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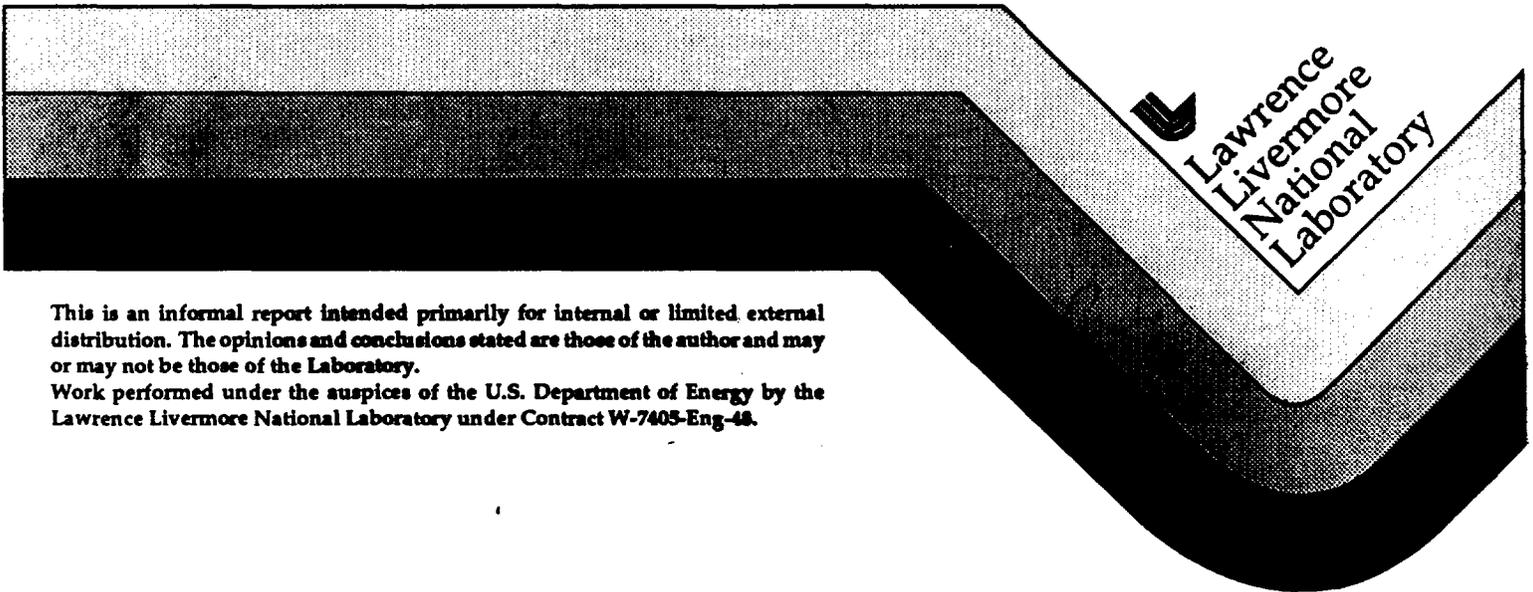
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**THERMAL CALCULATIONS PERTAINING TO A
PROPOSED YUCCA MOUNTAIN
NUCLEAR WASTE REPOSITORY**

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HYDROLOGY DOCUMENT NUMBER 699

February 1990



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Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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Accession Number: NNA.900925.0060

Abstract

In support to the Yucca Mountain Project waste package and repository design efforts, LLNL conducted heat-transfer modeling of the volcanic tuff in the repository. The analyses quantify: (a) the thermal response of a finite size, uniformly loaded repository where each panel of emplacement drifts contains the same type of heat source; (b) the response given a realistic waste stream inventory to show the effect of inter-panel variations; and (c) the intra-panel response for various realistic distributions of sources within the panel. The calculations, using the PLUS family of computer codes, are based on a linear superposition, in time and in space, of the analytic solution of individual, constant output point sources located in an infinite, isotropic, and homogeneous medium with constant thermal properties.

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ACRONYMS

APD	areal power density
ARRAYF	computer code
BWR	boiling water reactor
CDR	Conceptual Design Report
DAYLITE	computer code
DHLW	defense high-level waste
FD	finite difference
FE	finite element
FIFO	first in-first out
GWD	gigawatt-days
LLNL	Lawrence Livermore National Laboratory
MTU	metric tons of uranium
ORIGEN	computer code
ORNL	Oak Ridge National Laboratory
PLUS	computer code
PWR	power water reactor
SF	spent fuel
TWIGS	computer code
YMP	Yucca Mountain Project

1. Introduction

Researchers in the Yucca Mountain Project (YMP) are designing an underground facility and containers for the long-term disposal of spent nuclear fuel and high-level radioactive waste. It is proposed to bury these waste containers in a mined underground repository in the unsaturated volcanic tuff above the local water table under Yucca Mountain, Nevada. The underground portion of the repository is approximately 1000 ft below the surface and covers approximately three square miles. This repository is designed to accommodate about 63,000 metric tons of spent reactor fuel in more than 25,000 containers and about 7,000 tons of vitrified defense high-level waste (i.e., waste suspended in a glass matrix) in approximately 14,000 packages. The containerized waste is to be emplaced over a 25-year period. During the first 300 years after the repository is filled, the emplaced waste will deposit ~ 6 GW-yr of decay heat into the rock. This will raise the temperature of the rock well above ambient temperature for extended times.

Lawrence Livermore National Laboratory (LLNL) has been responsible for designing, modeling, and testing the waste forms and containment barriers. Data from these efforts will be incorporated in the final waste package designs and specifications. The current design approach for nuclear waste containment at the proposed Yucca Mountain Repository makes use of the thin wall of the metallic containers as a containment barrier. Ensuring acceptable waste containment periods with these containers is mainly dependent on minimizing the corrosion experienced during long-term disposal. The Yucca Mountain site, with its unsaturated volcanic tuff, was chosen because it is expected to provide with an environment with little movement of liquid water, well suited for disposal.

During the period when container wall temperatures are highest (i.e., approximately the first 300 years after emplacement), the presence of liquid water near the container would increase corrosive degradation of the containment barrier. A licensing strategy has established a tentative goal that 95% of the emplacement boreholes have no liquid water in contact with their containers for these first 300 years.

As a goal for our early design analyses, we chose to ensure this "no-liquid" condition in the heated boreholes by establishing a minimum-allowable borehole wall temperature of 97°C for the first 300 years. Since 97°C is about the boiling point of water at the altitude of the underground repository, this will preclude any liquid water from collecting in the borehole. Two other temperature conditions were also evaluated

during the early design analysis work to clarify whether the predicted peak temperature of the power water reactor (PWR) or boiling water reactor (BWR) fuel cladding ever exceeds 350°C and whether the tuff temperature 1 m (3.3 ft) from the borehole wall exceeds 200°C. The 350°C spent fuel (SF) cladding limit is set to minimize creep in the fuel rod's cladding, which provides another containment barrier for the radioactive material. The 200°C limit helps avoid stresses in the tuff from the dispersed mineral cristobalite which changes phase and expands by 5% between 200°C and 250°C.¹

Previous thermal analyses, documented in the Conceptual Design Report (CDR)², provided some preliminary evaluation of the effects of container load and spacing with variable areal power density (APD). The CDR thermal model assumes an infinite array of equally spaced and equally loaded containers in boreholes with no packing or borehole liner. The thermal effects are documented in terms of the temperatures in the mined drifts providing access to the emplaced containers, the peak cladding temperature of the SF waste, and the temperature of the tuff 1 m from the borehole wall. The CDR also documents the results of studies of the effects of horizontal and vertical emplacement. Some effort was made to model the effect of heat removal by the ventilation in the drifts. The CDR reports the transient thermal response during the first 100 years after emplacement. The analyses were done using the ARRAYF computer code from Sandia along with some simple finite element models.

To support the waste package and repository design effort, LLNL has conducted additional thermal modeling of the repository. This report documents the results of a series of transient conduction heat-transfer analyses to predict the thermal response of the tuff. These LLNL analyses quantified: (a) the panel edge and repository boundary effects if the model assumes a finite repository with each panel containing a distribution of the same heat sources; (b) the effect of inter-panel variations by using a realistic non-uniform panel-by-panel distribution of heat sources (where the modeled sources in any given panel are set equal to the panel average); and (c) the effect of intra-panel variations by using a realistic distribution of sources within the panel. These recent analyses are compared in terms of borehole wall (or inter-panel) temperature variations and determinations of the major contributing factors to the predicted temperature rises.

In this study, the PLUS family of computer codes was used to determine the temperature-time histories from emplacement up to 10,000 years after emplacement for the rock surrounding the waste containers. Evaluation of the performance limiting regions can be established by borehole wall temperature distributions at the time of peak local temperature, at 300 years after emplacement, and at 1000 years after emplacement.

2. Problem Definition

2.1 Panel and Source Description

The calculational models use a "nominal" set of repository dimensions and waste characteristics.² The panel and drift layout in the repository is shown in plan view in Fig. 1. The repository conceptual design contains 17 panels. Each panel contains 10 to 29 parallel emplacement drifts on 126-ft spacings. The major emplacement drifts contain 75 to 150 SF containers emplaced in vertical boreholes spaced up to 15 ft apart along the drifts. Some of these drifts have provisions for commingling the defense high-level waste (DHLW) in boreholes at midpoints between SF containers.

In this design, most of the SF containers contain groups of fuel rods consolidated to twice the density of an intact reactor fuel bundle. Panels 1 and 2 are filled before facilities are available for fuel rod consolidation. The fuel bundles in these panels (stored intact from the reactor) have one-half as much SF per container as do the other panels. Thus, the boreholes in each drift of these two panels are 7.5 ft apart to give the same local power density as the other panels. There are 340 drifts in this basic repository layout, containing the equivalent of 24,628 SF containers. Each container has an average of 2.64 metric tons of uranium (MTU), except in Panels 1 and 2, which have 1.32 MTU per container.

The APD is a parameter documenting the average energy deposited over the entire repository plane. It includes the effects of drift and panel geometry and nonstorage work areas. It basically controls the overall thermal response of the repository (in particular, the average wall temperature for boreholes in the repository). A given container's thermal output in addition to the thermal output and the proximity

(inter-borehole and drift spacing) of its neighbors govern its own borehole wall temperature.

Because of the relatively low thermal conductivity of the host rock, the short-term package temperature response (e.g., peak cladding temperature) is determined primarily by the container's own thermal output. The waves of heat from neighboring containers arrive years after the period of peak cladding temperature. Thermal output of SF waste is determined by its age (time out-of-core) and burn-up (energy output while in the reactor core). Centuries after emplacement, borehole wall temperature will be controlled chiefly by the spacings and thermal outputs of the array of surrounding containers. The burn-up of the SF waste primarily controls its long-term thermal output.

2.2 Source Thermal Output

The SF waste stream ranges in age from 5 to 35 years out-of-core and in burn-up from 5 to 60 gigawatt-days per metric ton of uranium (GWD/MTU).³ Figure 2 shows the distribution in burn-up of the oldest 63,000 tons of SF waste in the national inventory. Its average age is 18 years and its average burn-up is 33.6 GWD/MTU. By comparison, the analyses in the CDR usually assumed a waste stream 10 years out-of-core and with 30 GWD/MTU burn-up.

For this report's studies, the nominal thermal output at emplacement is 3300 W per package for the consolidated SF and 470 W per package for the DHLW. Packages containing only unconsolidated SF emit one-half of the consolidated value, or 1650 W. Table I, also derived from Ref. 3 and the emplacement schedule from Ref. 4, shows one possible "realistic" emplacement schedule with its waste characteristics. In this table, 5 years have been added to the emplacement dates used in Ref. 4. The SF burn-up, age, and emplacement date are based on a panel average. In reality, each panel will be filled over a year or two and will contain a distribution of fuel ages and burn-up. The column labelled "Areal Power Density" gives the initial kilowatts per acre at emplacement in each panel that would result if all the SF is 10 years out-of-core.

The thermal output from the PWR and the BWR SF derived from ORNL's ORIGEN calculations,³ is represented in terms of power vs time per MTU at various burn-ups. For ease of calculation, we further normalized the output from the 12 burn-

up ranges (over 20-40 GWD/MTU for both BWR and PWR SF) to a unit burn-up (Fig. 3). Figure 4 shows the corresponding power curve in terms of watts per canister for DHLW.⁵ In the case of SF, the power output per unit burn-up is approximately proportional to the age to the minus two-thirds power. The SF thermal output decreases very rapidly in the early years after removal from the reactor.

2.3 Additional Model Data

The thermal properties of the host rock (i.e., thermal conductivity, k , and thermal diffusivity, κ , of the unsaturated volcanic tuff) are given in the 1985 version of the Keystone document.⁶ These values are:

$$k = 1.84 \text{ W/m-K} \qquad = 0.5608 \text{ W/ft-K, and}$$

$$\kappa = 8.52 \times 10^{-7} \text{ m}^2/\text{s} \qquad = 289.36 \text{ ft}^2/\text{yr.}$$

This conductivity is about 10 percent lower than that used in the CDR.¹

An upper limit to a repository-wide APD can be set by varying the container spacing and loads such that the coolest borehole wall temperature always exceeds 97°C for the first 300 years. However, this would probably result in many containers whose SF cladding temperature exceeds the 350°C limit. A more acceptable repository-wide APD could be similarly set such that the average borehole wall temperature always exceeds 97°C for the first 300 years. But at this APD, there would be several sections where the borehole wall temperatures are less than the 97°C desired condition. These overcooled boreholes occur in groupings of containers with thermal loads well below the mean load (i.e., "cold" loads) or in groupings of containers located near the edges of drifts or panels in the repository (i.e., decreased communal warming).

