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COMPARISON OF PREDICTED FAR-FIELD TEMPERATURES FOR DISCRETE AND SMEARED HEAT SOURCES[a]

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ABSTRACT

A fundamental concern in the design of the potential repository at Yucca Mountain, Nevada is the response of the host rock to the emplacement of heat-generating waste. The thermal perturbation of the rock mass has implications regarding the structural, hydrologic, and geochemical performance of the potential repository. The phenomenological coupling of many of these performance aspects makes repository thermal modeling a difficult task. For many of the more complex, coupled models, it is often necessary to reduce the geometry of the potential repository to a smeared heat-source approximation. Such simplifications have impacts on induced thermal profiles that in turn may influence other predicted responses through one- or two-way thermal couplings. The effect of waste emplacement layout on host-rock thermal response was chosen as the primary emphasis of this study. Using a consistent set of modeling and input assumptions, far-field thermal response predictions were made for discrete-source as well as plate source approximations of the repository geometry. Input values used in the simulations are consistent with a design-basis areal power density (APD) of 80 kW/acre as would be achieved assuming a 2010 emplacement start date, a levelized receipt schedule, and a limitation on available area as published in previous design studies. It was found that edge effects resulting from general repository layout have a significant influence on the shapes and extents of isothermal profiles, and should be accounted for in far-field modeling efforts.

MODELS AND ASSUMPTIONS

For the purposes of this study, the potential repository site at Yucca Mountain was assumed to be composed of a single, homogeneous, isotropic material with constant properties. In addition, no open air spaces or variations in surface topography were considered. Using these simplifications, analytical solutions to the heat conduction equation can be derived.[1] The two approaches used in this study were chosen to represent the range of source types typically used in modeling the perturbed far-field thermal environment of the potential repository. Both are based on closed-form analytical solutions to the heat conduction equation for heat-generating sources isolated in a semi-infinite medium; the first assuming the uniform distribution of a heat-generating material throughout a right-circular cylinder and the second assuming the heat generating material to be distributed in a parallelepiped. By incorporating the principle of superposition, three-dimensional temperature histories were obtained for the far-field environment surrounding the potential repository.

Four sets of thermal calculations were carried out in this study. The first, denoted here as the discrete-canister model, explicitly accounts for each waste package by modeling them as finite-length right-circular cylinders. The remaining three simulations were based on areally extensive plate source representations of the heat-generating waste, and are referred to in terms of the number of plates modeled (e.g., single-plate model). Prior to a discussion of the modeled geometries used in the simulations, a brief description of the material properties, boundary and initial conditions, general layout of the potential repository, modeled waste stream, and emplacement scaling technique will be presented.

Material Properties

The properties of the rock surrounding the modeled waste was assumed to have the thermal properties of the second unit of the Topopah Springs member (TSw2) at Yucca Mountain, Nevada. Specifically, a thermal conductivity of 2.10 W/mK and a thermal capacitance of 2.20 J/cm^3K were used.

Boundary and Initial Conditions

The horizontal plane passing through the center of the heat generating material (plates or cylinders) was assumed to be located 350 m below the ground surface, with temperature sampling locations extending an additional 300 m below the potential repository horizon. A constant temperature of 18.7°C was applied at the ground surface for all sampling times. As an initial condition, a geothermal slope of 0.018°C/m-depth was used to a depth of 400 m and 0.030°C/m-depth for distances greater than 400 m below the modeled surface. The horizontal plane of the modeled region was assumed to be of infinite extent.

General Repository Layout

The geometry of the potential repository, as published in the Site Characterization Plan--Conceptual Design Report (SCP-CDR),[2] is composed of a series of emplacement panels (see

