27
6-23-80
2 4B NTIS

MMB

MASTER

SAND79-1265
Unlimited Release
UC-70

Preliminary One-Dimenional Thermal Analysis of Waste Emplacement in Tuffs

Bruce M. Bulmer, Allen R. Lappin

Sandia National Laboratories

2900-Q(3-80)

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

SAND79-1265
Unlimited Release
Printed April 1980

Distribution
Category UC-70

PRELIMINARY ONE-DIMENSIONAL THERMAL ANALYSIS OF WASTE EMPLACEMENT IN TUFFS

Bruce M. Bulmer
Exploratory Systems Division V, 5623

Allen R. Lappin
Geological Projects Division 4537

Sandia National Laboratories
Albuquerque, NM 87185

ABSTRACT

One-dimensional calculations of near-field temperatures resulting from waste emplacement in a multiple-layered tuff stratigraphy are presented. Results indicate a marked sensitivity of peak temperatures to assignment of in-situ fluid pressure, geothermal-heat flux, waste type, and location of waste relative to a specific stratigraphic discontinuity. Under the criterion that allowable initial-power densities are limited by the occurrence of boiling at a distance of 10 m from emplaced waste, allowable power densities are calculated to range up to 150 kW/acre or more, depending upon geothermal heat flux and waste type.

CONTENTS

ILLUSTRATIONS

TABLES

PRELIMINARY ONE-DIMENSIONAL THERMAL ANALYSIS OF WASTE EMPLACEMENT IN TUFFS

Introduction

Silicic tuff is one geologic medium for which the US Department of Energy (DOE) is currently conducting waste-management feasibility studies. In most occurrences, such tuff is inherently layered and may show broad variations in porosity and water content through a local stratigraphic section. Correlated with the broad variation in porosity is marked variability in thermal properties--in particular, thermal conductivity. There is a need to estimate the effects of such highly variable thermal properties, combined with the inherent layering of tuffs, on any temperature field that may result from the disposal of high-level nuclear wastes in tuffs.

The present one-dimensional thermal modeling study of waste emplacement in tuff is based on the stratigraphy encountered in the Yucca Mountain exploratory hole Ue25A#1 drilled on the DOE Nevada Test Site (NTS) in FY78 (Figure 1). This hole, drilled as part of an ongoing waste-management feasibility study (the Nevada Nuclear Waste Storage Investigation Project), reached a depth of ~765 m and penetrated a stratigraphically complex sequence of tuffs.

This analysis represents the first thermal study performed for waste emplacement in layered tuffs. The objectives of this study were to begin developing a methodology for determining acceptable areal power densities for disposal in tuffs, and to measure the effects of several parameters on acceptable power densities calculated according to a defined criterion. These parameters include

1. The temperature at which boiling of formation water is assumed to occur

2. Local geothermal heat flux

3. Depth of the heat-producing zone below a defined stratigraphic discontinuity, above which tuff has a considerably lower thermal conductivity than in the layer in which the heat-producing zone is located

4. Uncertainties in assigned material properties of the tuffs in which the waste is emplaced

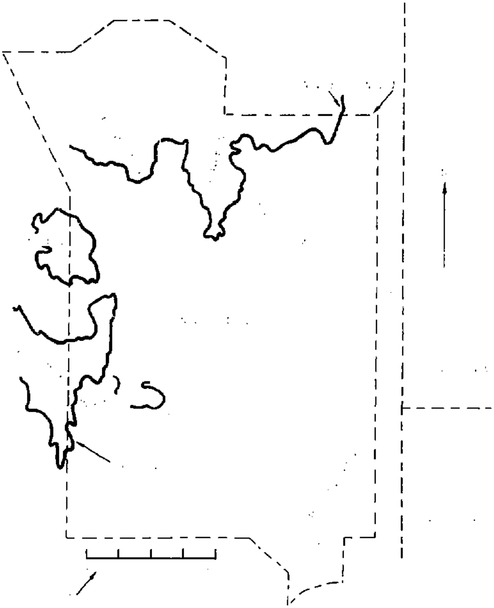

Figure 1. Generalized Map of NTS Showing Location of Yucca Mountain Exploratory Hole Ue25A#1

Calculations were made by using the one-dimensional finite-difference heat-conduction code CONDUCT.[1] The final result gives calculated maximum acceptable initial-power densities expressed as a function of geothermal heat flux, waste type, boiling criterion, and distance to a major stratigraphic interface.

Assumptions Made and Their Consequences

Inherent limits to the relevance of any phenomenological modeling study must be specified carefully; otherwise, the results can easily be taken out of context and interpreted to mean more (or less) than they should. This section discusses several assumptions made as part of this study and the consequences of these assumptions.