Table I.
Panel by Panel Heat Source Descriptions

**The areal power density is the initial kW/acre if all the SF is
10 years out-of-core at emplacement.**

Panel Thermal Source Location & Output Synopsis - NRP Repository Design / Plus Facility Model

(This is an extension of Montan case data/05/31jul87)

Units: temperature=deg.C, power=W, length=ft, time=yr, conductivity=W/ft-C, diffusivity=ft²/yr

Teff Properties		Diffusivity		Conductivity		T-ambient		Spent Fuel									
289.36		0.5608		75													
Panel No.	X _{mid} 1st row	Y _{mid} 1st row	Z _{mid} 1st row	No. drifts	Drift spacing	Source Spacing	Tot. len. source	No. source per drift	No. source per panel	RTU per container	RTU per panel	Average Burnup per panel	(RTU*BU) per panel	Year exit core	Age at emplacement	Year replaced	Areal Power Density
1	472.5	1914	-17.5	10	126	7.50	532.5	71	710	1.321	937.9	16.6	15569	1971.7	32.5	2004.2	33.7
2	1490.0	2512	-17.5	13	126	7.50	937.5	125	1625	1.321	2146.8	18.5	39713	1976.1	30.8	2006.9	37.6
3	2800.0	3161	-17.5	24	126	15.00	1125.0	75	1800	2.642	4755.6	26.3	125072	1980.8	28.0	2008.8	53.4
4	4200.0	3287	-17.5	25	126	15.00	1125.0	75	1875	2.642	4953.8	29.7	147126	1984.9	25.4	2010.3	60.3
5	5600.0	3035	-17.5	23	126	15.00	1125.0	75	1725	2.642	4557.5	32.3	147206	1988.1	23.9	2012.0	65.6
6	7000.0	2531	-17.5 17 (1+2 empty)	126	15 or 7.5	1125.0	75 or 151	1427	2.619	3737.4	33.4	124829	1990.4	22.8	2013.2	67.8	
6(A)	6445.0	2531	-17.5	4	126	15.00	1125.0	75	450	3.000	1350.0	33.4	45090	1990.4	22.8	2013.2	67.8
6(B)	6437.5	1775	-17.5	2	630	7.50	1125.0	151	302	1.200	367.4	33.4	12104	1990	22.8	2013.2	67.8
6(C)	6445.0	1649	-17.5	4	126	15.00	1125.0	75	300	3.000	900.0	33.4	30060	1990	22.8	2013.2	67.8
6(D)	6445.0	1019	-17.5	5	126	15.00	1125.0	75	375	3.000	1125.0	33.4	37575	1990.4	22.8	2013.2	67.8
7	8400.0	1775	-17.5	13	126	15.00	1125.0	75	975	2.642	2576.0	34.6	89128	1992	21.6	2014.5	70.2
8	9800.0	1649	-17.5	17	126	15.00	1125.0	75	900	2.642	2377.8	35.5	84412	1994.8	20.4	2015.2	72.1
9	10915.0	1901	-17.5	14	126	15.00	555.0	37	510	2.642	1368.6	35.8	48994	1995.6	19.4	2015.0	72.7
10	9800.0	-1397	-17.5	10	126	15.00	1125.0	75	750	2.642	1981.5	36.4	72127	1997.8	18.7	2016.5	73.9
11	8400.0	-2279	-17.5	17	126	15.00	1125.0	75	1275	2.642	3368.5	36.5	122952	1999.4	17.8	2017.2	74.1
12	7000.0	-2783	-17.5	21	126	15.00	1125.0	75	1575	2.642	4161.2	36.5	151882	2002.5	16.0	2018.5	74.1
13	5600.0	-3287	-17.5	25	126	15.00	1125.0	75	1875	2.642	4953.8	36.5	180812	2006.3	13.6	2019.9	74.1
14	4200.0	-3791	-17.5	29	126	15.00	1125.0	75	2175	2.642	5746.3	36.5	209742	2010.1	11.6	2021.7	74.1
15	2800.0	-3791	-17.5	29	126	15.00	1125.0	75	2175	2.642	5746.3	36.5	209742	2015.1	10.5	2023.6	74.1
16	1400.0	-3791	-17.5	29	126	15.00	1125.0	75	2175	2.642	5746.3	36.5	209742	2015.5	10.0	2025.5	74.1
17	285.0	-3791	-17.5	29	126	15.00	555.0	37	1073	2.642	2834.9	36.5	103673	2016.9	10.0	2026.9	74.1
Totals				340		D H L W		24628		61949.9	33.6	2082520		18.1		68.2	

Panel No.	X _{mid} 1st row	Y _{mid} 1st row	Z _{mid} 1st row	No. drifts	Drift spacing	Source Spacing	Tot. len. source	No. source per drift	No. source per panel	Year exit core	Age at replace.	Year replaced	
1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
3	2800.0	3161	-15.0	4	126	15.00	1140.00	76	304	1974.0	35.0	2009.0	
4	4200.0	3287	-15.0	9	126	15.00	1140.00	76	684	1975.4	35.0	2010.4	
5	5600.0	3035	-15.0	9	126	15.00	1140.00	76	684	1976.0	35.0	2011.0	
6	6437.5	2531	-15.0	6	126	15.00	1140.00	76	456	1978.4	35.0	2013.4	
7	8400.0	1775	-15.0	5	126	15.00	1140.00	76	380	1979.5	35.0	2014.5	
8	9800.0	1649	-15.0	5	126	15.00	1140.00	76	380	1980.5	35.0	2015.5	
9	10915.0	1901	-15.0	5	126	15.00	570.00	38	190	1981.2	35.0	2016.2	
10	9800.0	-1397	-15.0	4	126	15.00	1140.00	76	304	1981.6	35.0	2016.6	
11	8400.0	-2279	-15.0	5	126	15.00	1140.00	76	380	1982.5	35.0	2017.5	
12	7000.0	-2783	-15.0	6	126	15.00	1140.00	76	456	1984.4	34.2	2018.6	
13	5600.0	-3287	-15.0	9	126	15.00	1140.00	76	684	1993.4	26.6	2020.0	
14	4200.0	-3791	-15.0	11	126	15.00	1140.00	76	836	1998.6	23.2	2021.8	
15	2800.0	-3791	-15.0	11	126	15.00	1140.00	76	836	2000.8	23.0	2023.8	
16	1400.0	-3791	-15.0	11	126	15.00	1140.00	76	836	2002.9	23.0	2025.9	
17	285.0	-3791	-15.0	11	126	15.00	570.00	38	418	2004.4	23.0	2027.4	
Totals				340				7828		29.8			

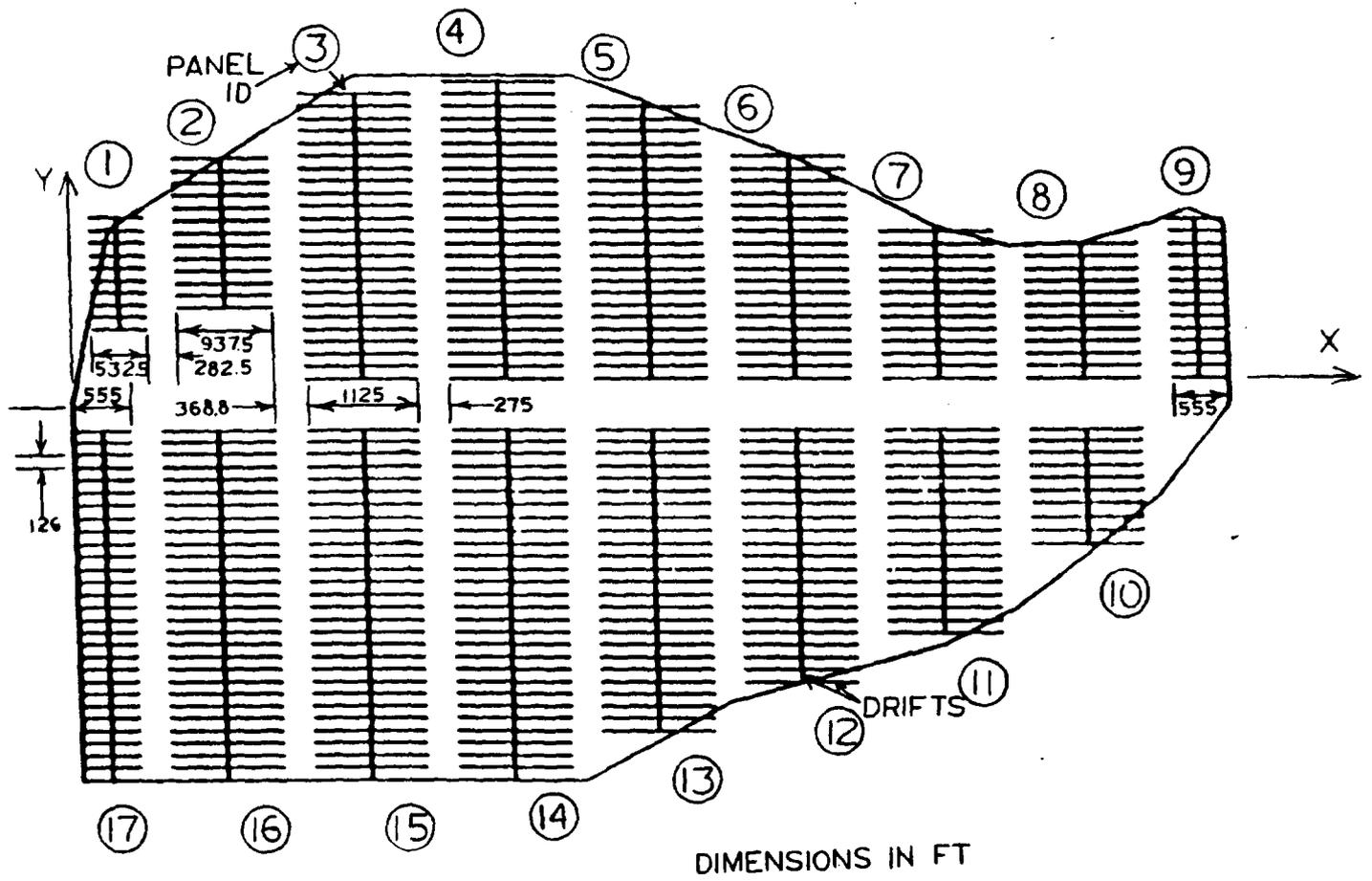


Figure 1. The layout of the modeled repository includes 17 panels.

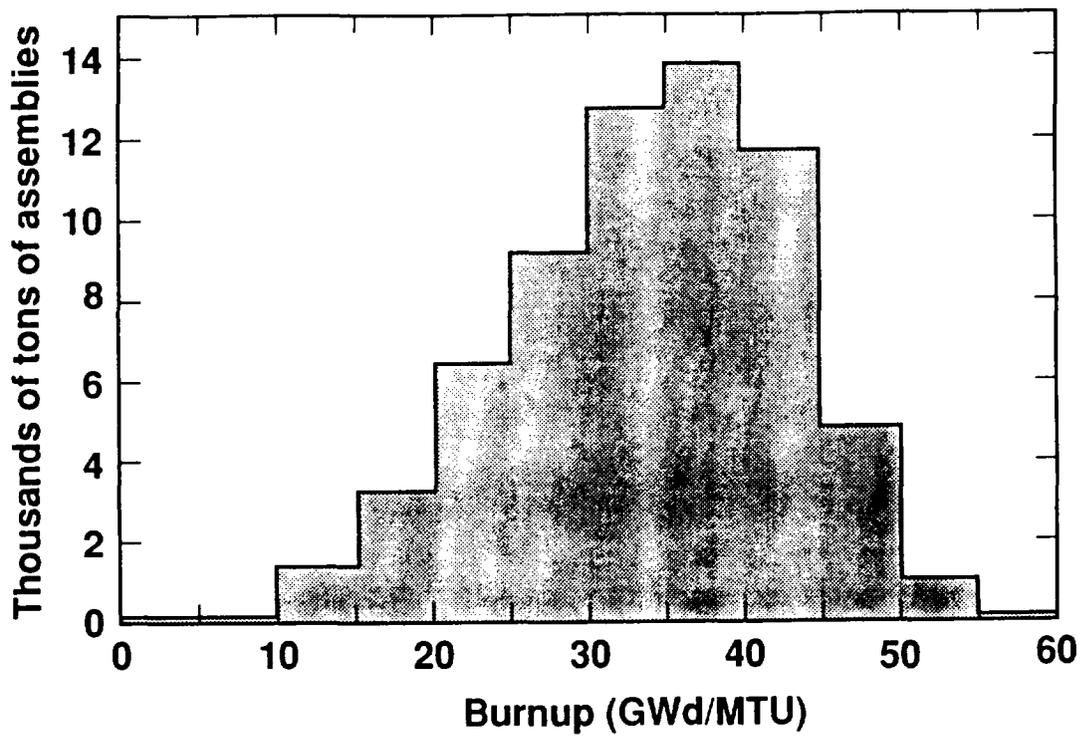


Figure 2. The distribution in terms of burn-up of the first 62K tons of SF waste inventory ranges from 3 to 57 GWD/MTU.

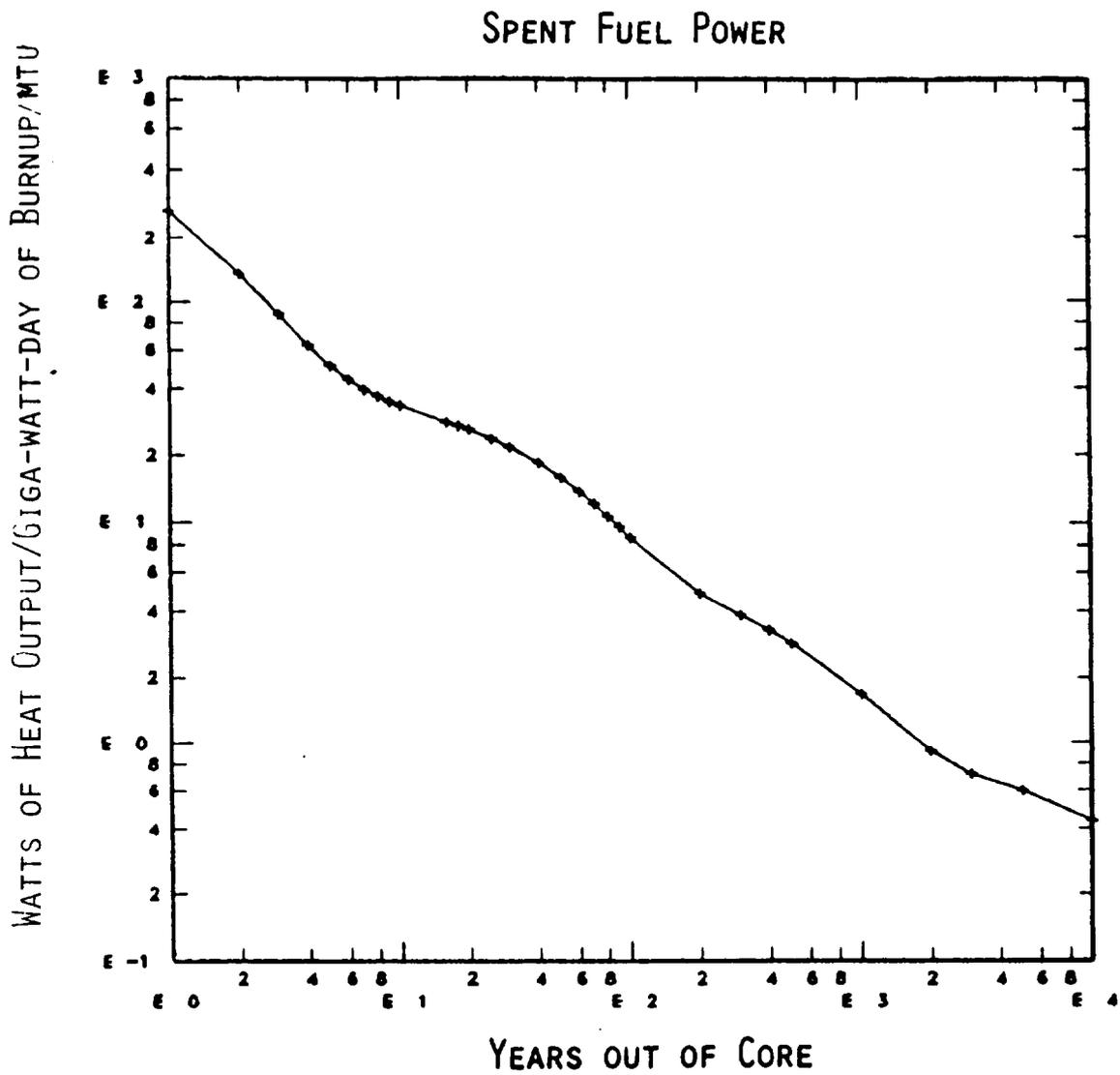


Figure 3. The power output of the spent fuel is modeled as a single curve per unit weight and burn-up vs its age.