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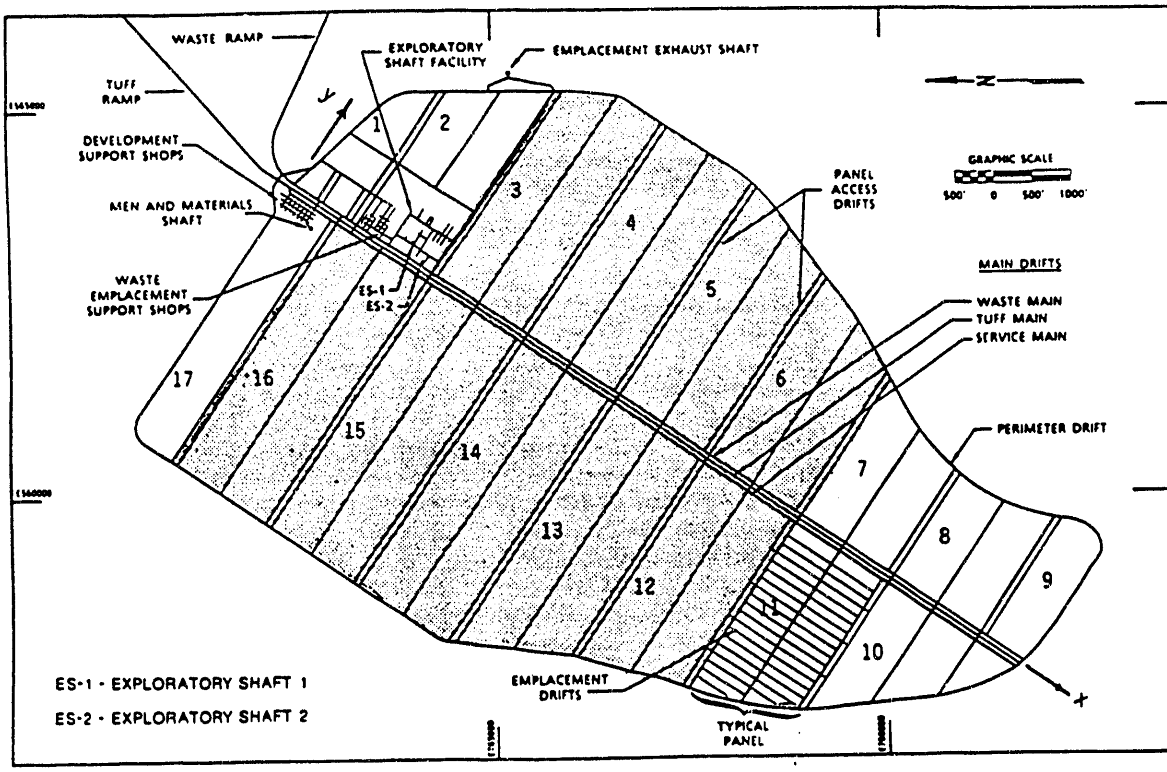

Figure 1. Conceptual Layout for Potential Repository[2]

Figure 1). Emplacement panels are typically 426 m (1400 ft) wide and extend from the main access to perimeter drifts. The panels vary from 457 to 1010 m (1,500 to 3,600 ft) in length and are approximately rectangular in shape. A total of 17 panels were designated in the SCP-CDR for waste emplacement, 14 full-width and 3 half-width. The principal access corridor to the emplacement panels is provided by a series of three main drifts that run the length of the developed region and combine to form a strip of unheated area 46 m (151 ft) in width. Associated with this main drift corridor is a thermal buffer zone between the outer main drift and the edge of what is considered the beginning of the actively heated region of a given panel. This buffer zone was defined to be 61 m (200 ft) wide in the SCP-CDR, but calculations carried out in support of this study indicated that a reduction to 45.7 m (150 ft) would be sufficient to meet the operational intent of the original SCP-CDR main drift standoff. Combining the main drift width with the modified main drift standoffs leads to an unheated zone 137.5 m wide (451 ft) running the length of the potential repository.

On a smaller scale, there exists a similar unheated zone between adjacent panels. Access to an emplacement panel is via a dual set of panel access drifts that run perpendicular to the mains and intersect the perimeter drift. Panel access drifts are 6.4 m (21 ft) wide and, between adjacent panel, are separated by a 19.2 m (63 ft) wide barrier pillar. When this is combined with a 25.9 m (85 ft) standoff between the first canister in an emplacement drift and the panel access drift, the actively heated drift length of an emplacement drift is reduced by 83.8 m (275 ft). The implications of the unheated zone defined about the mains, and the zones defined between panels will form the basis of later discussions.

