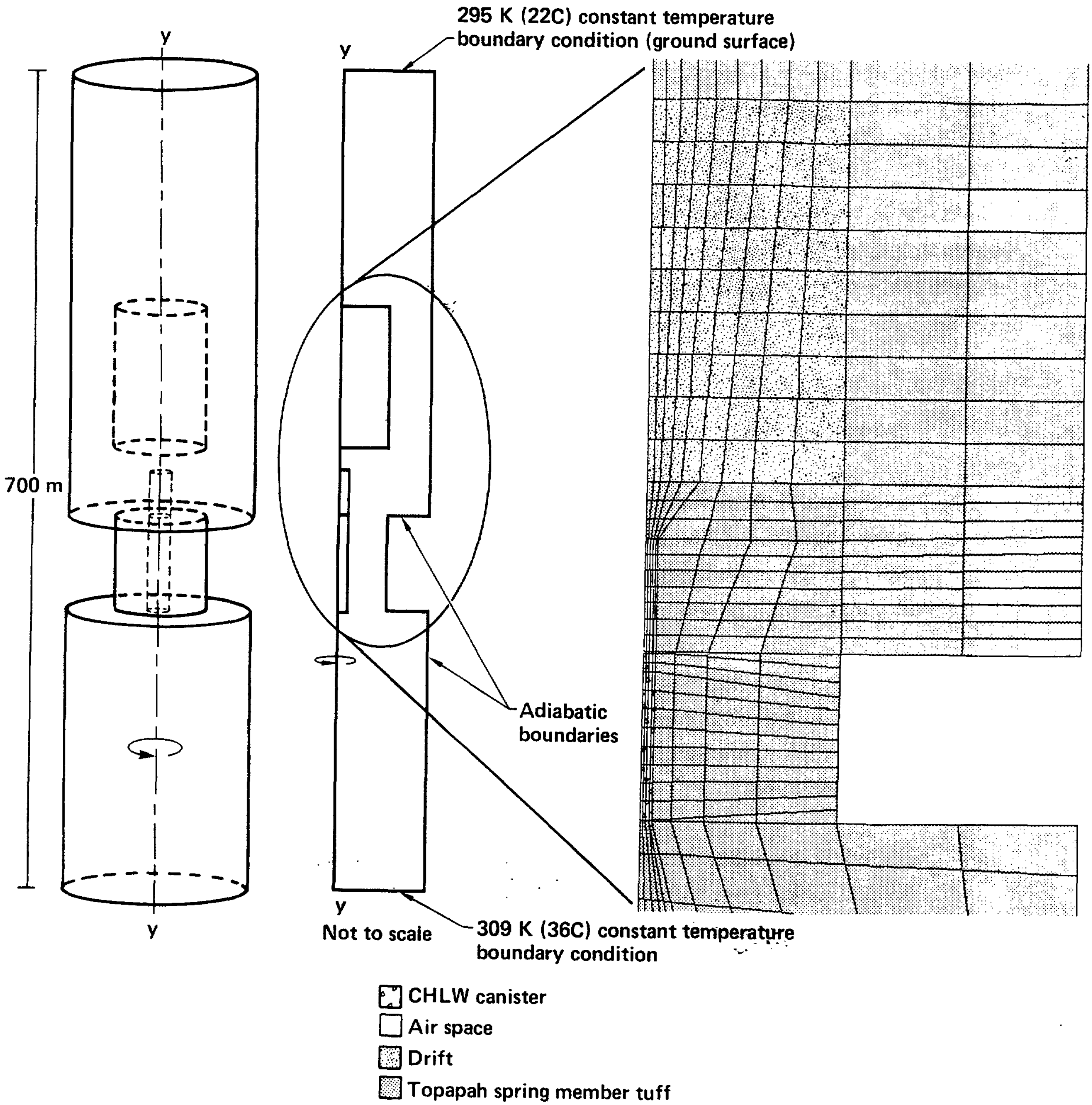


Figure 3. A portion of the finite element mesh for the axisymmetric model used in the thermal analysis of a vertically emplaced CHLW package. The 2D mesh is rotated 360 degrees about the y-y axis to produce the axisymmetric model shown on the far left.