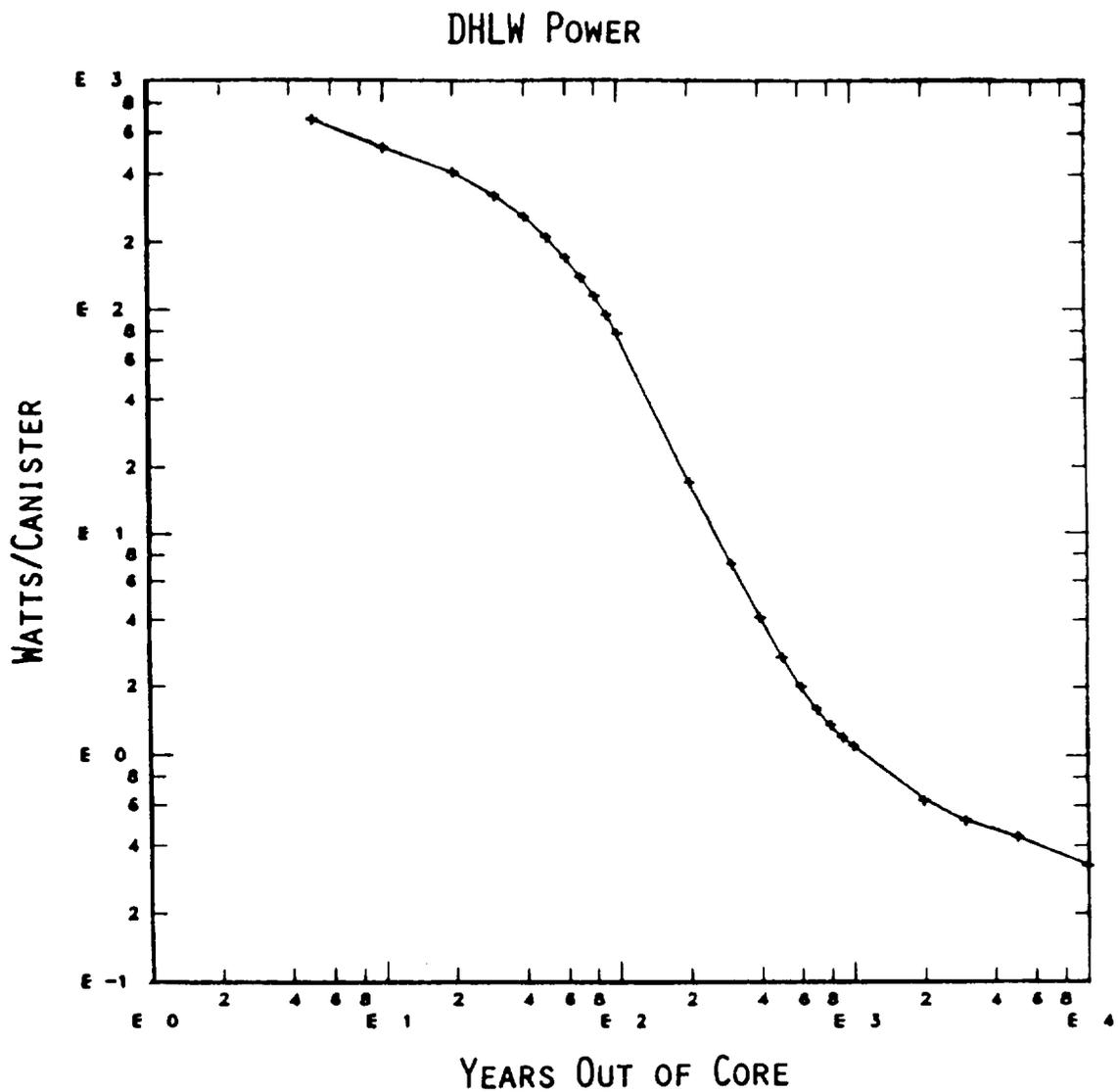


Figure 4. The power output per canister of the DHLW was modeled vs its age.

3. Calculational Models

3.1 Numerical Model Requirements

To determine the temperature rise of repository rock heated by the energy emitted from a non-uniform array of nuclear decay heat sources of varying age, burn-up, and emplacement time, our calculational model must include the effects of:

1. The source thermal output nearest the point of interest and the sources in neighboring boreholes,
2. Additional sources farther from the point of interest at later times,
3. Variation of each source's output with time,
4. Variation in output from source to source, and
5. Variation in source emplacement date.

Consideration of these effects rule out some common thermal modeling techniques. One such technique would represent the thermal response of the repository's host rock and its array of heat-emitting sources by the response of a "representative" section of the heat source array. This model would accurately predict the response everywhere in the repository only if it houses an infinite array of uniformly spaced, identically loaded sources. One such representative section for this repository model might be a single container buried in host rock bounded by the planes midway to adjacent sources.

Finite-difference (FD) or finite-element (FE) numerical methods use this "infinite array" technique to determine the thermal response at a discrete number of locations in the representative section for a discrete number of times. Usually only one source is modeled when using FD or FE methods. The fine discretization required by these methods for good accuracy requires an inordinate amount of computer storage space and calculational time if more than one source is modeled. In our case where heat conduction is slow and the rate of power deposition drops off rapidly with time, these infinite array models of the repository have been used to predict accurately the temperature-time histories or steady-state distributions in regions of tuff near the

source being modeled. Experience has shown that the peak borehole wall temperature occurs relatively soon after emplacement (e.g., 3 - 10 years in our case). Again, only the local source contributes significantly to the short-term thermal performance. These discretized volume models are especially useful to determine the effects of voids in the conduction medium and the effects of temperature- and location-dependent material properties.

3.2 Analytical Model Description and Limitations

For our study, we have chosen to use a simple, yet powerful, technique to determine the thermal response of the repository. It models the response of the repository's volcanic tuff with its diverse array of containerized heat sources by linearly superimposing, in time and in space, the individual contributions of a series of constant output sources. The contribution of each source is based on the analytical solution for conduction of heat from a constant-strength point source into an infinite, isotropic, and homogeneous medium with constant thermal properties. The equation used to evaluate the contribution to the overall temperature change is

$$\Delta T = \frac{Q}{[4\pi kr]} \operatorname{erfc} \left[\sqrt{\frac{r^2}{4\kappa(t-t_0)}} \right],$$

where ΔT equals a point heat source's contribution to the total local temperature rise at time t and at a distance r away from that heat source of strength Q , initiated at time t_0 . The ability of the material to conduct heat is defined by its thermal diffusivity, κ , and its thermal conductivity, k . The parameter **erfc** is the complementary error function. Solutions embodying this equation are available in the PLUS family of computer programs.⁷ The change in decay heat output with time is modeled by initiating the heat flow from a package at emplacement, $t_{0,0}$, with a source equal its average thermal output over some initial time period, Q_0 . At the end of this initial time period and at appropriate later times, $t_{0,i}$, additional negative sources of constant strength, $-Q_i$, are linearly superimposed on the initial constant strength source to provide the appropriate lower average heat output over the next time period. A more detailed description of this process is found in Ref. 7. We have used the programs TWIGS and DAYLITE from the PLUS family of computer programs.

No voids, such as those representing tunnels or empty boreholes, can be modeled with this equation. Heat transfer is only by conduction. Neither radiative nor

convective heat transfer can be included. The effect of heat loss/gain by phase change of the water in the pores and fractures of the tuff also cannot be modeled. This effect is negligible at short times and less than 10°C at about 300 years.⁸

3.3 Analytic Model Application

In the repository model, rows of buried waste packages are located in the walls or floor of a series of underground tunnels (called drifts). These heat-emitting containers can be modeled by a series of point sources along a finite-length line. These discrete groups of point sources will hereafter be called "line" sources. A drift containing a series of packages is generally represented by a larger single, horizontal line source of appropriate length and strength to represent all the packages containing the heat sources in that drift. An additional, parallel line source may be added in the drifts containing commingled DHLW. The depth of the line sources is set to what would be the midpoint of the vertically emplaced container (i.e., 17.5 ft below the plane of the repository for SF containers and 15 ft for DHLW). The thermal output from the SF in a drift or container source is determined by multiplying its age-defined normalized output (given in Fig. 3) by its total weight of uranium and its average burn-up.

The heat sink provided by a constant 25°C earth's surface is modeled as an isothermal condition 1000 ft above the repository plane. It can be generated in the thermal model by creating a "mirror-image" of container sources with equivalent heat-absorbing strength at 2000 ft above the repository plane and by assuming a 25°C initial tuff temperature. For model simplicity, we defined each of the mirror-image panels as an equivalent single line source at the mirror-image-panel centerline.

Modeling waste containers in the repository as drift-averaged line sources is acceptably accurate everywhere except close to a borehole. When the thermal response in the rock near a borehole is to be determined, the heat from the emplaced sources in the local drift must be modeled as a series of vertical line sources, one for each container in the drift. Sources in adjacent drifts are far enough away that they may be represented as drift-averaged line sources. Representation of the entire local drift as individual container line sources is really not required. Detailed modeling of a few sources on each side of the point of interest is adequate. For our analyses, all sources in the entire drift are modeled for input convenience.

Our analyses look at three distinct vertical emplacement models. In the first model, the "Uniform Source Model", all containers, (except those stored in Panels 1 and 2 of the repository) are stored along the drift on 15-ft centers. These exhibit a thermal output representing mean age and burn-up (17.9 years out-of-core and 30.8 GWD/MTU for consolidated SF rods). This type of model is used in the CDR. The added thermal output of the commingled DHLW is spread uniformly among all the repository containers. Panels 1 and 2 are assumed to contain only packages of intact SF on 7.5-ft centers, generating one-half of the thermal output of a mean container of consolidated SF. Thus, the local power density in all panels is the same. All the sources are emplaced in the year 2017 (the middle point of the planned emplacement period, which is 2003 - 2027).

The second model, the "FIFO (First In-First Out) Variable Source Model", assumes the same spacing and emplacement orientation as in the first model. However, the SF packages contain fuel with a distribution in age and a burn-up at emplacement closer to the actual waste inventory. It uses the expected inventory for the oldest 63,000 MTU from both BWRs and PWRs. The waste stream is emplaced oldest first in sequential panels (First In-First Out), filling roughly one panel per year. A drift may be composed of only consolidated SF on 15-ft centers, or of consolidated SF commingled with DHLW on 7.5-ft centers, or of close-spaced intact SF on 7.5-ft centers. Panels 1 and 2 contain intact SF as in the first model. The first waste fuel to be emplaced is older (approximately triple the age of the last fuel to be emplaced) and of lower burn-up (less than one-half that of the last fuel). These conditions were expected to exaggerate the effects seen in the mean thermal load results.

The third model, the "Enhanced Variable Source Model", looks at "heat tailoring" the emplacement schedule of the waste stream in a given panel. Heat tailoring the emplacement schedule arranges for the containers with low thermal output to be kept away from the panel and repository edges where possible. Containers of high burn-up fuel are commingled near panel centers with those containers with lower thermal output. Where the waste stream permits, the intact SF occupies the other third of a drift and the commingled DHLW occupies the center two thirds.

4. Results

The results of the calculations are presented in two formats. The first presents the thermal response as temperature-time histories at selected locations in the repository. These temperature-time histories document the analyses of both the Uniform Source Model (SF of mean age and burn-up for all containers) and the FIFO Variable Source Model (realistic variation of fuel age and burn-up at emplacement). The second format displays the results as temperature distributions for selected panels at various times and for all three models.

4.1 Temperature-Time Histories

The temperature-time histories are plotted for locations within or near Panels 1, 6, 9, and 14 for times up to 10,000 years after emplacement. Table II and Fig. 5 provide detailed information on the respective locations. Locations A, B, and R are located on the midline between adjacent panels. The other locations, all at 1.21-ft radius from the center of the nearest source, are intended to represent the temperature of an emplacement borehole wall. Locations H, P, and C are located at a panel center. Locations S and T lie on the panel centerline at panel ends. Where appropriate, "300 years" after emplacement time and the "97°C" minimum desired borehole wall temperature level are indicated.

For the Uniform Source Model, Panels 3 through 17 vary only in size and location. Thus, variations in their response would result only from differences in their size and the fraction of their boundaries that lie on the cooler perimeter of the repository. For the Variable Source Models, the four monitored panels define the total range of thermal response. Panel 1, with its older intact SF, was chosen because we expected that it would help define the borehole lower temperature limit in all models. Panel 6 represents a mean panel in the repository. Panel 9, located in the farthest corner of the repository, tracks the effect of a high heat loss at the perimeter of a small panel with mean power output sources. Panel 14, containing mostly high burn-up SF, usually defines the upper temperature limit.

The effect of source array size was determined by a comparison of the response near the source at the center of an "infinite" panel (about one mile square) with that of Location C in the "finite" Panel 14. The model assumes uniform sources. Figure 6 shows no perceptible difference for the first 150 years and only a 10 percent

overprediction of temperature rise after 1000 years for the "infinite" panel. On panel boundaries, the difference is more significant.

As mentioned in the discussion on calculational methods, a set of negative source, mirror-image panels are included in the model to simulate the effect of the isothermal conditions at the ground surface 1000 ft above the repository. To check the effect of including this isothermal ground surface, we ran a calculation on the uniform source model with the repository mirror sources removed. The result, shown in Fig. 7, indicates that including the isothermal earth's surface in the model is important only at late times after emplacement. We kept the mirror source array in the model because its presence did not significantly increase the computation time. This calculation comparison also suggests that possible heat removal by the water table 700 ft below the repository would similarly be of concern only at late times after emplacement (i.e. > 1000 yr).

For our Uniform Source Model (uniform power density, age and burn-up) in a finite repository with individual panels, Tables III(a) and III(b) gives the temperatures: (1) at peak temperature conditions; (2) at 300 years after emplacement; and (3) at 1000 years after emplacement. Plotted temperature-time histories are given in Figs. 8 to 11. These analyses show the following results **at 300 years after emplacement**.

1. The borehole wall temperature in the repository ranges from 55 to 125°C.
2. The borehole wall temperatures near the center of most "full-sized" panels are greater than 97°C. Most of the boreholes in Panels 1 and 2 drop to below the 97°C limit.
3. In Panels 1 and 2, the panel center temperature is 27°C cooler than the panels containing the youngest, hottest fuel.
4. In Panel 6 (the "average" panel in the repository), the borehole wall temperature might vary by as much as 60°C between the coolest borehole and the hottest.
5. The temperatures for points between the panels rise very slowly. They reach a peak of less than 80°C well after 300 years.

6. At the time of peak temperature rise, about 70% of the borehole wall temperature rise is due to the source in its hole. After 1000 years, only 10% of the rise is due to the output of its local source.
7. Emplacement of the sources in the repository over a 25-year period does not significantly affect the characteristic borehole wall temperatures at 300 years. At this late time, when sources in most of the repository contribute to the local tuff temperature rise, conditions are changing so slowly that the few years difference in emplacement time is insignificant.

The temperature-time histories also show a maximum 100°C difference in peak borehole wall temperature. The peak borehole wall temperature occurs shortly after emplacement.

One current SF waste disposal plan assumes that the oldest SF in the waste stream will be emplaced in the repository first (as in our FIFO Variable Source Model). The back-log of the older SF temporarily stored at reactor sites would be dissipated until an approximate steady-state influx of the younger, more recent fuel waste stream is reached. In this scenario, the first waste emplaced will be three times older than the average and about one-half the burn-up of the last emplaced waste. The expected consequences of including this distribution of emplacement sources on the thermal response of individual panels exaggerates the results discussed previously.

The results for the FIFO Variable Source Model analyses are plotted in Figs. 12 to 15 (see also Tables III(c) and III(d)). Review of the temperatures **at 300 years after emplacement** shows the following results.

1. The resultant hottest borehole wall for this emplacement scheme has increased by 11°C while the coolest has decreased by 19°C. This increases the borehole wall temperature range by 47% (42 to 136°C compared with 61 to 125°C for the Uniform Source Model).
2. All of Panels 1 and 2 and much of Panel 9 drop below 97°C. For Panels 6 and 14, only edges and corners drop below 97°C.
3. The representative panel (6p) has a 53°C variation in borehole wall temperature.

4. Panels with the same spacing, layout, and average burn-up give the same long-term thermal response regardless of age of fuel.

During the period of peak borehole wall temperatures, boreholes in Panels 1 and 2 are lower by up to 83°C from the uniform source case. In Panels 6 and 14, the highest and lowest values of peak borehole wall temperature from the uniform source case have changed by -10°C to +25°C, respectively.

Table II.

Locations where Time-Histories are Described

ID	Panel No.	Location within Panel ^a	Remarks
A	Betw. 4 & 14	Inter-panel main drift	Hot panel
B	Betw. 14 & 15	Inter-panel aux. drift	Hot panel
C	14	Panel center	Hot panel
D	9	End of edge drift	Exposed panel
E	1	End of edge drift	Intact SF only
H	1	Panel center	Intact SF only
P	6	Panel center	Average panel
Q	6	End of middle drift	Average panel
R	Betw. 5 & 6	Inter-panel aux. drift	Average panel
S	6	Middle of central drift	Average panel
T	6	Middle of edge drift	Average panel
U	6	End of edge drift	Average panel
V	6	End of central drift	Average panel

^a Within panels, the actual location is at the borehole wall radius from the centerline of the nearest source (1.21 ft).