1. One-dimensional geometry is assumed. The main consequence of this assumption is that the calculations are valid only at distances great enough from a repository such that isotherms are essentially planar and parallel to the repository. Calculations made at Sandia Laboratories as part of the Waste Isolation Project Plant (WIPP) Program indicate that this distance is ~ 12 m, measured from the center line of a horizontal plane of vertical canisters emplaced in salt and assuming individual canisters are 5 m long.[2] Therefore, criteria developed in this study apply only at distances greater than 10 m from the top of the waste within the horizon of waste disposal. An additional result of this geometric assumption is that the waste must be treated as a uniform heat source; i.e., "smeared out" evenly within a heat-producing zone. Thus, no intrarepository information can be gleaned directly from these calculations. Because temperatures above the top of the heat-producing zone are a function only of the total thermal flux and thermal properties of the rock, the assignment of a 25-m thickness to this zone has no effect on the calculated temperatures in this area. In subsequent discussion, the plane forming the upper boundary of the heat-producing zone is denoted the "waste-rock interface."

2. Thermal properties of the tuffs are assumed temperature-independent. The primary result is that calculated results are

not valid beyond the initiation of in-situ boiling. The possible temperature effects of water volatilization and of liquid and vapor transport are thus not considered. Decreased conductivity above the boiling temperature would markedly affect temperatures inside the boiling isotherm but not those outside it. Since the beginning of boiling was used as a cutoff in these calculations (as explained below), this limitation is consistent with the goals of the study. It is not a limitation inherent in the CONDUCT code. The slight decrease in thermal conductivity characteristic of most rocks between ambient temperature and the boiling point is also ignored. This should have only a limited effect on the computed thermal field below the boiling temperature.

3. The waste types considered in this study are UO_2 spent fuel (SF) and conventional borosilicate high-level waste (HLW) with 30% fission-product loading. Both are assumed 10 yr out-of-core at the time of emplacement. The main consequence of these assumptions is that they allow use of two unique thermal-power histories, shown in Figure 2. At this stage of the study, it was inappropriate to consider a more varied suite of waste types (compare Reference 3).

4. It is assumed that the repository is perfectly backfilled; i.e., that the heat-producing zone has the same thermal conductivity as the surrounding emplacement medium. Thus, heat-transfer effects during the operational phase of the repository are ignored. Since the repository excavations are included within the thickness assigned to the heat-producing zone in these calculations and since the temperatures in the overlying strata are controlled by thermal flux only, lower thermal conductivity of possible backfill materials after the operational phase should have no effect on the calculations.

5. It is assumed that all thermal fluxes are perpendicular to the stratigraphy. This assumption ignores the possibility that the tuff layering might be inclined to the repository and/or the

earth's surface. In fact, the stratigraphy at the Yucca Mountain Hole Ue25A#1 is inclined ~10° to the horizontal. As a result of this inclination, the geometry at the site is two-dimensional, even in the first approximation.

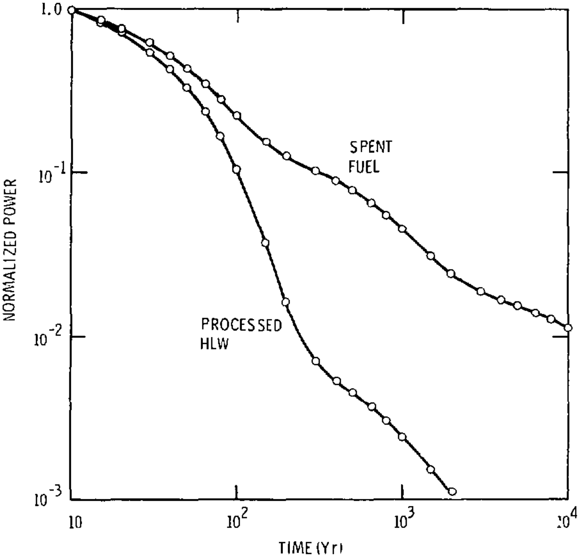

Figure 2. Normalized Power vs Time for UO_2 Spent Fuel and Processed HLW as a Function of Time. (Both waste forms assumed 10 yr out-of-core at time of emplacement)

Input Parameters

This section discusses the various parameters input into the assumed model as well as limits placed on the range of variable parameters.