The use of the 2D axisymmetric model results in two additional modeling approximations. The access drift is forced into the shape of a solid cylinder, and, when modeling spent fuel, the internal heat conducting fins which normally run axially through the waste are modeled horizontally. For the vertically emplaced spent fuel analyses reported in this paper, the fins were input in the horizontal direction with the equivalent total volume as would be present in the reference canister. We have not yet evaluated the effect these two approximations have on the temperature histories of interest though we think it is minimal.

Aside from the modeling approximations, a number of other assumptions and approximations have been made which are thought to have a minimal effect on the accuracy of the results. (Forced convection in the drifts was not modeled and could have a significant effect on waste package temperatures.)

- The thermal properties of dry air were used for gaps inside the outermost containment barrier.

- The thermal properties of one hundred percent humid air were used for gaps between the outermost containment barrier and the surrounding tuff up to a temperature of 373 K (100°C) at which time the properties of one hundred percent steam were used.

- Heats of vaporization and recondensation, and fluid transport were not included in the analyses, however, changes in the thermal conductivity and specific heat due to fluid phase changes in the rock were considered.

- No initial geological temperature gradient in the tuff was used. An initial value of 302 K (29°C) was used throughout the rock with the exception that a constant temperature boundary condition of 295 K (22°C) was used to represent the earth's surface 350 m above the repository. In addition, for the runs modeling vertically emplaced waste a constant temperature boundary condition of 309 K (36°C) was used to represent a plane 350 m below the repository. Calculations showed that the effect on the waste package of not including the thermal gradient in the rock from the problem was negligible.

- An initial temperature of 373 K (100°C) was assumed for each waste package at emplacement.

- The boiling point of water was assumed to be 373 K (100°C) although estimates show the true boiling point to be near 368 K (95°C) when altitude and impurity effects are considered.

- All air gaps and spaces (including the access drift) include the effects of conduction, natural convection and thermal radiation by means of a temperature dependent equivalent thermal conductivity. This approach has been successfully used by others [3,4].

- All materials (including the consolidated spent fuel rod assemblies) were assumed to be isotropic. Tables 1 and 2 show the material property values used for spent fuel and tuff respectively. The values in Table 1 reflect the fact that the consolidated spent fuel rod assemblies are not truly isotropic due in part to the air gaps between the rods.

TABLE I Equivalent Spent Fuel Material Properties Used for Thermal Analyses [5, p. 337, 340]

Density		2000 [kg/m^3]
Specific Heat		2640 [J/kgK]
Thermal Conductivity	T [K]	k [W/mK]
	273	0.060
	323	0.070
	373	0.093
	423	0.135
	473	0.190
	523	0.263
	573	0.355
	623	0.460
	673	0.590

TABLE 2 Tuff Material Properties Used for Thermal Analyses

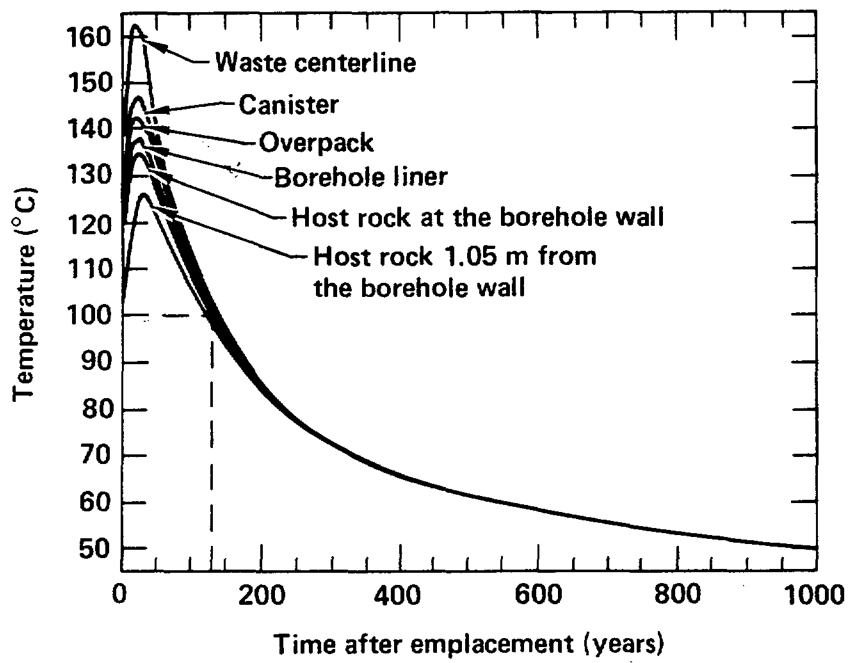
Density		2244 [kg/m^3]
Specific Heat	T [K]	Cp [J/kgK]
	273	971.4
	372	971.4
	373	689.0
	673	689.0
Thermal Conductivity	T [K]	k [W/mK]
	273	1.8
	372	1.8
	373	1.6
	673	1.6