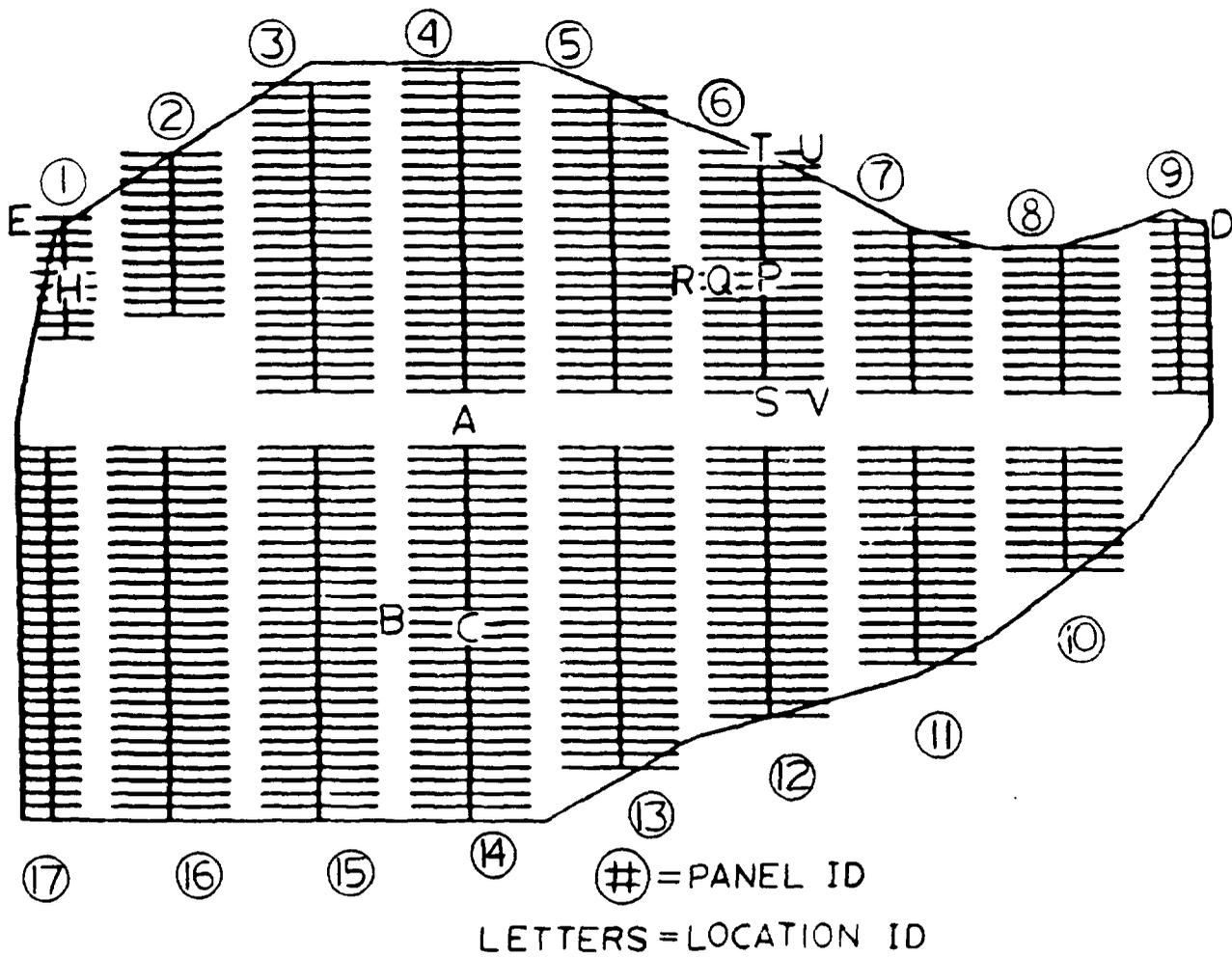


Figure 5. There are 13 locations where temperature-time history results are described (see Table II).

Table III(a)
Temperature Results
for Uniform Source Model / Cases "ac"

Panel ID	Source Location	Peak Temperature (°C)	Time of Peak Temperature	Temperature @ 300 yr (°C)	Temperature @ 1000 yr (°C)
1	H	162	19	98	98
1	E	110	7	61	49
9	D	147	4	68	51
14	C	193	13	125	99
4, 14	A	64	1000	57	64
14, 15	B	78	1000	73	78

Table III(b)
Temperature Results
for Uniform Source Model / Cases "6p"

Panel ID	Source Location	Peak Temperature (°C)	Time of Peak Temperature	Temperature @ 300 yr (°C)	Temperature @ 1000 yr (°C)
6	P	212	30	135	101
6	Q	167	20	105	91
5, 6	R	77	1000	74	77
6	S	202	20	105	84
6	T	202	19	103	76
6	U	163	22	75	60
6	V	168	20	87	77

Table III(c)
Temperature Results
for FIFO Variable Source Output / Cases "be"

Panel ID	Source Location	Peak Temperature (°C)	Time of Peak Temperature	Temperature @ 300 yr (°C)	Temperature @ 1000 yr (°C)
1	H	80	25	59	46
1	E	59	10	42	37
9	D	164	7	72	53
14	C	219	16	136	107
4, 14	A	63	1000	57	63
14, 15	B	85	720	79	85

Table III(d)
Temperature Results
for FIFO Variable Source Model / Cases "p6"

Panel ID	Source Location	Peak Temperature (°C)	Time of Peak Temperature	Temperature @ 300 yr (°C)	Temperature @ 1000 yr (°C)
6	P	191	30	127	99
6	Q	152	20	98	88
5, 6	R	75	1000	67	75
6	S	199	20	102	76
6	T	187	19	101	83
6	U	151	22	83	76
6	V	162	20	74	60

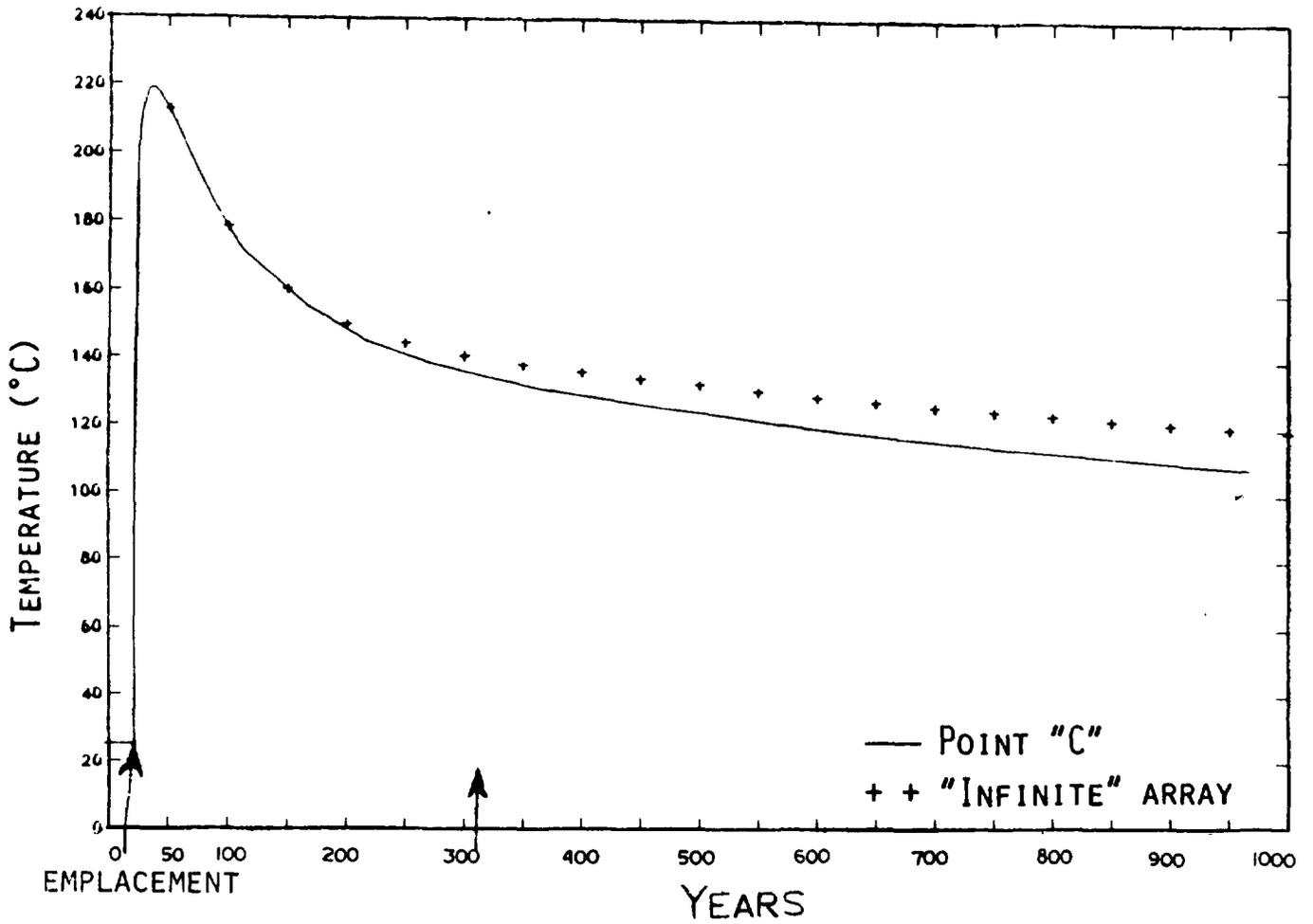


Figure 6. The effect of using a "finite" array of sources, such as in Panel 14, vs a simulated "infinite" array of sources is noticeable after 300 years of emplacement.

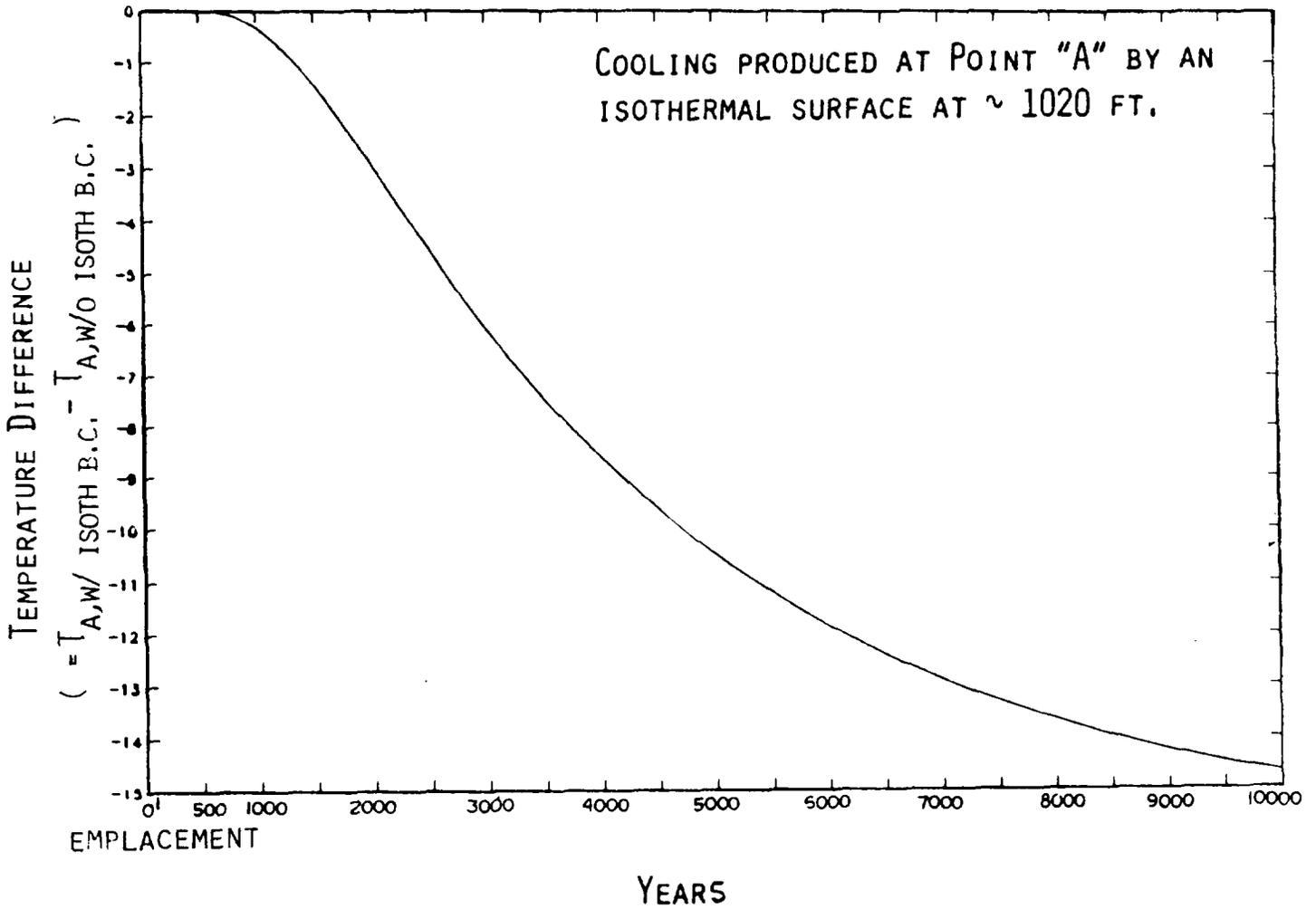


Figure 7. The effect of using an equivalent sink, mirror image of the repository sources to model an isothermal ground surface is noticeable 1000 years after emplacement.

Uniform Source Model: Panels 1, 9, and 15

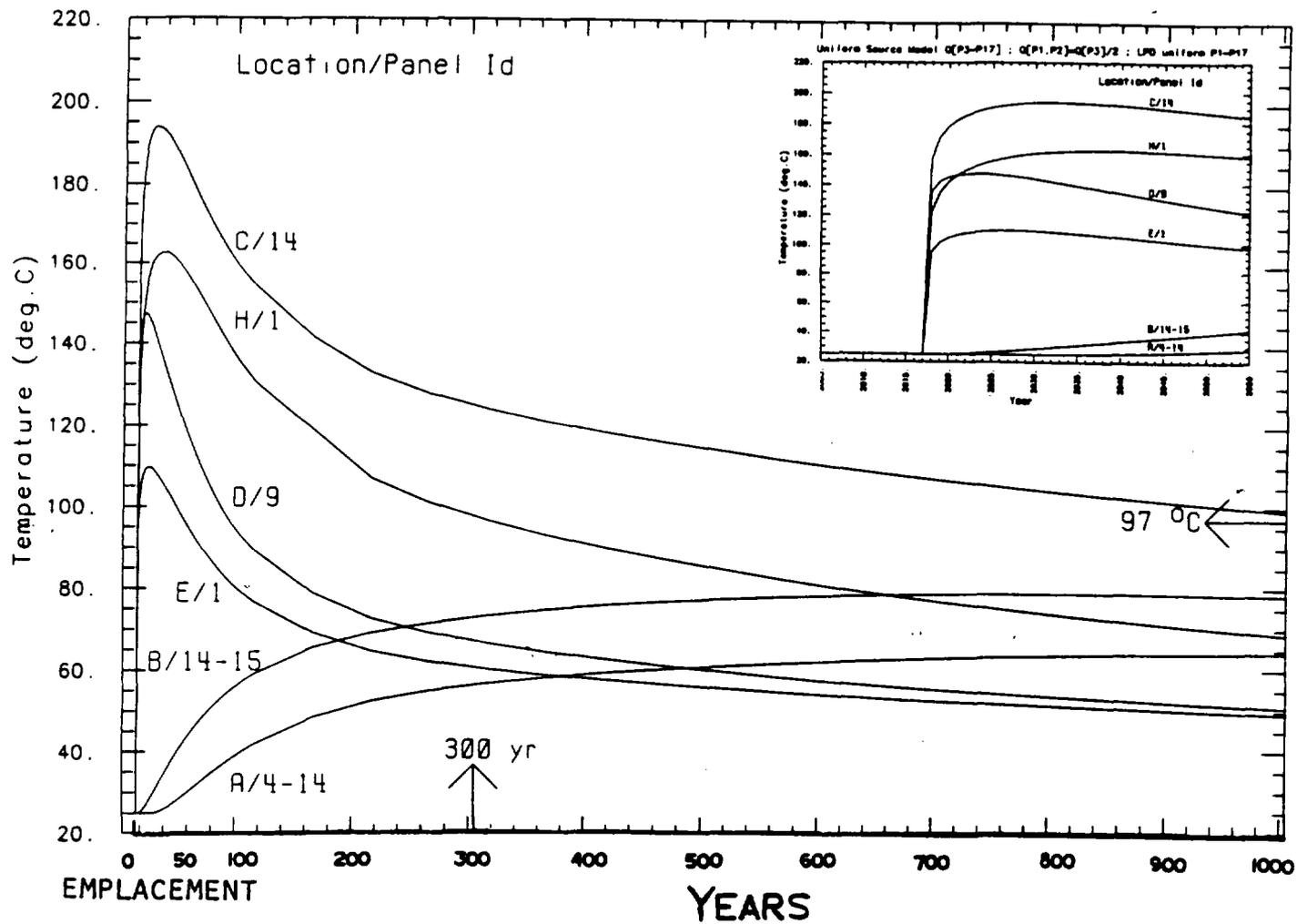


Figure 8. Uniform source temperature-time histories; Panels 1, 9, and 14.