Stratigraphy

The stratigraphic breakdown used for this study (Figure 3) is based on the original lithologic logs of Hole Ue25A#1 compiled during and shortly after drilling activities. More recent lithologic logs of the hole, based on overall examination of the core, agree well with the boundaries selected here.[4] Extensive variations in the apparent material properties of the tuffs were generalized by subdividing the entire stratigraphy into 10 distinct layers, as shown. Little advantage appears likely by more extensive subdivision of the layering at the present level of detail of available material property data. One-dimensional modeling does not apply near the heat-producing zone, where more detailed stratigraphic subdivisions might well be pertinent.

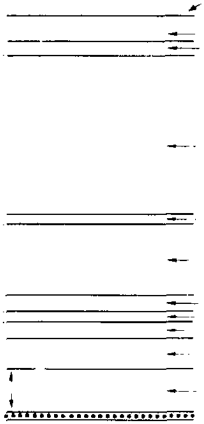

Figure 3. Generalized Stratigraphic Breakdown From Hole Ue25A#1 Used in Thermal Modeling

Thermal Properties

At the time of this modeling, thermal data on tuffs were very limited. These data[5] were consistent with assumption of a nearly linear relationship between thermal conductivity (K) and saturation at constant porosity (as shown in Figure 4), and with a nonlinear relation between porosity and conductivity, also shown. That the tuff conductivity data at zero saturation were collected at 110°C is ignored in generating Figure 4 because thermal conductivity above this temperature is temperature-independent. In assigning thermal conductivities to be used in this study, 80% saturation was assumed for tuff layers above the level of standing water in Ue25A#1 (470 m) and 100% below this level. Estimated thermal conductivities assigned to each generalized layer are given in Table 1.

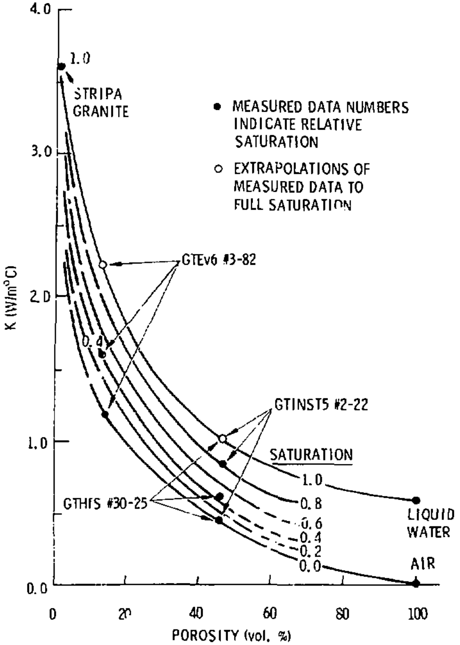

Figure 4. Porosity, Saturation, and Ambient-Temperature Thermal Conductivity Relationships Used in Assigning Thermal Conductivities to Tuffs From Hole Ue25A#1 (thermal conductivity of Stripa Granite taken from Reference 6)

TABLE 1

Generalized Stratigraphy and Material Properties Assumed, Based on Stratigraphy of Yucca Mountain Exploratory Hole Ue25A#1

Depth Interval					
m	ft	Lithology and Unit	ρ_b (g/cm^3)	K (W/m°C)	Porosity (approx.)
0 to 61	0 to 200	Density welded tuff--Tiva Canyon Member of Paintbrush Tuff	2.40	2.2	8
61 to 84	200 to 276	Nonwelded or bedded tuff--base of Tiva Canyon and separate bedded tuffs	1.70	0.75	50
84 to 401	276 to 1316	Welded Tuff--Topopah Spring Member of Paintbrush Tuff	2.30	1.8	14
401 to 414	1316 to 1358	Partially welded tuff--lower part of Topopah Springs	2.25	1.6	20
414 to 560	1358 to 1837	Nonwelded or bedded tuff	1.95	1.2	35
560 to 594	1837 to 1949	Partially welded tuff--Prow Pass Member of Crater Flats Tuff	2.10	1.5	25
594 to 614	1949 to 2014	Welded tuff--Prow Pass Member of Crater Flats Tuff	2.35	1.9	16
614 to 647	2014 to 2123	Partially welded tuff--Prow Pass Member of Crater Flats Tuff	2.25	1.7	20
647 to 711	2123 to 2333	"Slightly" welded tuff--Prow Pass Member of Crater Flats Tuff	2.0	1.3	30
711 to 1000	2333 to 3280	Partially welded tuff--Bullfrog Member of Crater Flats Tuff	2.35	1.8	18

If depths >1000 m are needed for long-term modeling, assume continuation of uniform Bullfrog

After this study, limited additional data became available on the thermal conductivity of tuffs from Hole Ue25A#1.[7] Table 2 compares measured and estimated ambient-temperature thermal conductivities and porosities within two depth zones of Hole Ue25A#1.