Results

Figures 4, 5 and 6 show typical temperature history curves for three different waste forms under specific emplaced conditions. Refer also to Tables 3 and 4 for a summary of all the significant input and output parameters for the thermal analyses completed to date.

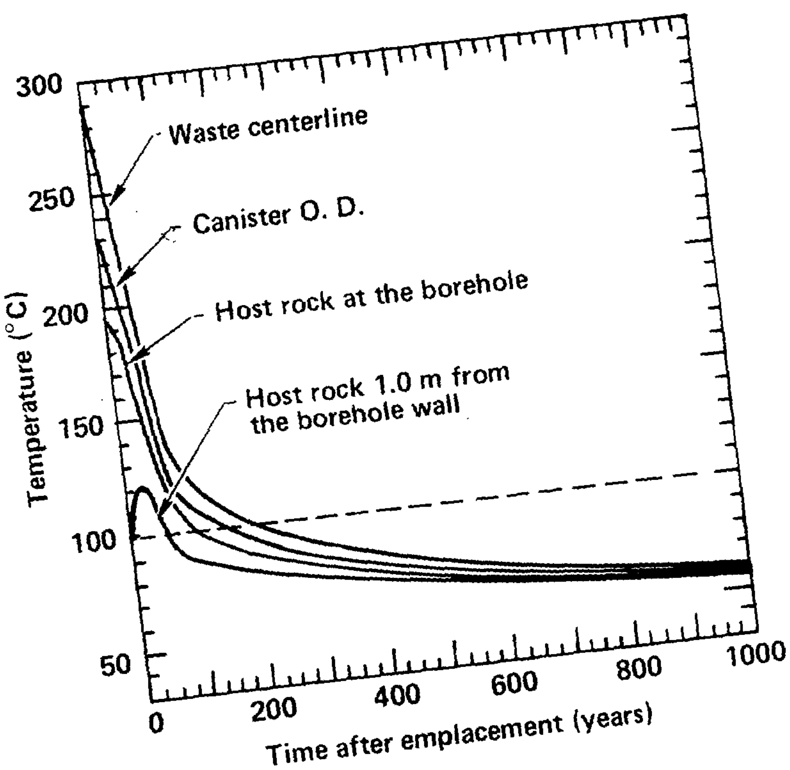
Special attention should be paid to the two sets of analyses completed which gave the thermal effects of the introduction of packing into the design. The first analysis encorporated compressed crushed tuff packing 15 cm thick on the radius (k = 0.65 [W/mK], experimentally measured) around horizontally emplaced canisters containing PWR spent fuel. The results showed that with no packing the peak fuel temperature was about 613 K (340°C) but when packing was included the peak fuel temperature was 681 K (408°C) which is above the design limit of 623 K (350°C) for spent fuel.

The second set of analyses modeled vertically emplaced canisters containing CHLW with and without 14.5 cm of loose crushed tuff packing (k = 0.185 [W/mK] for T < 372 K and k = 0.114 [W/mK] for T > 373 K). The peak centerline temperature for the analysis without the packing was 568 K (295°C). With packing included in the model the peak centerline temperature was near 1123 K (850°C) which is well above the design limit of 673 K (400°C) for CHLW.