Uniform Source Model: Reference Panel No. 6

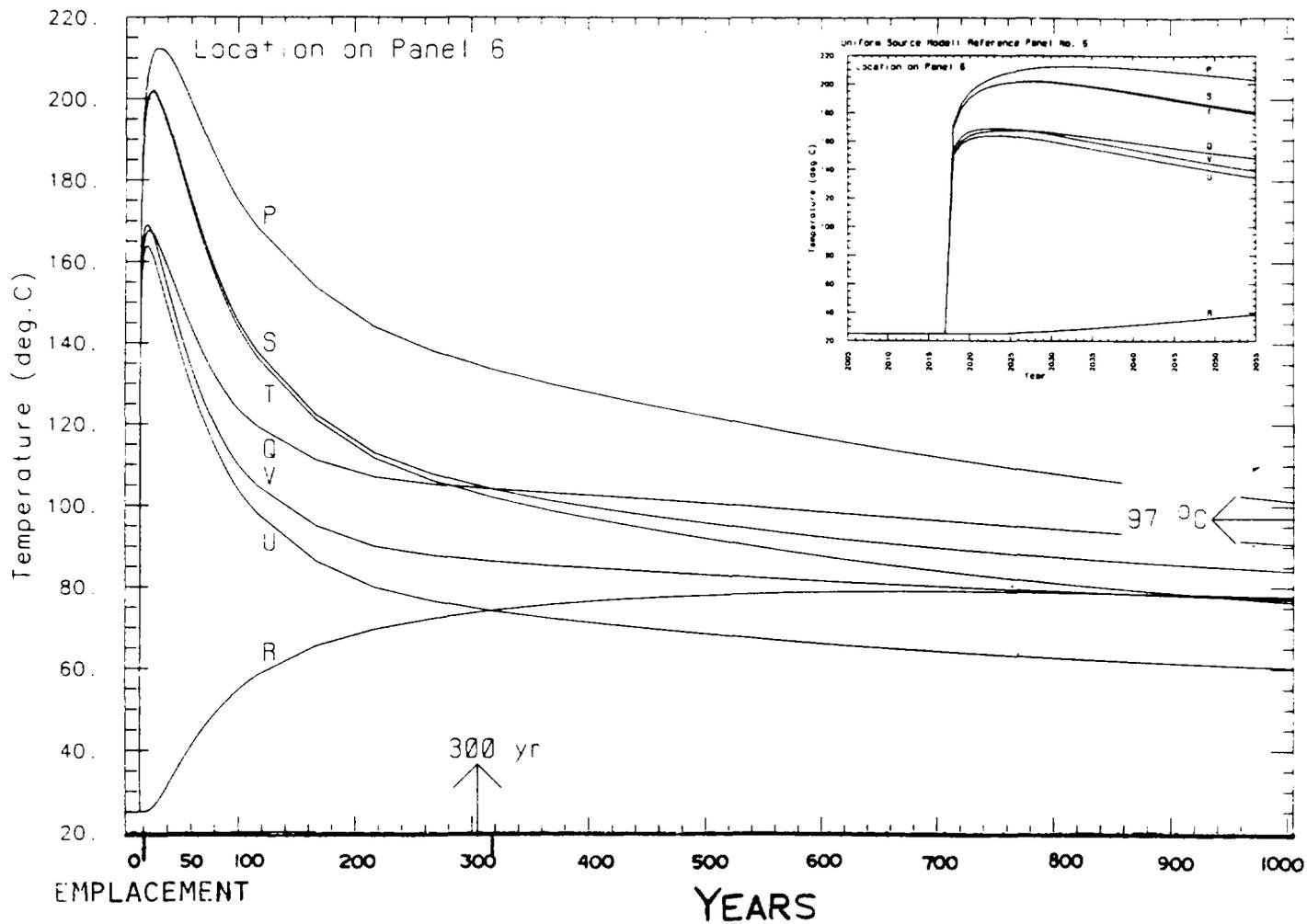


Figure 9. Uniform source temperature-time histories; Panel 6.

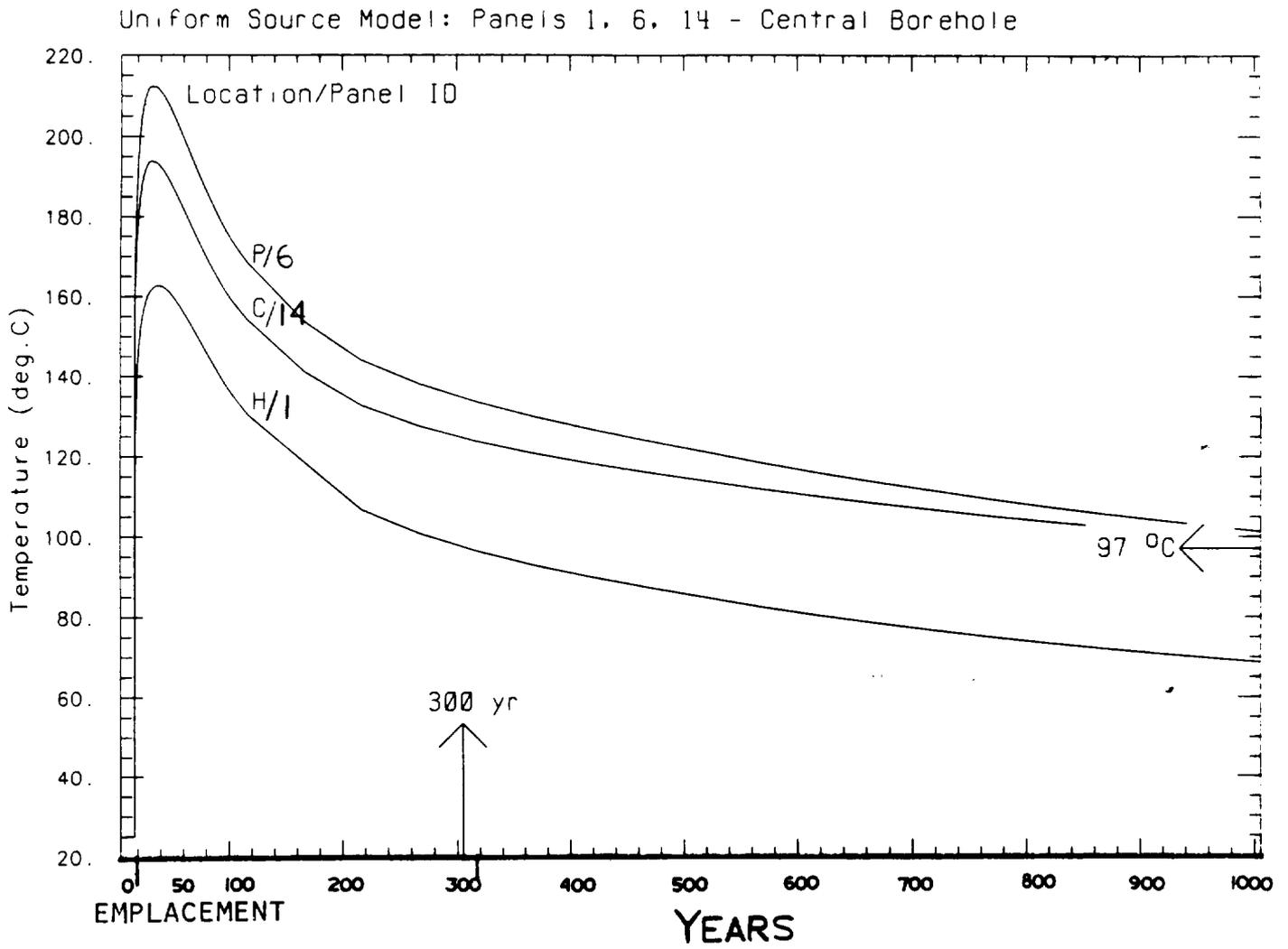


Figure 10. Uniform source temperature-time histories; Panels 1, 6, and 14; centers.

Uniform Source Model: Panels 1, 6, 9 - Panel Corner/Repository Edge B/A

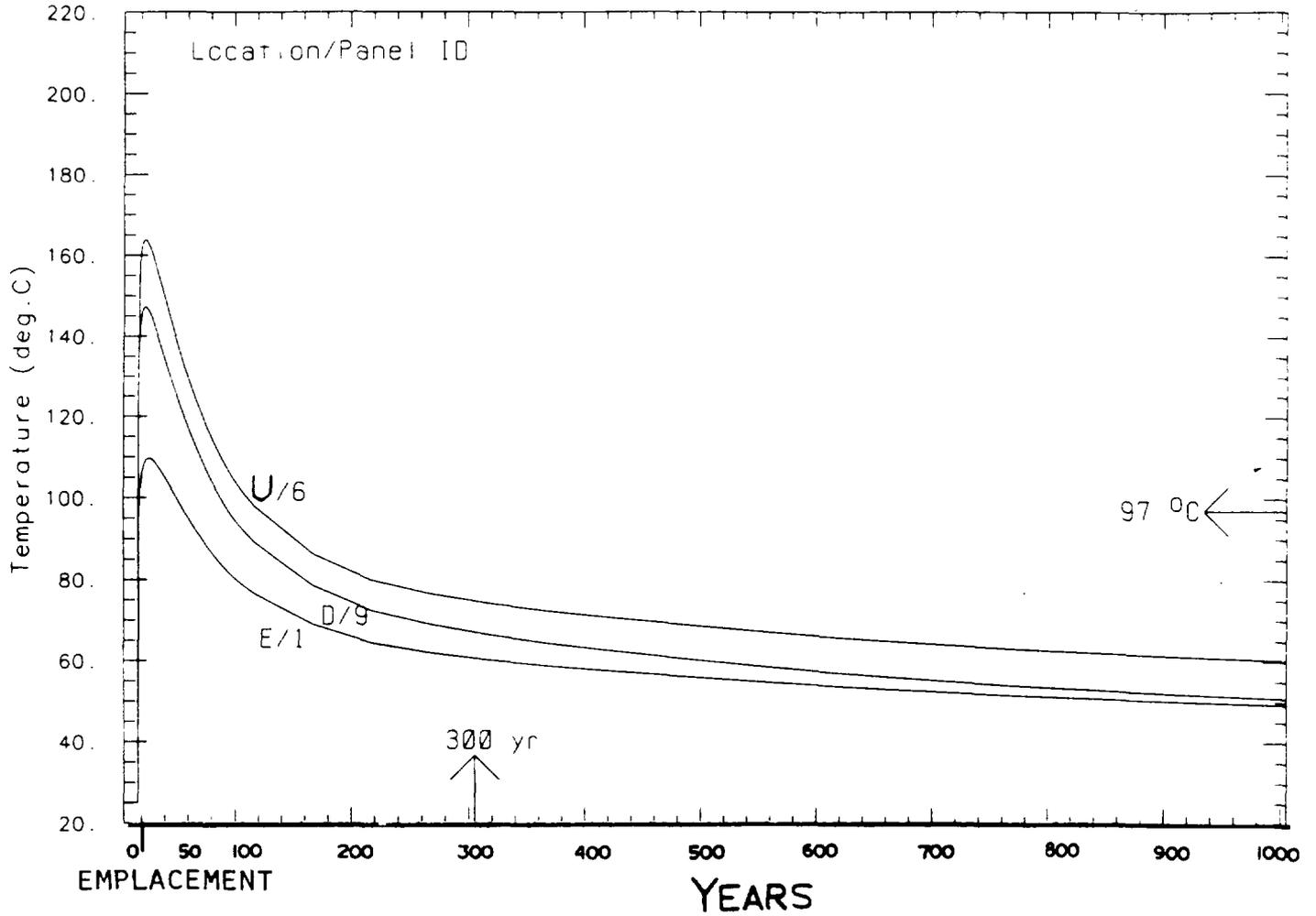


Figure 11. Uniform source temperature-time histories; Panels 1, 6, and 9; edges.

FIFO Variable Source Model: Panels 1, 9, 14

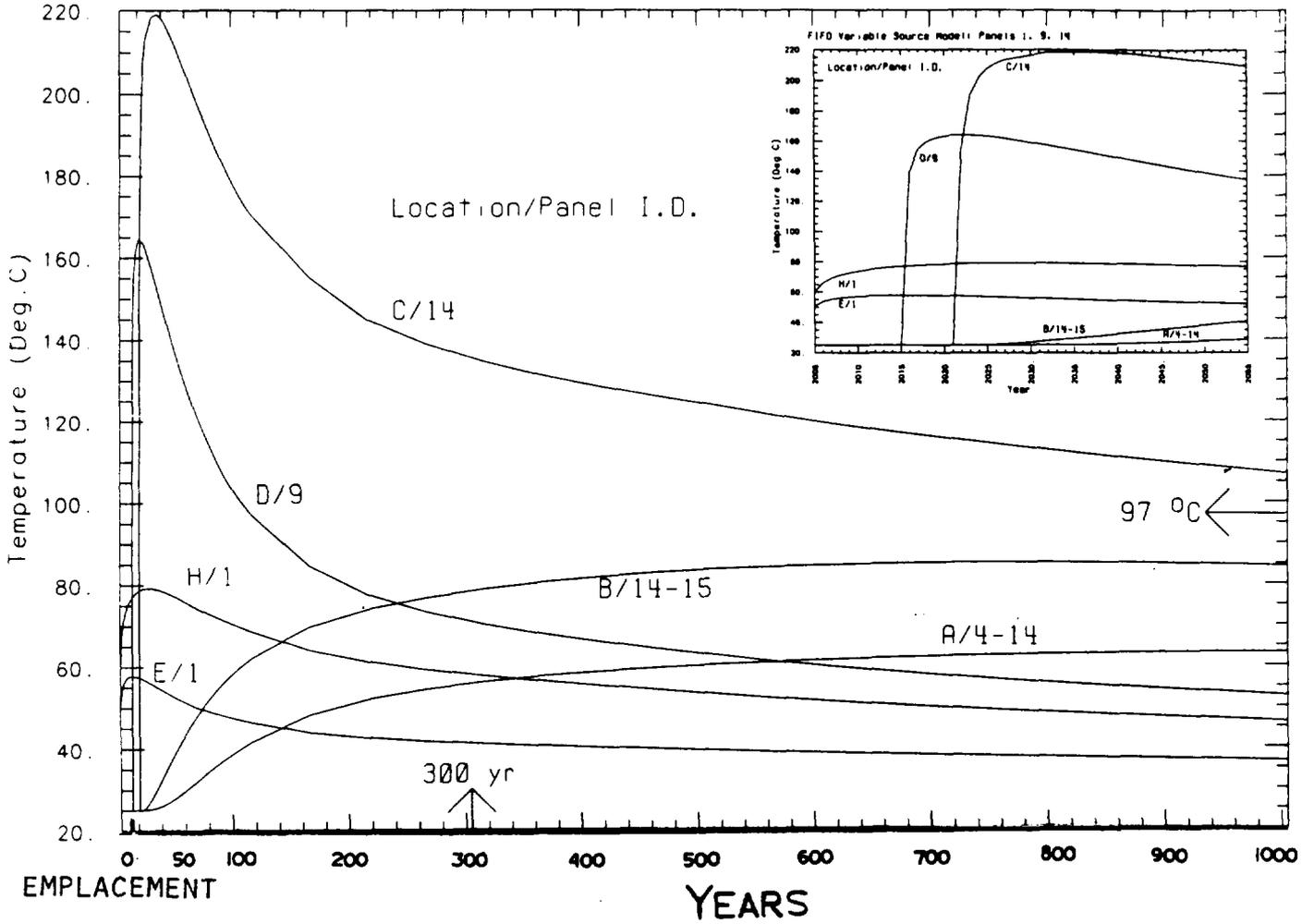


Figure 12. FIFO variable source temperature-time histories; Panels 1, 9, and 14.