TABLE 2

Comparison of Estimated and Measured Thermal Conductivities for Two Tuffs From Hole Ue25A#1, NTS

Depth Zone (m)	Porosity (%)		Thermal Conductivity, (W/m°C)	
	Estimated	Measured (No. of samples)	Estimated	Measured (Depth of sample, m)
414 to 560	35	28-35 (6)	1.2	1.3 (473)
711+	18	18-24 (7)	1.8	2.2 (741)

As shown, there is very good agreement between estimated and measured conductivity values for the nonwelded tuffs. For the welded tuff below 711 m, the estimated value is about 20% low compared to the one sample for which conductivity has been measured. The sensitivities of computed temperatures to uncertainties in thermal conductivity and specific heat were also analyzed for an initial power density of 150 kW/acre, a waste thermal half-life of 27 yr, and one-dimensional geometry. These calculations indicate that for an average rock conductivity of 2 W/m°C, a 20% uncertainty in conductivity would lead to a 21°C uncertainty in the maximum temperature at the "waste-rock interface." The sensitivity of predicted temperatures to relative uncertainty in conductivity increases rapidly with decreasing conductivity. At lower power densities, the sensitivity of peak temperatures to material property uncertainties decreases.

In these calculations, the specific heat of all rocks is assumed to be 0.20 cal/g°C. This, as stated above, limits the validity of the calculations to the subboiling regime since the vaporization heat of contained water is not included. A 20% uncertainty in this value would result in a 13°C uncertainty in peak temperatures at the "waste-rock interface" under the assumed conditions.[8] The value used is among the lowest of the measured values of specific heat of tuffaceous rocks. Any error because of this assumption would therefore result in calculation of higher temperatures. Note also that the temperatures at the "waste-rock interface" are more sensitive to uncertainties in thermal-property assignments than are temperatures at points farther from the waste.

Geothermal Heat Flux

One goal of this study was to assess the effects of different geothermal heat fluxes on the maximum allowable initial-power densities. Fluxes measured within Nevada[9] generally fall between 1 and 3 HFU (1 HFU = 1×10^{-6} cal/cm^{2}s), except for Battle Mountain High, where values at least as high as 3.8 HFU have been measured. In the case of Yucca Mountain, the measured flux is reported as 1.6 HFU.[9]

Depth of Burial

A major goal of this study was to assess the effects of stratigraphic layering. It was assumed that the conductivity of nonwelded tuffs is too low to be acceptable for waste emplacement at reasonable power densities, and further that the Bullfrog Member of the Crater Flat Tuff was the target welded tuff (burial) zone. Under these assumptions, the stratigraphic contact of greatest interest is between the Bullfrog and the overlying Prow Pass Member of the Crater Flat Tuff. This contact occurs at a depth of 711 m in Hole Ue25A#1. Most depths used in the figures therefore refer to the depth of the top of the heat-producing zone (waste-rock interface) below the 711-m level. Additionally, the Bullfrog was assumed uniform in thermal properties and infinite in depth below 711 m.*

---

*This assumption was made to limit the study to the effects of one major interface and because of original uncertainties concerning the stratigraphic distances over which interface effects would operate. As discussed below, the interval over which this assumption is relevant to calculated temperatures is limited to 200 m; this interval includes the generalized repository.

Boiling Criteria

Three different assignments of boiling temperature were considered as part of this study, as shown in Figure 5. If it was assumed that boiling will occur at a fluid pressure of 1 atm, the boiling temperature is nearly insensitive to the depth of burial. This assignment of boiling temperature is equivalent to the assumption that the repository is located above the water table, and that the surrounding rocks are sufficiently permeable on the time scale of in-situ heating to avoid any volatile overpressuring. The assumption of atmospheric boiling has no direct applicability to disposal beneath the water table.