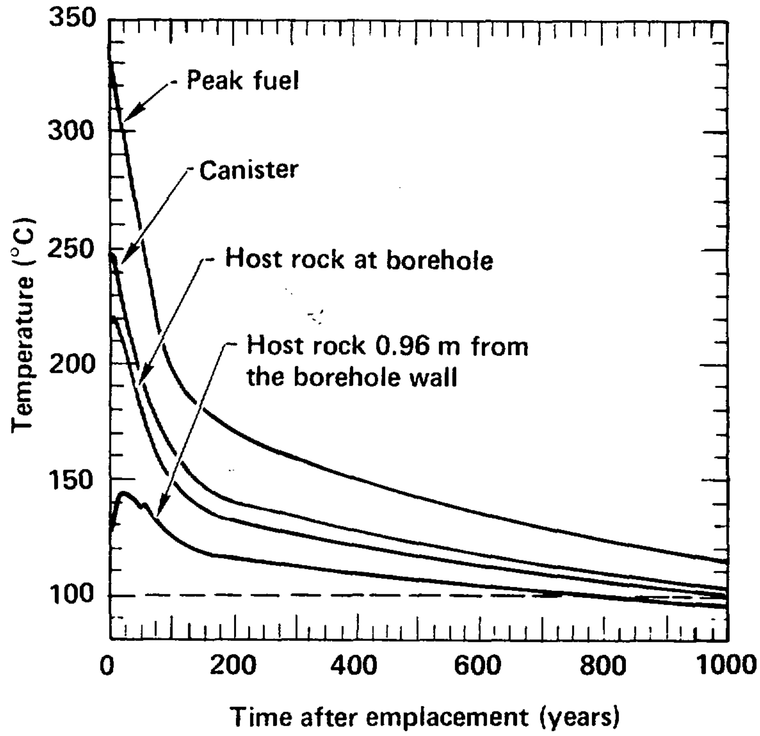
WF .... DHLW
APD .... 57.3 kW/acre
10 year power .... 0.680 kW
C_{diam} .... 81 cm
P_{bh} .... 11.40 m
P_{pkg} .... 3.5 m
Directory# D69HO.68A

Figure 4. Temperature histories of waste package components and host rock for horizontally emplaced DHLW (TACO2D infinite cylinder model)



WF........................CHLW
APD........................42.6 kW/acre
10 year power...........2.21 kW
C_{diam}...................32 cm
P_{drift}...................30.5 m
P_{pkg}....................5.9 m
Directory#...............C50V2.21C

Figure 5. Temperature histories of waste package components and host rock for vertically emplaced CHLW (TACO2D axisymmetric model)



WF .... BWR·SF

APD .... 43 kW/acre

10 year power .... 3.42 kW

C_{diam} .... 57 cm

P_{drift} .... 30.5 m

P_{pkg} .... 9.1 m

Directory# B50V3.42A

Figure 6. Temperature histories of waste package components and host rock for vertically emplaced BWR spent fuel (TACO2D axisymmetric model)

TABLE 3 Significant Input Parameters and Output Results for the 10 Year Old DHLW and CHLW Thermal Analyses Completed to Date