In recent years several modifications have been proposed to the basic SCP-CDR layout, some of which were incorporated into this study. First, changes in the proposed size of the exploratory studies facility (ESF) have indicated that panels 1 and 2 may no longer be viable for waste emplacement. Thus, they were excluded from consideration in this study. Furthermore, the specific spacings of 38.4 m (126 ft) between emplacement drifts and 4.57 m (15 ft) between spent fuel containers defined in the SCP-CDR is an artifact of the specific initial canister power outputs and target areal power density (APD) under investigation at the time of the SCP-CDR. For this study, drift sizes as defined in the conceptual design were adhered to as well as maximum extraction ratio limits considered to be appropriate for the rock of the target horizon. Specifically, assuming a 4.88 m (16 ft) drift width and a 30% extraction ratio limit, a minimum drift spacing of 16.3 m (53.4 ft) was calculated for use in this study. Regarding the target APD of 57 kW/acre published in the SCP-CDR, more recent investigations have indicated that changes from consolidated fuel packages to a reference package containing 4 intact boiling-water and 3 intact pressurized-water reactor assemblies (BWR and PWR, respectively) would allow an increase in design-basis APD to approximately 80 kW/acre without violating currently published thermal goals for the potential repository.[3] As a result, the loading chosen for investigation in this study was a design-basis APD of 80 kW/acre. One of the main geometric implications of altering the drift spacings and increasing the overall design-basis loading is that fewer panels are required to accommodate the expected tonnage of waste. Referring to the shaded regions of Figure 1, only the development of panels 3, 4, 5, 6, 12, 13, 14, 15, and 16 were necessary given the assumptions of this study.

Modeled Waste Stream

As reported in the Characteristics Database maintained by Oak Ridge National Laboratories,[4] the Energy Information Administration's historical and projected data indicate that almost 87,000 tons of spent fuel will be available for permanent disposal by the end of discharge year 2037. This inventory of spent fuel represents the discharge from approximately 115 commercial reactors and assumes a No New Orders-Extended Burnup scenario. Although 87,000 tons of spent fuel will be ultimately available for disposal, the Mission Plan Amendment[5] (MPA) specifies that 63,020 metric tons of spent fuel and 6,980 tons of defense high level waste (DHLW) are to be emplaced in the nation's first repository. Table 1 shows the MPA's tonnage schedule for the emplacement of spent fuel. In addition, if the current reference internal canister loading configuration of 4 intact BWR and 3 intact PWR assemblies is observed, average assembly weights translate these tonnage values into the yearly number of canisters received documented in Table 1.

With the tonnage and canister configurations established, numerous assembly selection criteria can be applied to the projected inventories to produce a wide range of waste stream characteristics. For this study, a selection criteria known as "levelized" was chosen. In the levelized scenario, assemblies are chosen from the available inventory such that the yearly average spent fuel ages and burnups are constrained, and essentially equal to the overall averages over the 25-year emplacement life of the potential repository. Table 1 documents the yearly average ages, and initial container heat outputs for the waste stream calculated for use in this study. For the discrete canister models, yearly averages were used directly with four-term exponential decay curves fitted to the yearly average burnup values. For the plate source models, however, the overall emplacement average characteristics were used.

Scaling for Waste Age and Burnup

Although the levelized approach to waste selection tends to eliminate extreme variations in yearly thermal decay characteristics, even small yearly variations can cause noticeable variations in predicted thermal profiles. For this reason, the application of a scaling technique to account for variations in waste age and burnup is often used in thermal design calculations. For this study, the equivalent energy density (EED) concept[6,7] was applied. The EED concept bases its equivalent loading criteria on the assumption that a given waste will produce worst-case thermomechanical effects equal to worst-case thermomechanical effects produced by some baseline waste, provided that the thermal energy deposited over a specific "deposition period" is the same for both waste descriptions. For this study, a 300-year deposition period was used to scale emplacement densities.

Table 1: Mission Plan Amendment Spent Fuel Tonnage Requirements and Levelized Waste Stream Characteristics

Acceptance Year	Tons of Spent Fuel	Number of Spent Fuel Containers	Levelized Selection: Average Age (years)	Levelized Selection: Average Burnup (GWd/MTU)
2010	400	200	38.5	16.5
2011	400	200	37.7	15.2
2012	400	200	37.5	13.8
2013	900	447	37.5	20.0
2014	1,800	894	36.7	22.3
2015	3,000	1,489	35.4	25.7
2016	3,000	1,489	33.8	27.3
2017	3,000	1,489	32.5	29.0
2018	3,000	1,489	31.5	27.3
2019	3,000	1,489	30.8	31.3
2020	3,000	1,489	29.9	30.4
2021	3,000	1,489	29.5	34.8
2022	3,000	1,489	28.9	34.6
2023	3,000	1,489	28.4	38.2
2024	3,000	1,489	27.7	38.2
2025	3,000	1,489	27.2	40.1
2026	3,000	1,489	26.5	39.1
2027	3,000	1,489	26.0	40.0
2028	3,000	1,489	25.4	40.9
2029	3,000	1,489	24.8	39.4
2030	3,000	1,489	24.3	40.8
2031	3,000	1,489	23.7	39.5
2032	3,000	1,489	23.3	38.1
2033	2,700	1,340	23.0	39.5
2034	2,420	1,200	22.8	36.4
TOTALS/ AVERAGES	63,020	31,283	28.5	35.4