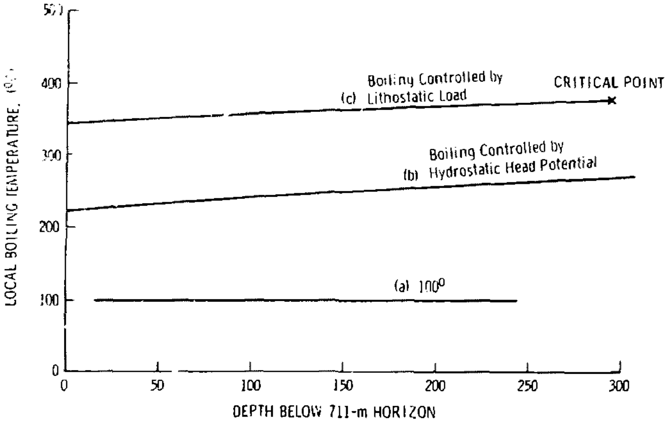

Figure 5. Three Different Assignments of Boiling Temperature

At the other extreme, it can be assumed that the boiling point is determined by the lithostatic load (ignoring additional, thermally induced confining pressure); i.e., the fluid and solid confining pressures are identical. This is equivalent to assuming that the rocks are totally impermeable on the time scale of the in-situ heating, and that the tuffs have no tensile strength. This assumption could apply both above and below the water table, given suitable in-situ permeabilities. It ignores the possibility of venting into any underground excavations, consistent with the requirements of one-dimensional modeling.

A third boiling criterion is that the boiling temperature is controlled by the potential height of a column of standing water between the disposal horizon and the local water table; i.e., by the hydrostatic head potential. This is equivalent to the assumption of fissure equilibrium, as defined by Thompson.[10] Any possible effects an actual repository would have on the local water table (as well as potential drainage of the underground excavations) are ignored. As shown in Figure 5, this assumption leads to intermediate boiling temperatures.

Results

The initial temperature distributions in the layered stratigraphy, calculated as a function of geothermal flux, are given in Figure 6. Specifically noted are the temperatures* at the interface at 711-m depth, and the calculated temperature gradients in the tuff below. These values were used in all later calculations and were simply added to the ΔT predicted to result from waste emplacement via linearity of the heat-conduction equation.

Figures 7, 8, and 9 show the temperature rises that are calculated to occur at the "waste-rock interface," and which result from disposal at the indicated initial power densities. These temperature rises are a function of increasing depth of the "waste-rock interface" below 711 m. These results have two main implications.

---

*Referenced to the "surface" temperature; i.e., the mean temperature at the shallowest depth that is free of significant diurnal and annual fluctuations.

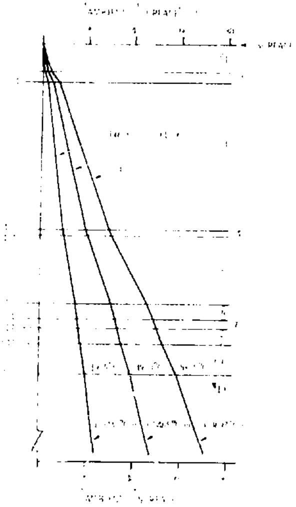

Figure 6

Calculated Temperature Increases with Depth in Generalized Yucca Mountain Stratigraphy as a Function of Geothermal-Heat Flux

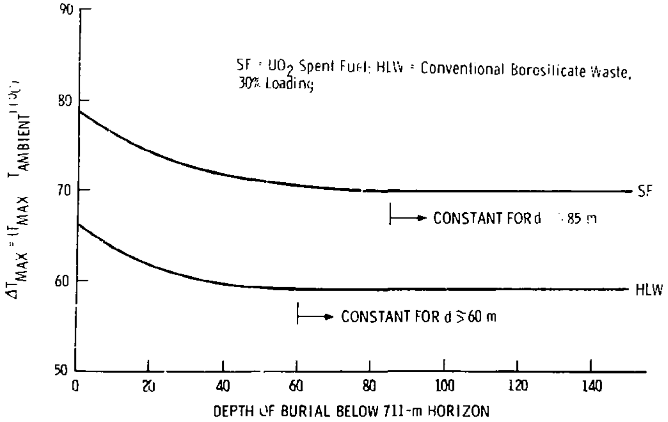

Figure 7. Calculated Temperature Rises at "Waste-Rock Interface" as a Function of Burial Depth Below 711 m (Initial Power Density = 50 kW/acre)

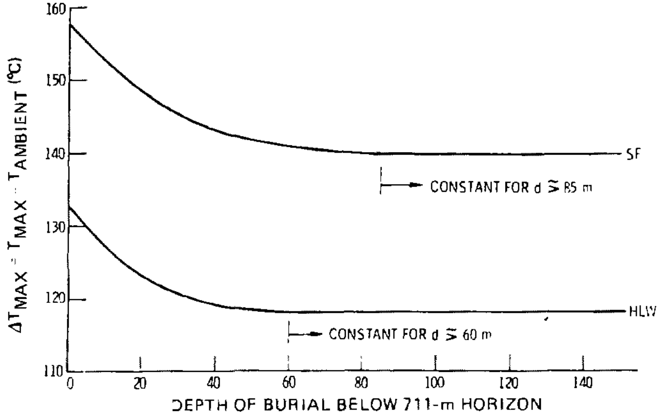

Figure 8. Calculated Temperature Rises at "Waste-Rock Interface" as a Function of Burial Depth Below 711 m (Initial Power Density = 100 kW/acre)