	DHLW			CHLW					
Directory Number	D50H0.38B	D69H0.56A	D69H0.68A	C50H2.21A	C50V2.21B	C50V2.21C	C50V2.21D	C75V2.21A	C100V2.21A
Emplacement Mode	H	H	H	H	V	V	V	V	V
Areal Power Density [kW/acre]	41.5	56.8	57.3	44.9	42.6	42.6	42.6	63.6	84.5
Package Power at Burial [W]	380	556	680	2210	2210	2210	2210	2210	2210
Canister diam [cm], material	61 SST	81 SST	81 SST	32.4 SST	32.0 SST	32.0 SST	32.0 SST	32.0 SST	32.0 SST
Overpack diam [cm], material	66 SST	86.1 SST	86.1 SST	37.5 SST	-	-	-	-	-
Borehole liner diam [cm] material	72.4 CS	92.4 CS	92.4 CS	43.8 CS	-	-	-	-	-
Packing outer diam [cm], material	-	-	-	-	-	-	61.0 LCT	-	-
Borehole diam [cm]	81.3	101.6	101.6	54.0	42.2	61.0	61.0	42.2	42.2
Borehole pitch [m]	8.8	9.4	11.5	44.0	-	-	-	-	-
Package pitch [m]	3.5	3.5	3.5	4.0	5.9	5.9	5.9	3.91	2.94
Drift pitch [m]	-	-	-	-	30.5	30.5	30.5	30.5	30.5
Number of internal fins, material	-	-	-	-	-	-	-	-	-
Model	IC	IC	IC	IC	AS	AS	AS	AS	AS
Temperature Limit [°C]	500	500	500	400	400	400	400	400	400
Peak waste temp [°C], time [yrs.]	121 17.5	154 30	165 17.5	333 2.0	330 1.0	293 1.0	849 0.5	355 1.5	391 2.0
Waste temp at 300 yrs [°C]	62	78	73	101	92	88	115	114	139
Waste temp at 1000 yrs [°C]	44	54	50	59	60	59	63	74	87
Peak borehole temp [°C], time [yrs.]	101 35	136 35	135 30	206 4.2	220 2.5	193 2.5	178 3.5	256 3.5	304 7.0
Peak temperature ∿ 1 m from borehole surface [°C]	96	129	127	145	124	121	118	171	235

Abbreviations:

H = Horizontal
V = Vertical
SST = 304L Stainless Steel
CS = Carbon Steel
LCT = Loose Crushed Tuff (K = 0.15 [W/mK], estimated)
IC = 2D Infinite Cylinder
AS = 2D axisymmetric

TABLE 4 Significant Input Parameters and Output Results for the BWR and PWR 10 Year Old Spent Fuel Thermal Analyses Completed to Date

	BWR			PWR								
Directory Number	B50V3.42A	B75V3.42A	B99V3.42A	P56H3.3A	P56H3.3B	P56H3.3C	P57H3.3C	P57H3.3B	P115H3.05A	P57H3.56A	P57H3.3A	P57H2.2A
Emplacement Mode	V	V	V	H	H	H	H	H	H	H	H	H
Areal Power Density [kW/acre]	43.0	63.7	84.5	43.2	43.2	43.2	43.6	43.6	82.5	43.8	43.6	42.0
Package Power at Burial [W]	3420	3420	3420	3300	3300	3300	3300	3300	3050	3560**	3300	2200+
Canister diam [cm], material	57.0 SST	57.0 SST	57.0 SST	45.0 SST	45.0 SST	45.0 SST	50.0 SST	50.0 SST	50.0 SST	65.0 SST	50.0 SST	40.0 SST
Overpack diam [cm], material	-	-	-	-	-	-	-	-	-	-	-	-
Borehole liner diam [cm] material	-	-	-	51.4 CS	86.4 CS	86.4 CS	62.2 CS	62.2 CS	62.2 CS	76.2 CS	86.0 CS	76.4 CS
Packing outer diam [cm], material	-	-	-	-	80.1 CCT1	80.1 CCT1	-	-	-	-	82.4 CCT1	72.5 CCT2
Borehole diam [cm]	67.2	67.2	67.2	61.0	96.5	96.5	69.0	69.0	69.0	86.4	92.8	81.3
Borehole pitch [m]	-	-	-	48.9	48.9	48.9	52.0	52.0	24.0	56.3	52.0	34.7
Package pitch [m]	9.1	6.1	4.6	4.8	4.8	4.8	4.5	4.5	4.5	4.5	4.5	4.5
Drift pitch [m]	30.5	30.5	30.5	-	-	-	-	-	-	-	-	-
Number of internal fins, material	*	*	*	6 SST	6 SST	-	6 CS	12 CS	12 CS	14 CS	24 CS	12 CS
Model	AS	AS	AS	IC	IC	IC	IC	IC	IC	IC	IC	IC
Temperature Limit [°C]	350	350	350	350	350	350	350	350	350	350	350	350
Peak waste temp [°C], time [yrs.]	336 2.0	357 4.0	394 9.0	342 2.5	379 2.0	449 2.5	343 3.0	327 3.0	345 13.0	330 5.0	374 2.5	326 3.0
Waste temp at 300 yrs [°C]	159	197	240	148	155	185	153	144	231	152	156	152
Waste temp at 1000 yrs [°C]	115	147	184	109	111	129	109	105	180	107	112	108
Peak borehole temp [°C], time [yrs.]	220 7.0	264 12.0	321 16.0	237 4.0	215 7.0	223 7.5	252 4.0	246 3.5	300 27.0	278 8.0	242 7.0	188 12.0
Peak temperature ~ 1 m from borehole surface [°C]	142	195	258	170	158	167	175	175	252	202	178	147