In the Unit Evaluation Study performed by Johnstone et al.[8] thermal decay characteristics for 10-year-old, PWR-type spent fuel as described by Kisner[9] were used to represent the heat generation of the entire inventory of spent fuel anticipated for potential emplacement at the Yucca Mountain site. Since the time of the Unit Evaluation Study, the Kisner waste description has been used to represent the baseline thermal decay characteristics in many repository thermal design effort, including this study. Table 2 documents the initial thermal loadings, design-basis and scaled, as applied to the discrete-canister, single-plate, two-plate, and nine-plate models run in this study.

Table 2: Initial Loadings for Models

Model	Initial Areal Power Density (kW/acre)		
	Design-Basis	Local	Scaled Local
Discrete-Canister	80	97	70.7 to 79.0
Single Plate	80	80	60.6
Two-Plate	80	80	60.6
Nine-Plate	80	97	73.5

Discrete-Canister Model Geometry

In the discrete representation of the potential repository, the contribution of 31,283 spent fuel containers and 13,500 DHLW containers were explicitly accounted for in the prediction of the perturbed far-field thermal environment. Spent fuel containers were modeled as right-circular cylinders with diameters of 0.74 m (29 in) and lengths of 4.76 m (187.5 in). Similarly, the DHLW package was assigned a diameter of 0.61 m (24 in) and a length of 3.0 m (118 in). These values are consistent with reference dimensions presented for spent-fuel and DHLW packages in the SCP-CDR.

Unlike the fully commingled case presented in the SCP-CDR design, it was assumed that the DHLW canisters would be segregated into the first five drifts of each panel, and emplaced in a staggered, double row configuration. Each DHLW canister was assumed to be spaced 2.28 m (7.5 ft) from its nearest neighbor with an initial power output per container of 200 W and an initial age of 30 years.

Activation of the heat-generation of the spent fuel canisters was timed to mimic a fully stepped emplacement scheme consistent with expected operations. Specifically, canisters were activated on a yearly basis beginning at the perimeter drift and working toward the main drift accesses. Each panel took anywhere from 2 to 6 years to fill, with the DHLW drifts being activated in the last year of spent-fuel emplacement within a given panel.

Single-Plate Model Geometry

For the single plate model, the size and orientation of the plate was chosen so that it encompassed the entire set of heat-generating panels defined in the discrete-canister model. The plate was aligned so that, where practical, the edges of the plate coincided with the edges of the discrete-canister model's heat-generating areas. The overall x-dimension of the plate was defined as 2,134 m (7,000 ft), the distance from the edge of panel 16 to the edge of panel 12. Similarly, the distance from the outermost emplacement drift in panel 16 to the outermost drift in panel 4 was used to define the y-dimension of the plate. The depth of the plate was defined as 4.76 m, equal to the length of a reference spent fuel canister.

Two-Plate Model Geometry

As discussed earlier, there is a 137.5 m strip of non-heated rock running down the approximate center of the repository block. In order to account for this in a plate-source model, a minimum of two plates is required. Both plates were assigned a thickness of 4.76 m. Plate 1 was defined to encompass the discrete-canister model's definitions of panels 3 through 6, with plate 2 extending over panels 12 through 16. The x-dimension of plate 1 was set at 1,707 m (5,600 ft) with the y-dimension determined by the area of spent-fuel emplacement in panel 4, 864 m (2,835 ft). The x-dimension of plate 2 was defined as 2134 m (7,000 ft) and the y-dimension set at 1,011 m (3,317 ft), corresponding to the distance between the edges of panel 12 and 16 and the y-extent of the spent-fuel emplacement area in panel 16, respectively. The area encompassed by the DHLW was not accounted for in this model, since it was determined in the discrete-canister model that the DHLW's contribution to the perturbed far-field environment was negligible.

Nine-Plate Model Geometry

While the two-plate model does account for the non-heated region defined about the main accesses, it is unable to account for the thermal buffer zones between adjacent panels. For this, a nine-plate model was adopted. The dimensions and orientations of the plates were defined so that they coincided with the areas of actual spent fuel emplacement defined in the discrete-canister model. DHLW emplacement was once again ignored. The effects of this assumption will be discussed in the following section.

RESULTS

The three-dimensional thermal profiles generated in this study were examined from two standpoints. First, isothermal surface profiles were generated at various times including the preclosure period of up to 100 years following emplacement and the postclosure period out to 2,000 years following initial waste emplacement. In addition to comparing general shapes, extents, and durations of specific isothermal surfaces, the solutions obtained for the various plate source models were subtracted from those obtained for the discrete-canister model to identify and quantify areas of temperature differences.