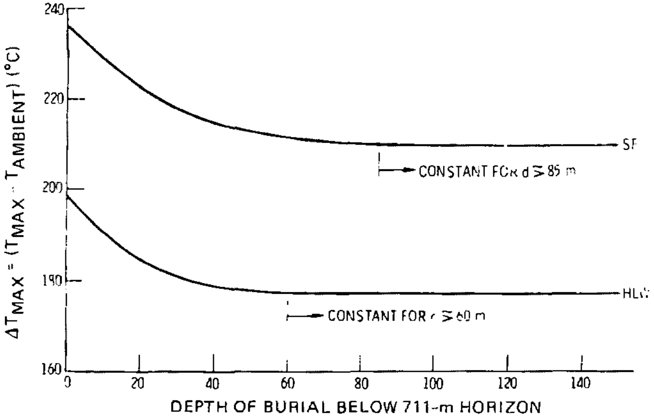

Figure 9. Calculated Temperature Rises at "Waste-Rock Interface" as a Function of Burial Depth Below 711 m (Initial Power Density = 150 kW/acre)

In the case of reprocessed HLW, a half-thickness of homogeneous disposal medium of ~60 m appears sufficient to damp out any major stratigraphic effect on the peak temperatures occurring at the "waste-rock interface." However, the inherent limitations of the one-dimensional calculation increase the required thicknesses. Allowing a total thickness of 25 m for the region within which isotherms are distinctly nonplanar (see Assumption 1), it appears that a unit thickness of 145 m (60 + 60 + 25) suffices to eliminate the effects of stratigraphy on peak temperatures at the "waste-rock interface." Since temperatures of the waste itself are expected to peak earlier than points beyond this distance, even thinner layers could be considered without any effect on the maximum temperature of the waste. Such detail cannot, however, be defined by one-dimensional modeling. The requisite layer thicknesses do not appear to be a function of initial areal power density but of the waste type. By the same logic as used in the case of HLW, a layer thickness of 195 m (85 + 85 + 25) would appear to eliminate stratigraphic effects on peak temperatures in disposal of spent fuel. There is no requirement to completely eliminate stratigraphic effects on temperatures resulting from emplacement; the objective here is merely to estimate the distance over which stratigraphic effects may need to be considered.

Figures 10 and 11 indicate maximum calculated temperatures (including effects of variable geothermal fluxes) for two representative cases: disposal of HLW at 150 kW/acre and disposal of UO_2 spent fuel at 100 kW/acre. Results are shown as a function of both depth and geothermal flux for an assigned "surface" temperature of 20°C. As shown, there is in all cases a unique depth at which the resultant absolute temperatures are predicted to be a minimum; this is because the lower temperatures resulting from increased distance from the stratigraphic interface at 711 m are eventually offset by the increasing initial temperatures resulting from the geothermal gradient. Note that the observed minima (denoted by arrows) are very shallow in nature. Also shown in these figures is the calculated boiling temperature, assuming the boiling criterion is based on the hydrostatic head potential.

As indicated in Figure 11, disposal of spent fuel at a power density of 100 kW/acre is not predicted to result in boiling under this assumption except very near (within 21 m) of the interface considered here (711 m), and for high-geothermal-heat flux (3 HFU). In the case of disposal of HLW at an initial-power density of 150 kW/acre (Figure 12), boiling would occur for all burial depths at a geothermal flux of 3 HFU, also at the lower assumed fluxes in some cases, depending on the distance of the repository from the interface being considered.

For both cases shown in these figures, no boiling is predicted for any burial depth, assuming that boiling is controlled by the lithostatic pressure. Extensive boiling at all burial depths is predicted if volatilization occurs at a fluid pressure of 1 atm. The fact, as shown in Figure 12, that the calculated temperature increases that result from waste emplacement are linearly proportional to the initial power density permits linear interpolation to be used in estimating power densities at which boiling would occur.