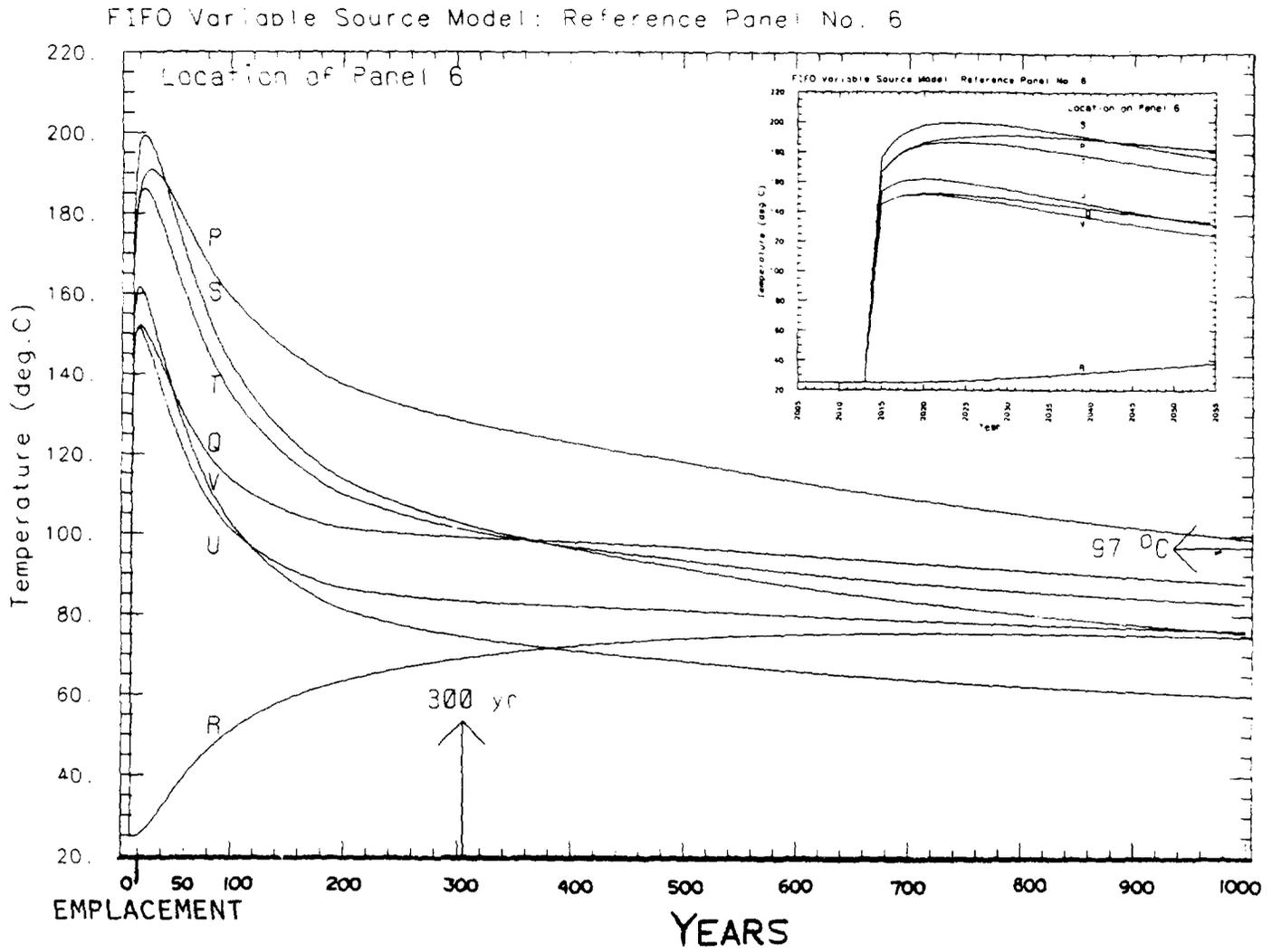


Figure 13. FIFO variable source temperature-time histories; Panel 6.

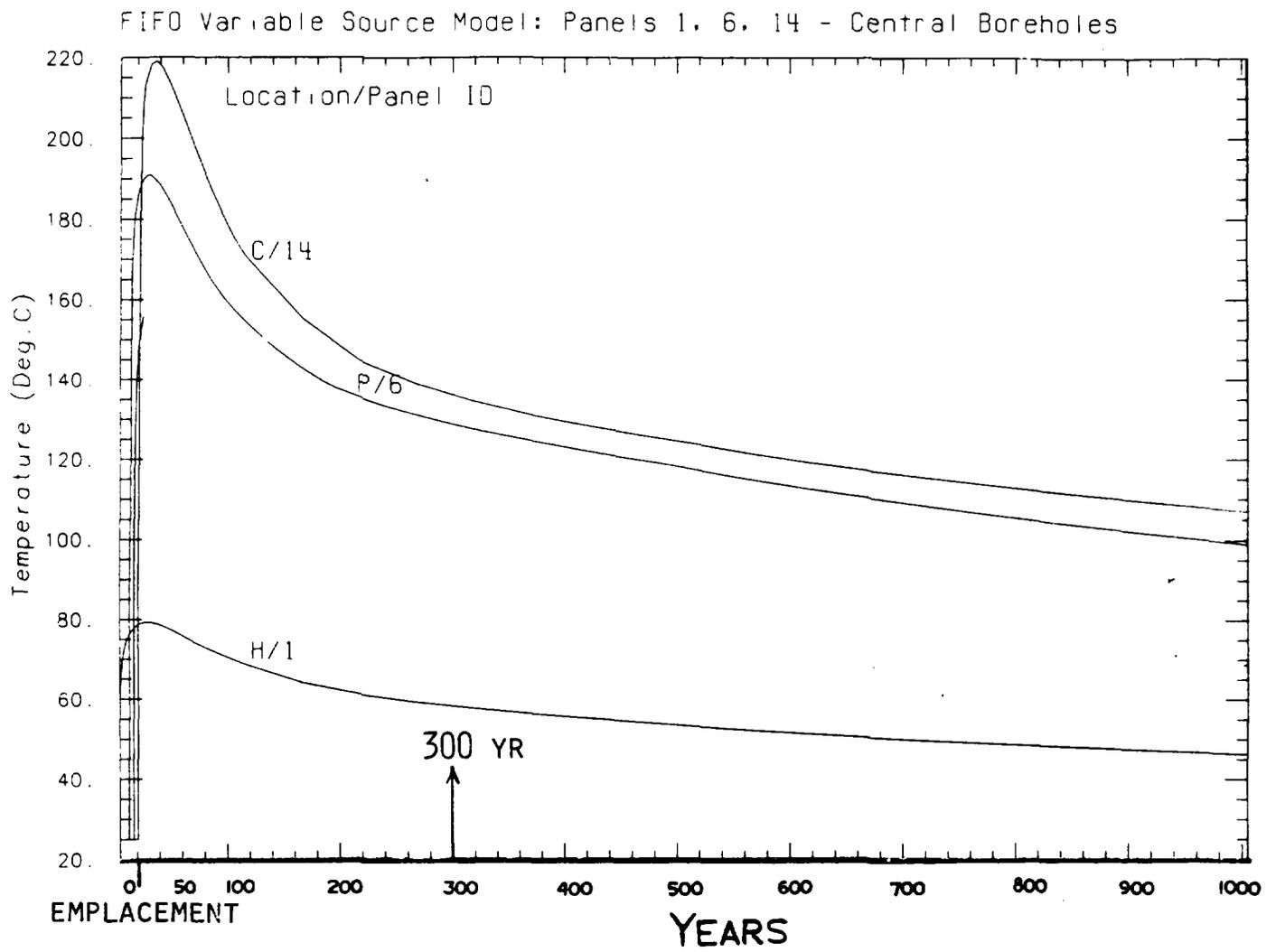


Figure 14. FIFO variable source temperature-time histories; Panels 1, 6, and 14; centers.

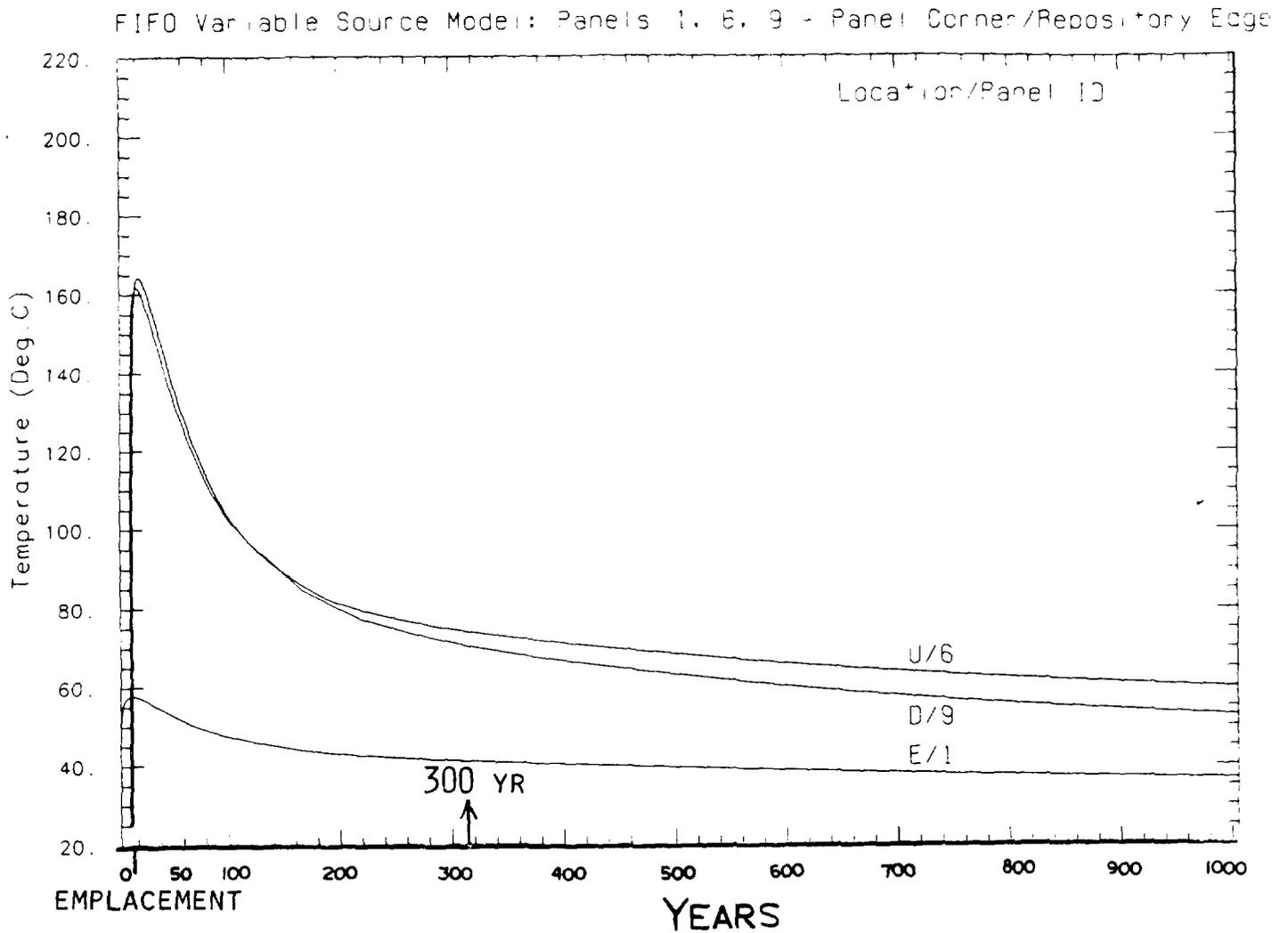


Figure 15. FIFO variable source temperature-time histories; Panels 1, 6, and 9; edges.

4.2 Intra-Panel Temperature Distributions

After examining the temperature-time histories of "representative" points discussed in the Section 4.1, we examined the temperature distributions of "representative" panels at particular fixed times. Temperature distributions in the centuries time frame is of interest from the standpoint of containment of radioactive materials in the repository.

An example of the borehole temperature distribution along an emplacement drift is shown in Fig. 16. These curves present the temperature conditions at 1000 years after assumed repository closure. They occur in one of the warmest places in the repository, i.e., the middle drift of Panel 14 which contains point "C". The model generating the first curve (smooth) assumes all 75 of the packages contain the same amount of SF, 2.64 MTU. In a more realistic situation, about 20% of the packages may contain unconsolidated SF and, thus, generate 33% to 50% as much heat as the consolidated fuel containers in the drift. In this case (shown by the second curve in Fig. 16), every fifth package contains 1.2 MTU while the remaining 80% contain 3 MTU. The average remains 2.64 MTU. For the drift-averaged case, only one or two packages at the ends are below the boiling point of water (about 97°C at the repository elevation) for the uniform source case. For the case with dispersed intact SF, five to seven packages on each end fall below this temperature.

Panel 6 was chosen to investigate the edge effects of finite panels, non-uniform source output distribution, and heat-tailored emplacement on borehole wall temperature distributions. This panel is of average size, stores average burn-up waste, and is located near the middle of the repository. It uses 17 of the 19 emplacement drifts, storing 1425 SF containers loaded with an average of 2.64 MTU (i.e., 3 MTU in consolidated SF containers and 1.2 MTU in intact SF containers) and 456 containers of DHLW. The SF consists of 80% consolidated fuel containers and the remaining 20% intact fuel assembly containers. The first six emplacement drifts contain consolidated SF commingled with DHLW. The intact SF containers are stored on 7.5-ft centers in Drifts 7 and 12. Drifts 8 through 11 and Drifts 13 through 17 store only consolidated SF. The layout is shown in Fig. 17.

Isotherms of the borehole wall midplane temperatures at 300 years after repository closure for the Panel 6 array of SF sources are shown in Fig. 18. The contributions of the DHLW heating are included in the thermal load calculations. The

shaded portion of the drift shows the part of the panel where the borehole midplane temperatures at 300 years are less than 97°C. The lower temperatures for the two drifts containing intact SF only (Nos. 7 and 12) are observable. The containers near the ends of a large number of drifts in the middle of the panel fall below the 97°C limit, especially near the "intact SF" drifts and at the panel ends.