* = 17 horizontal fins with the equivalent volume as would be found in the reference vertically finned canister.
** = 7 fuel assemblies instead of six.
\+ = 4 fuel assemblies instead of six.

Abbreviations:
H = Horizontal
V = Vertical
SST = 304L Stainless Steel
CS = Carbon Steel
CCT1 = Compressed Crushed Tuff (K = 0.97 [W/mK], estimated)
CCT2 = Compressed Crushed Tuff (K = 0.65 [W/mK], measured)
IC = 2D Infinite Cylinder
AS = 2D axisymmetric

Any reasonable amount of packing necessitates redesign of the reference spent fuel canisters to avoid raising the peak fuel temperature above allowable limits. Further analysis showed that a canister containing only four PWR spent fuel rod assemblies would be required to satisfy the temperature limit. The thermal penalty of such a design would result in 50% more packages with the additional economic effects of larger boreholes, additional costs per packing assembly as well as the additional handling required per assembly.

Furthermore, an analysis of a horizontally emplaced PWR spent fuel canister with six radial internal heat conducting fins can be compared with an analysis of an identically emplaced canister but with twelve fins. Results show that doubling the number of fins reduces the peak waste temperature by about 16 K. This may or may not be a significant amount depending on how close the peak temperature of the spent fuel is to the design limit of 623 K (350°C) after uncertainty studies are conducted.

Conclusions

- Current reference conceptual designs do not exceed temperature limits.
- A significant thermal penalty may result if a packing is introduced into the waste package design. This effect is highly dependent on the material properties of the particular packing used. To stay within the temperature limits when packing is used, a lower heat output per package (implying more and smaller packages) will be required.
- The use of 6 heat transfer fins in a spent fuel canister with packing reduces the peak temperature by about 70°C.
- Doubling the number of heat transfer fins (from 6 fins to 12) in spent fuel canisters results in the reduction of the peak fuel temperature by about 16°C.

- Results from the WAPPA thermal submodel compare quite favorably with results from the thermal analyses reported here. The WAPPA thermal submodel predicted temperatures a maximum of 7% higher than the results from TACO2D.

Recommendations for Future Work

Before the conceptual design process is completed, a number of additional analyses will have to be done. Perhaps the most significant of these would be some form of uncertainty analysis. Questions as to the accuracy of the results remain with respect to the two-dimensional modeling of a three-dimensional canister/repository and including possible end effects not considered where boreholes of finite length are modeled as having infinite length. Once the number of conceptual designs are reduced then three-dimensional analysis could be utilized in a more economical way (both time and money) so as to answer some of these questions.

In addition, some uncertainty is involved in the choice of material properties used in the calculations. This is due in part to uncertainties in the experimentally measured tuff properties and in part to assumptions concerning air, water and steam behavior near emplaced canisters. Parameter studies may be used to bound the effects of some of these material property uncertainties.

Other parameter studies should be employed so that cost effectiveness is reflected in the final designs. Thermal analyses including additional variation in areal power density and canister diameter, are examples of potential studies which, when completed, could influence final designs.

Lastly, TACO2D should be documented using methods acceptable to regulatory agencies [6].

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