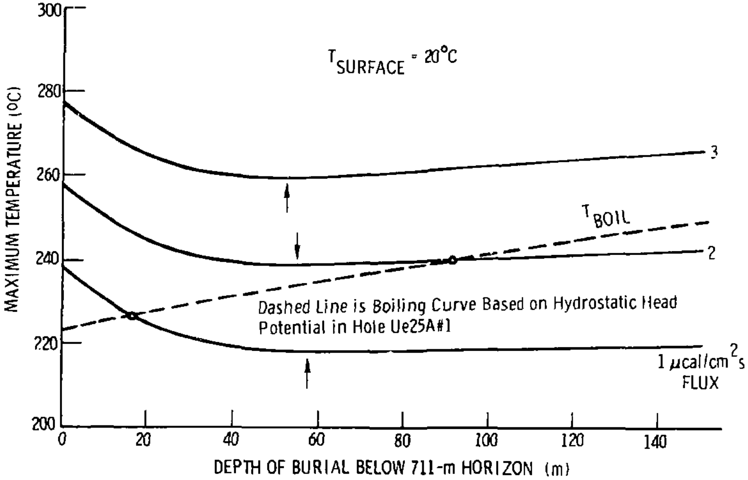

Figure 10. Maximum Temperatures at the "Waste-Rock Interface" as a Function of Burial Depth Below 711 m (emplacement of HLW at 150 kW/acre)

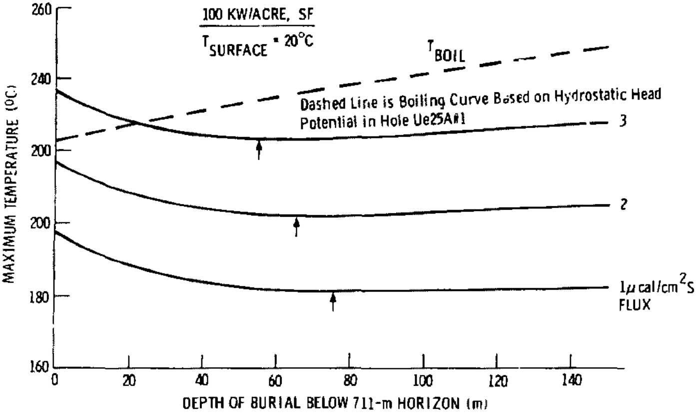

Figure 11. Maximum Temperatures at the "Waste-Rock Interface" as a Function of Burial Depth Below 711 m (emplacement of SF at 100 kW/acre)

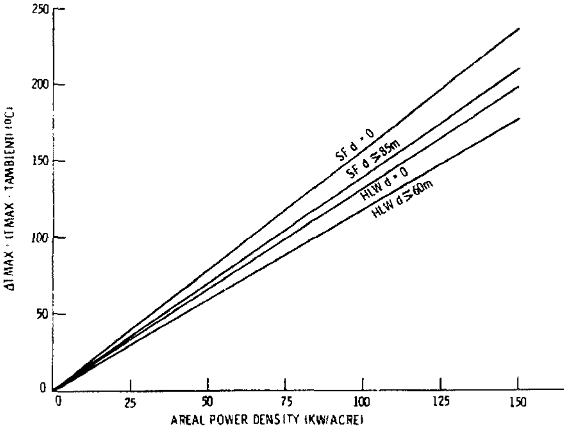

Figure 12. Calculated Temperature Rises Resulting From Waste Emplacement as a Function of Waste Type, Initial-Power Density, and Burial Depth

Conclusions

Figure 13 presents a general summary of the calculations made as part of this study, assuming that boiling is controlled by the hydrostatic head potential and that the permissible power density is dictated by the occurrence of boiling at the "waste-rock interface" at a level ~10 m above the waste. As shown, there is a fairly complex interplay of burial depth, geothermal flux, permissible power density, and waste type. Regardless of waste type, allowable power densities are strongly affected by the stratigraphy only for burial depths within about 50 m of the interface at 711 m. For depths exceeding this, there is a slight but continuous increase in permissible loadings. The boiling temperature increases more rapidly at this depth because of increasing hydrostatic head than does the ambient temperature. The effects of near proximity to the stratigraphic interface appear greater in the case of conventional HLW than for spent fuel because the time-to-peak temperature is shorter for HLW. At a given depth of emplacement, there is a linear relation between geothermal-heat flux and allowable power density, permitting extrapolation of these results to higher and lower fluxes than for those fluxes considered here. In all cases, allowable power densities are lower for spent fuel than for HLW for a given geothermal-heat flux because of the slower decay of the thermal power of spent fuel. Assuming a constant temperature uncertainty, resulting from the difference between the estimated and measured thermal conductivity of the Bullfrog Tuff (1.8 vs 2.2 W/m°C), calculated permissible densities estimated here for both waste forms would appear to be low by ~15 kW/acre.