At any given time, the fraction of boreholes with temperatures less than 97°C is very sensitive to the assumed conductivity of the tuff. Temperature distributions for this source layout were calculated at 200, 300, 500, 700, and 1000 years after closure to determine the fraction of the boreholes with wall temperatures below 97°C. The results of these calculations are plotted in Fig. 19 for the three package types and the overall value. The most obvious feature in this figure is the high percentage of DHLW packages with borehole wall temperatures below 97°C. Also, after 200 years, more than 10% of all the boreholes are cooler than 97°C. At 300 years, this percentage has risen to 15%, and at 1000 years nearly all the boreholes in the panel are less than 97°C. The fraction of boreholes greater than 97°C is extremely sensitive to the assumed value of thermal conductivity of the tuff. A variation of 10% in the value used by these analyses ($k=1.84$ W/m-K) can vary that fraction by a factor of two or more.

We ran an additional model where the source distribution is arranged to keep as many boreholes as hot as possible for as long as possible (i.e., heat-tailored emplacement). In this arrangement (Fig. 20), the low output sources are isolated from the panel edges as much as possible. The layout is symmetrical with intact SF occupying the center third of a drift, alternating with DHLW occupying the other two-thirds of a drift. The results of the thermal calculations are shown in Figs. 21 and 22. They show a marked reduction in the number of containers occupying boreholes with wall temperature below 97°C. The fraction below 97°C, for this configuration, is one-half that for the previous layout up to about 400 years after emplacement. This suggests that, given the real inventory, the early storage period temperatures of the low power boreholes could be kept acceptably warm by emplacing them near the center of the panel. The fraction of boreholes with temperatures less than 97°C could be further reduced by decreasing the inter-container spacing in the drifts near the panel corners.

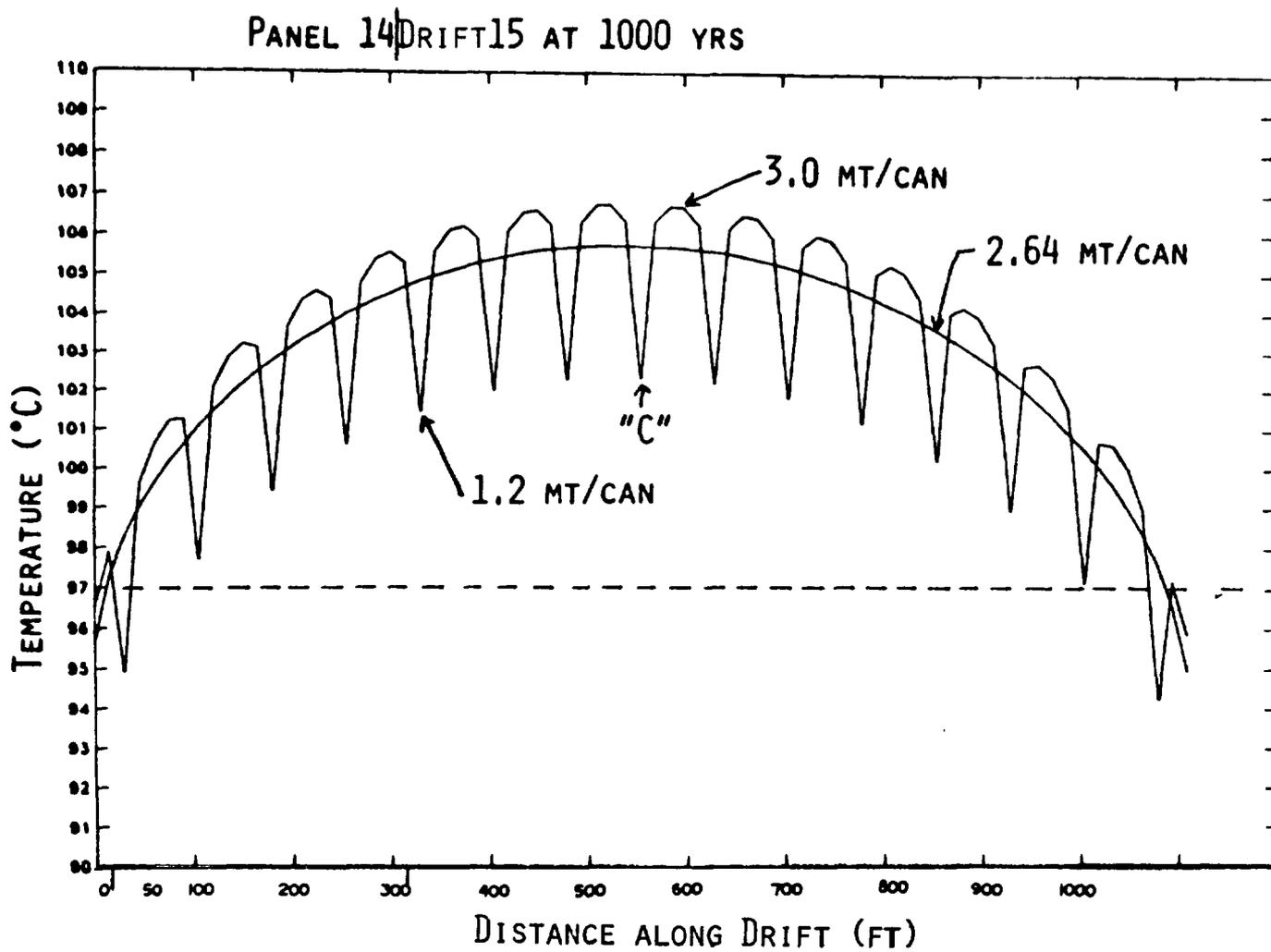


Figure 16. Temperature distribution along a drift.

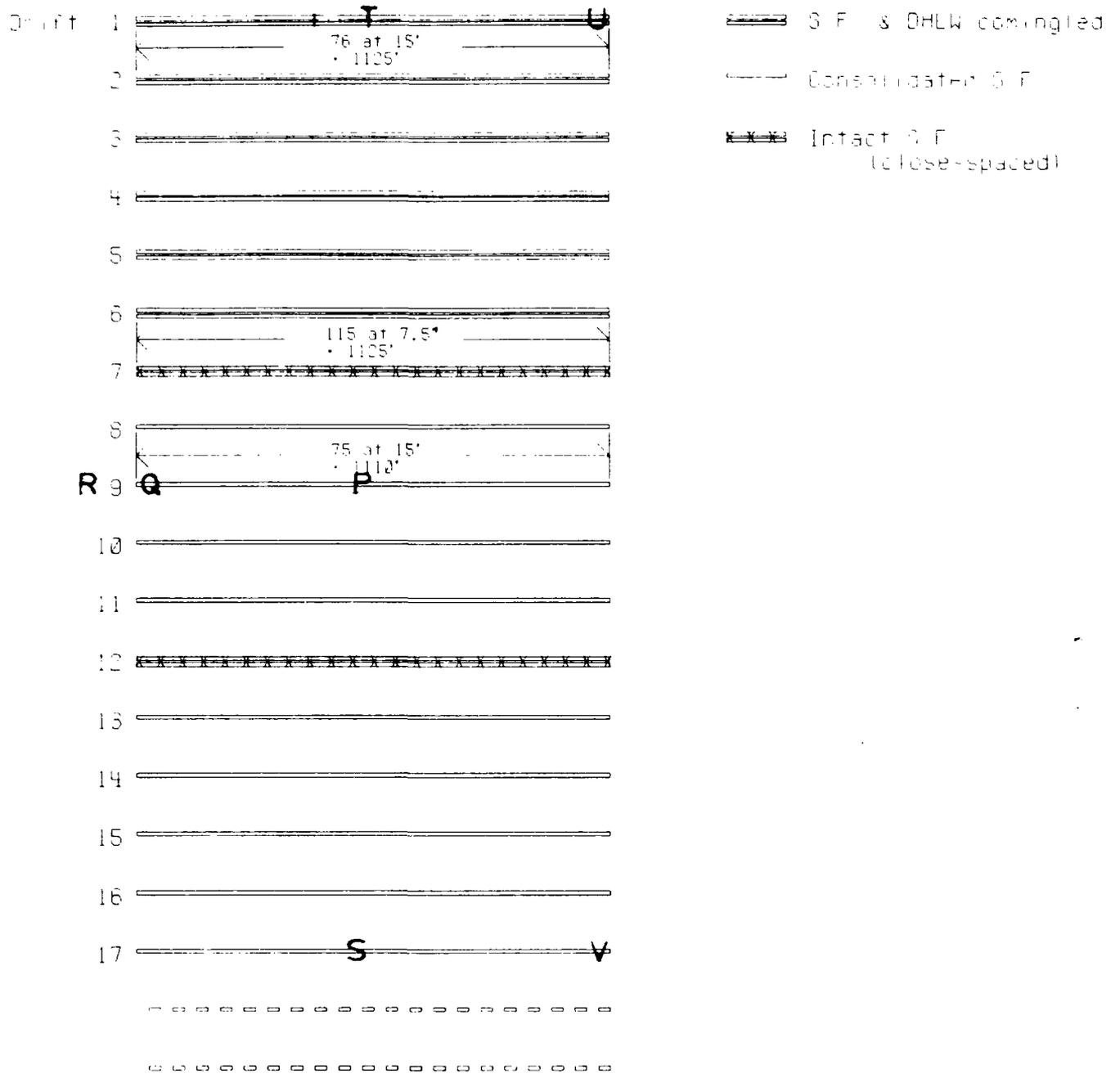
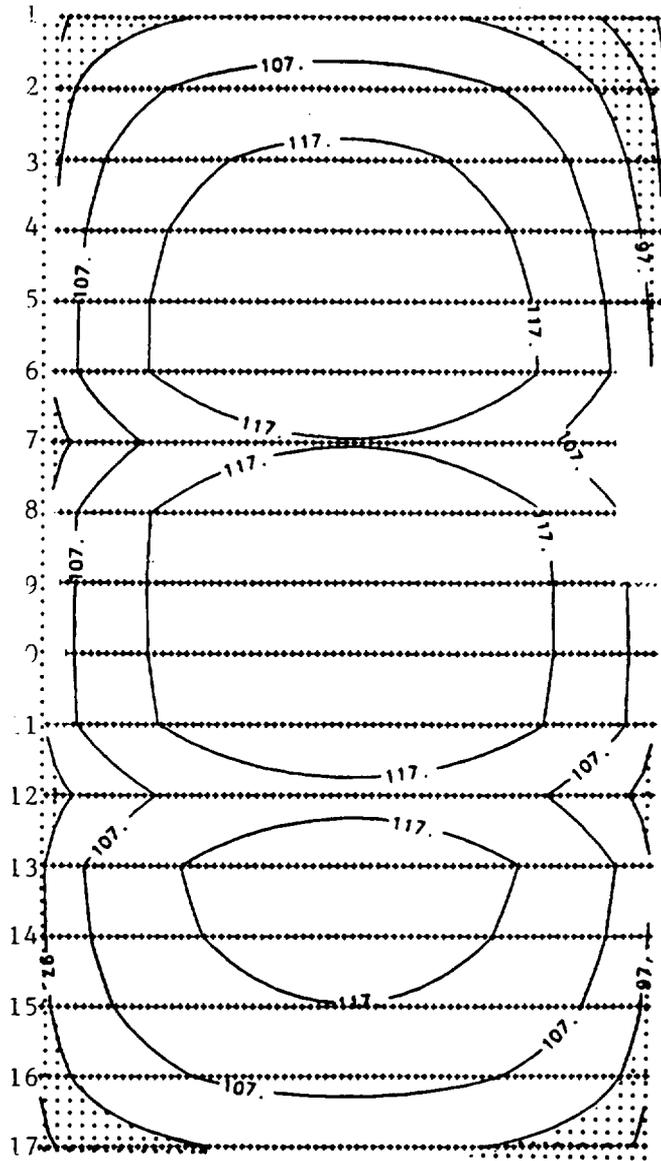


Figure 17. Source layout for the FIFO variable source case.



PANEL 6 - 300 YEARS AFTER CLOSURE

Figure 18. Isotherms for the FIFO variable source case.

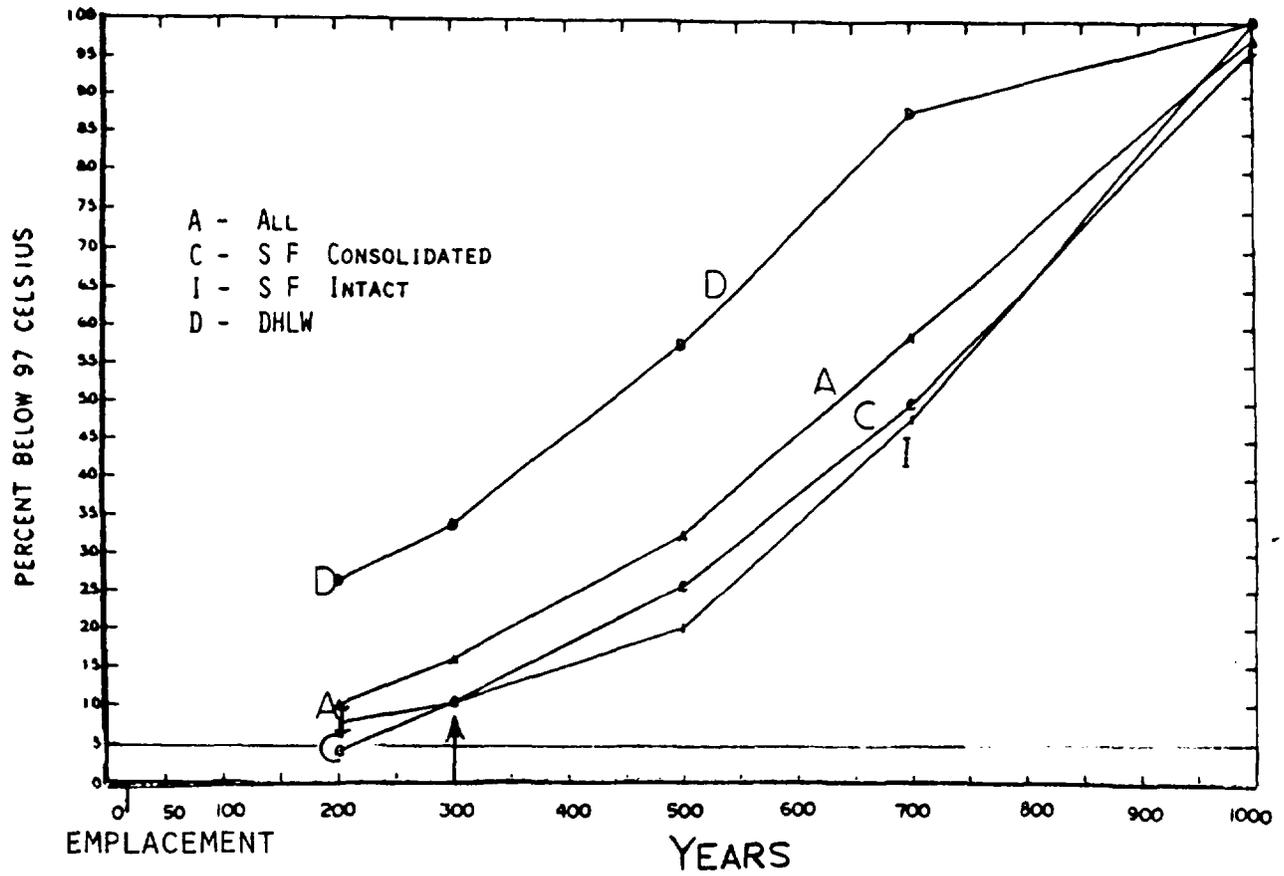


Figure 19. Fraction of boreholes below 97°C at various times after emplacement for the FIFO variable source case.

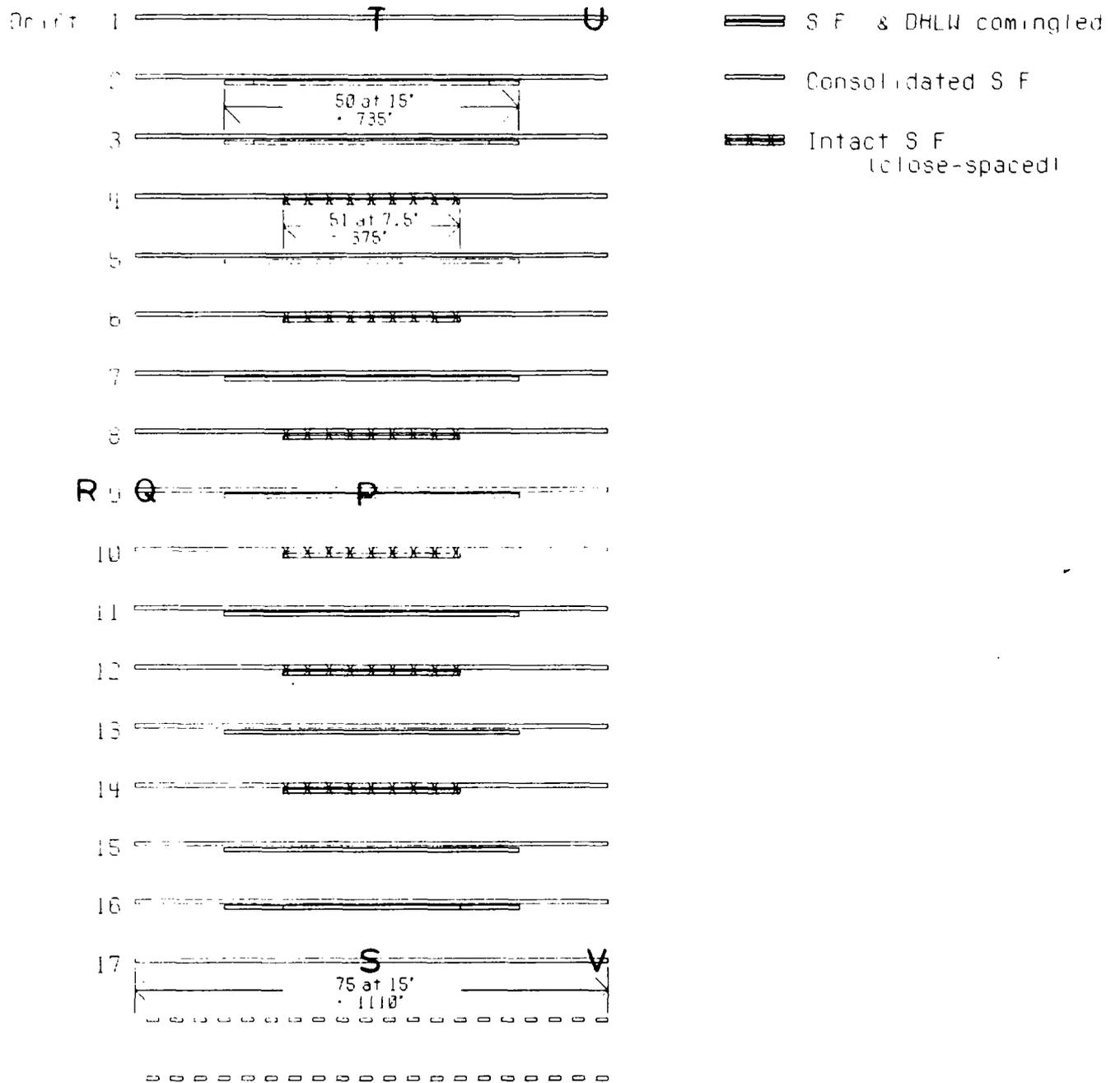
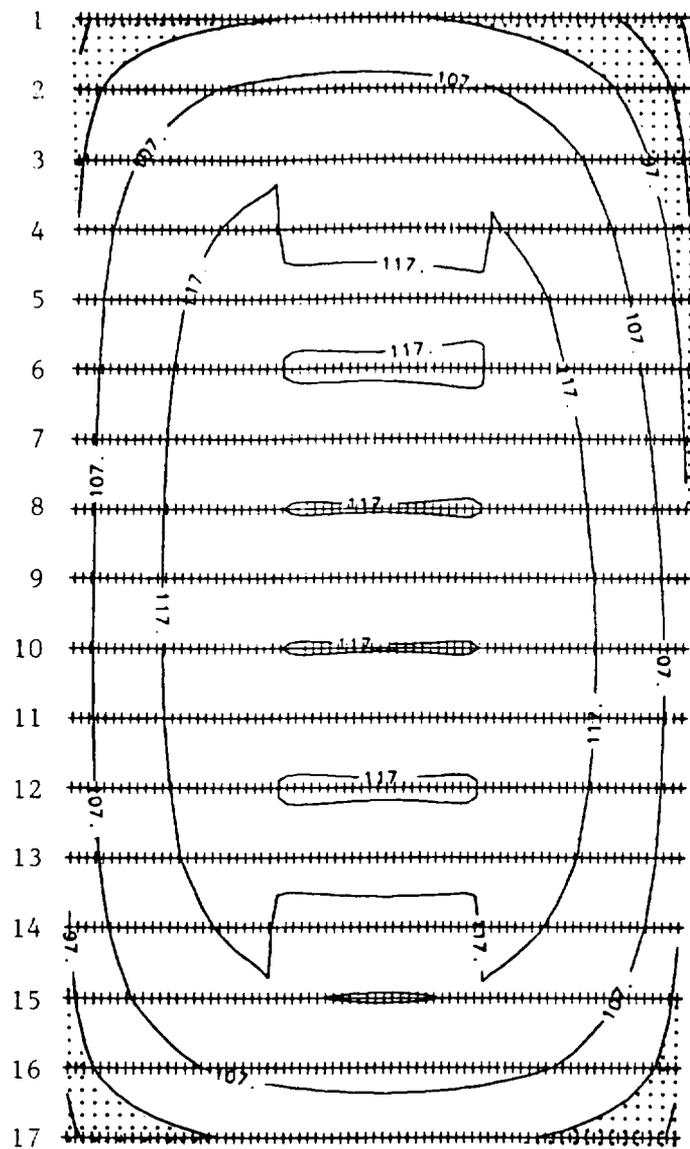


Figure 20. Source layout for the enhanced variable source case in a panel.



PANEL 6 - 300 YEARS AFTER CLOSURE

Figure 21. Isotherms for the enhanced variable source case.

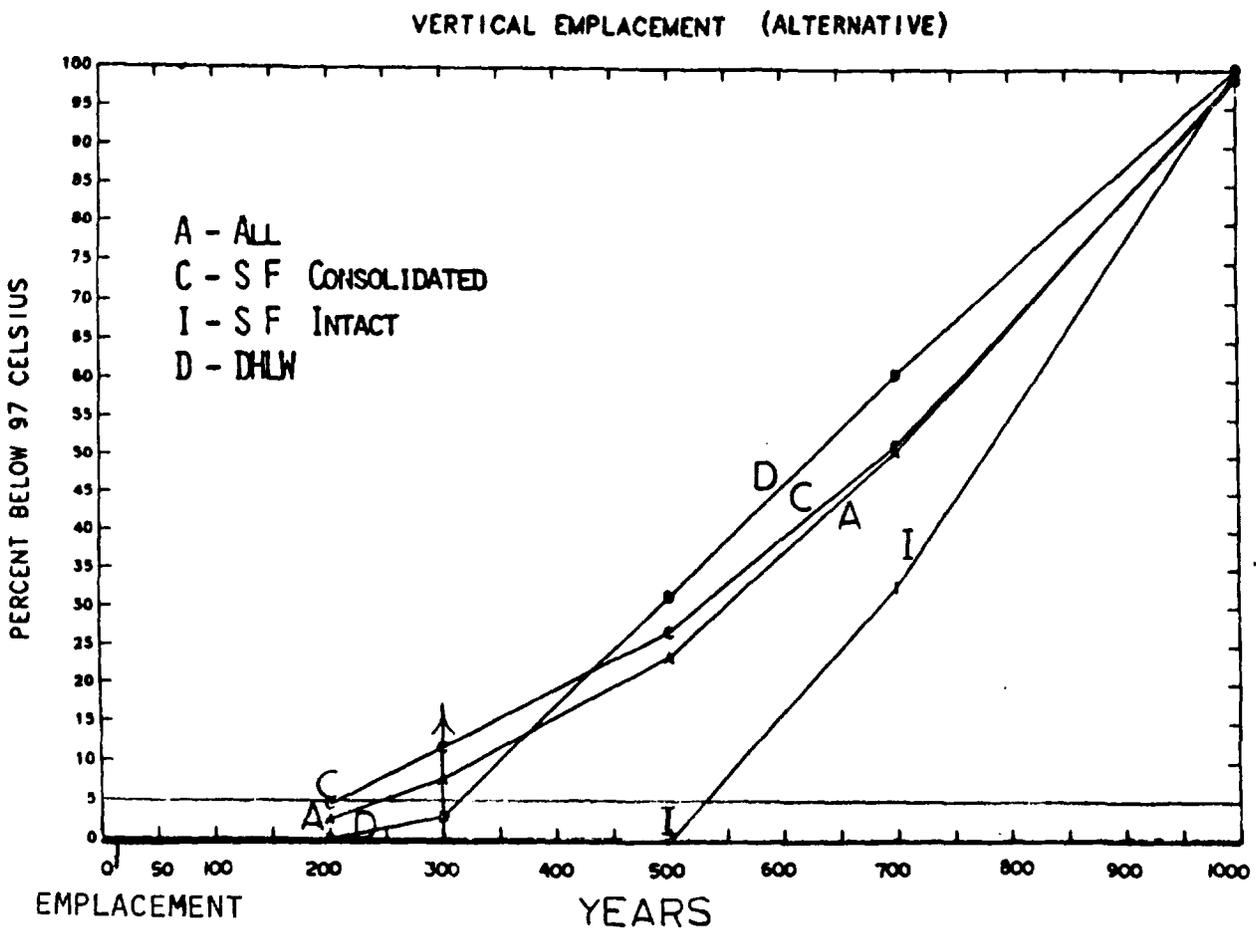


Figure 22. Fraction of boreholes below 97°C at various times after emplacement for the enhanced variable source case.

5. Conclusions

To support the Yucca Mountain Project nuclear waste disposal package and repository design efforts, LLNL has modeled conduction heat-transfer of the nuclear-decay-heated volcanic tuff in the repository. These analyses extend the analyses documented in the CDR by quantifying the thermal response for a finite, uniformly loaded repository with each panel containing a distribution of the same heat sources; the response for a realistic panel-by-panel distribution of heat sources (where the sources in a given panel have been averaged to some uniform value) to show the effect of inter-panel variations; and the intra-panel change in response for various realistic distributions of sources within the panel.

For this study, the tuff's response to the heat sources in the repository is modeled by linearly superimposing, in time and in space, individual contributions of an analytically defined series of constant output point sources located in an infinite, uniform, and constant property medium. No voids, such as drifts or empty boreholes, are modeled. However, the "constant temperature" surface 1000 ft above the repository is modeled. Heat transfer is only by conduction.

Calculational results show that the effect of using an infinite array model to predict the local temperature rise in the center of finite-size panels in the repository is barely perceptible during the first 150 years and only 10% high after 1000 years. This error would increase substantially near the ends of drifts and edges of panels.

For the case of a finite repository model with uniform power density, age and burn-up, the following conditions are observed at 300 years after emplacement. Although the borehole wall temperatures near the center of most "full-sized" panels are greater than 97°C, most of the boreholes in Panels 1 and 2 drop to below the 97°C limit. In an "average" panel, the borehole wall temperature can vary by as much as 60°C between the coolest and the hottest borehole. At the time of peak borehole wall temperature (~ 20 years after emplacement), there is up to 100°C variation in the peak borehole wall temperature in a panel. At this time, about 70% of a borehole wall's temperature rise is due to the source in its hole. After 1000 years, only 10% of this temperature rise is due to the output from the source in its borehole.

Assuming an emplacement schedule where the oldest SF from the actual expected waste inventory is emplaced in the repository first, the following thermal

response is noted at 300 years after emplacement. The hottest borehole wall for this emplacement scheme has increased by 11°C while the coolest has decreased by 19°C, which is an increase of 47% in the borehole wall temperature range. A representative panel has a 53°C variation in borehole wall temperature. Many more boreholes than the uniform source model have predicted temperatures less than 97°C at 300 years. Thus, although only the load of an isolated borehole need be used to predict its peak borehole wall temperature, the actual emplaced inventory in the repository should be used to predict whether a given borehole will remain above the unconfined boiling point at 300 years.

Finally, calculations for a representative panel involved determining characteristic intra-panel borehole temperature distributions at 300 years after repository closure to detail the local effects of finite panels, non-uniform source distributions, and heat-tailored emplacement layout. The model includes detailed descriptions of drifts with commingled consolidated SF and DHLW and drifts with intact SF only. The containers near the ends of a large number of drifts in the middle of the panel fall below the 97°C limit, especially near the "intact SF" drifts. Also, a high percentage of DHLW packages have borehole wall temperatures below 97°C. At 200 years after emplacement, greater than 10% of all the boreholes are cooler than 97°C. At 300 years, this percentage has risen to 15%. At 1000 years, nearly the whole panel is less than 97°C.

Altering the source distribution to keep as many boreholes as hot as possible as long as possible (heat-tailored emplacement) results in a marked reduction in the number of containers occupying boreholes with wall temperature below 97°C. The fraction below 97°C, for this heat-tailored configuration, is one-half that for the untailed layout up to about 400 years after emplacement. A relative variation of 10% in the thermal conductivity of the tuff can vary these fractions by a factor of two or more.

References

1. **Site Characteristic Plan, Yucca Mountain Site, Nevada Research and Development Area, Nevada**, Volume III, U. S. Department of Energy, Office of Civilian Radioactive Waste Management, DOE/RW-0199, 1988. HQ0.881201.0002
2. SNL (Sandia National Laboratories), **Site Characterization Plan Conceptual Design Report**, SAND84-2641, Sandia National Laboratories, Albuquerque, NM, 1987. NNA.880902.0014, NNA.880902.0015, NNA.880902.0016, NNA.880902.0017, NNA.880902.0018, NNA.880902.0019
3. U.S. Department of Energy, **Integrated Data Base for 1987: Spent Fuel and Radioactive Waste Inventories, Projections, and Characteristics**, DOE/RW-0006, Rev. 3, Oak Ridge National Laboratory, Oak Ridge, Tennessee (September 1987). NNA.900403.0377
4. DOE (U.S. Dept. of Energy), **Mission Plan**, Office of Civilian Radioactive Waste Management, Washington, D.C., 1985, DOE/RW-0005 (Table 2-2). NNA.870519.0050
5. Baxter, R.G., **Defense Waste Processing Facility Wasteform and Canister Description**, Savannah River Plant, SC, 1988, DP-1606, Rev. 2 (Table 19). NIVA.890327.0057
6. F.C. Nimic, S. J. Bauer, J. R. Tillerson, **Recommended Matrix and Rock Mass Bulk, Mechanical, and Thermal Properties for Thermal-Mechanical Stratigraphy of Yucca Mountain**, Sandia National Laboratory- Albuquerque, NM, Keystone Document 6310-85-1, 1985. NNA.891129.0284
7. D.N. Montan, **The Plus Family - A Set of Computer Programs to Evaluate Analytical Solutions of the Diffusion Equation**, Lawrence Livermore National Laboratory (University of California), Livermore, CA, UCID-20680, February 1986. NNA.900430.0044

8. **J.J. Nitao, Numerical Modeling of the Thermal and Hydrological Environment around a Nuclear Waste Package using the Equivalent Continuum Approximation: Horizontal Emplacement, Lawrence Livermore National Laboratory (University of California), Livermore, CA, UCID-21444, 1990. NNA.890317.0021**

Appendix A

This report does not use any information from the Reference Information Base nor contain any candidate information for the Reference Information Base or the Site and Engineering Properties Data Base (SEPDB).