Under the assumption of hydrostatically controlled boiling, allowable power densities range from 110 to >150 kW/acre for HLW, depending upon the burial depth and the geothermal-heat flux. For spent fuel, the range is from 92 to 150 kW/acre. Little or no boiling would occur under the assumption of lithostatically controlled boiling up to power densities of >150 kW/acre for either waste form. In the case of boiling at 100°C, extensive boiling would occur for almost any waste loading considered here.

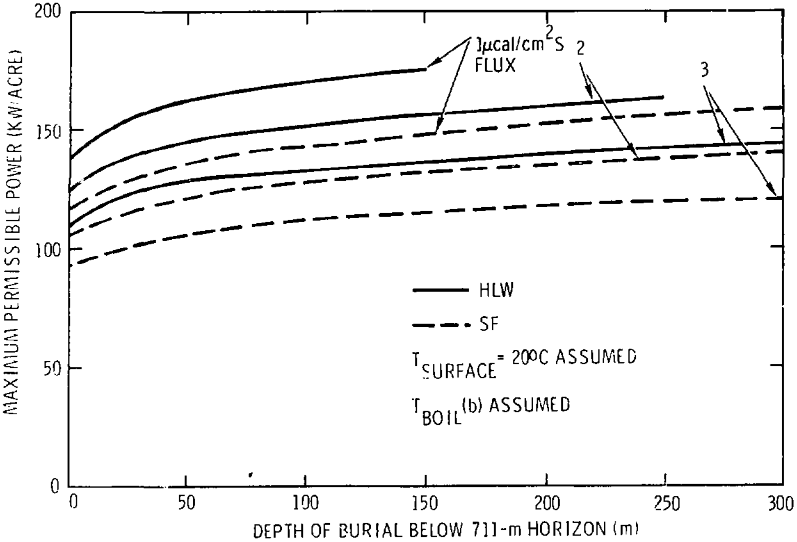

Figure 13. Calculated Maximum Permissible Initial-Power Densities for Waste Disposal in the Bullfrog Member of the Crater Flat Tuff. (Factor limiting power density is assumed occurrence of boiling at a distance of 10 m from emplaced waste)

Great care must be taken in interpreting these results. Specifically, it must be understood that the consideration of boiling at the "waste-rock interface" 10 m above the waste is only a calculational device. This device allows study of the effects of variable assumptions about the temperature at which boiling would occur and is dictated by the requirements of one-dimensional modeling. Any criterion of acceptable power densities based upon boiling would appear to have a similar sensitivity to in-situ fluid pressures, which are largely unknown at depth and are a function of in-situ water head and both liquid and steam permeabilities.

References

1. B. M. Bulmer, "User's Instructions for Program CONDUCT," Sandia Laboratories, Unclassified Internal Memorandum, RS 5511/1000, September 1978.

2. J. Tillerson, personal communication. Sandia Laboratories, Albuquerque, NM, September 1978.

3. R. C. Lincoln, D. W. Larson, and C. E. Sisson, *Estimates of Relative Areas for the Disposal in Bedded Salt of LWR Wastes From Alternative Fuel Cycles*, SAND77-1816 (Albuquerque, NM: Sandia Laboratories, 1978).

4. "Preliminary Lithologic Log of Drill Hole Ue25A#1," US Geological Survey Internal Communication, R. W. Spengler to W. W. Dudley, Jr., January 12, 1979.

5. N. B. C. Yelamanchili, "Thermal Conductivity and Physical Properties of Rock Cores From G-Tunnel," Laboratory Report 173, Holmes and Narver, Inc., NTS, to A. R. Lappin, Sandia Laboratories, July 24, 1978.

6. H. Carlsson, *A Pilot Heater Test in the Stripa Granite*, LBL-7086(SAC-06, UC-70), (Berkeley: Lawrence Berkeley Laboratory Report, August 1978).

7. N. B. C. Yelamanchili, "Thermal Conductivity Tests on Tuff Samples from Ue25A#1 Drill Hole," Laboratory Report 206B, Holmes and Narver, Inc., NTS, to A. R. Lappin, Sandia Laboratories, July 31, 1979.

8. B. M. Bulmer, "Thermal Properties Sensitivity in Geologic Media Surrounding Buried Heat Sources," Sandia Laboratories Internal Memo, February 28, 1978.

9. J. H. Sass et al, "Heat Flow in the Western United States," *Geophy Res*, 76:6376-6413, 1971.

10. J. B. Thompson, "The Thermodynamic Basis for the Mineral Facies Concept," *Am J Sci*, 253:65-103, 1955.