Beginning with an examination of the isothermal profiles generated by the four simulations, Figures 2 through 4 document a plan view of the 95°C isosurface for the single-plate, two-plate, and discrete-canister models at 100 years following initial emplacement. The nine-plate model results are not included since they are virtually indistinguishable from the discrete-canister results at this time step. Rectangles representing the locations of active spent fuel and DHLW emplacement from the discrete-canister model are included in the figures for reference.

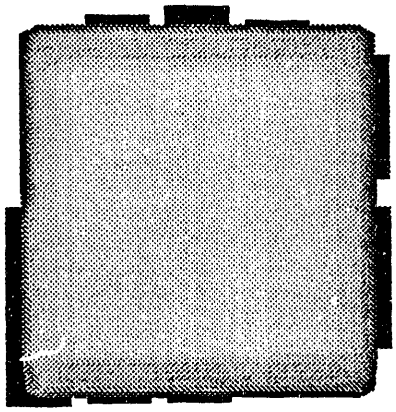

Figure 2. Plan View of 95°C Isotherm for the Single-Plate Model 100 Years Following Emplacement

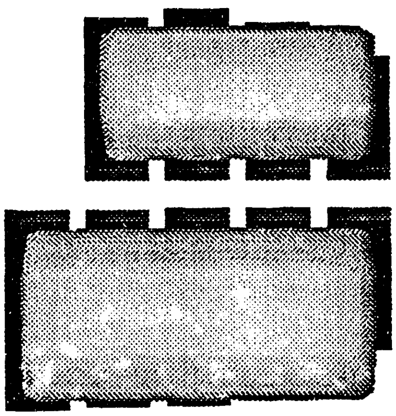

Figure 3. Plan View of 95°C Isotherm for the Two-Plate Model 100 Years Following Emplacement

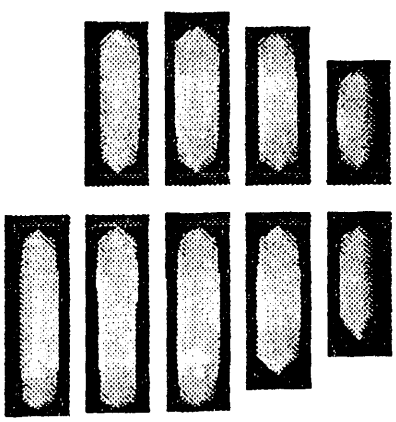

Figure 4. Plan View of 95°C Isotherm for the Discrete-Canister Model 100 Years Following Emplacement

Comparing Figures 2 and 3, it is obvious that the increase in plate sources from 1 to 2 allows the modeler to capture the thermal influence of the major geometric feature of the potential repository, the nonactively heated main drift corridor. As witnessed by Figures 5 and 6, the imposed edge effects of this corridor become more important as time increases into the postclosure period.

Despite the marked improvement in going from 1 to 2 plates, the large areal extent of the plates predicts what, in the discrete-canister simulations, would be equivalent to early coalescence of the isotherms across panels. Figure 4 shows that this is not the case. In order to account for the edge effects inherent in the discrete-canister model, a minimum of nine plates coincident with the actively heated regions of the potential repository would be required.

This is not to say that the nine-plate model is entirely equivalent to the discrete-canister model. Over the time span examined, however, the differences are considered to be insignificant. In the preclosure period, a comparison of results indicated that the nine-plate model underpredicted the discrete-canister model by as much as 8°C in the regions of the unmodeled DHLW. Based on the 5 to 7°C thermal contribution of the DHLW calculated in the discrete-canister model, this early-time underprediction can be discounted. Regions were also identified in which the nine-plate model predicted temperatures up to 7.5°C greater than those obtained for the discrete-canister model. These areas of overprediction were highly localized, with the majority of the modeled region falling well within a 5°C temperature difference. The close correspondence between the nine-plate and discrete-canister models is maintained throughout the 2,000 year time period examined. It is noted, however, that a trend toward the degradation of the agreement between the two models was observed as the sampling time exceeded 1,500 years.

Beyond 1,000 years, the effects of the DHLW are no longer an issue, with main drift temperatures agreeing between the discrete-canister and nine-plate models to within 1 to 3°C. From 1,000 to 2,000 years, the underprediction of the nine-plate model compared to the discrete-canister model increases from approximately 4 to over 11°C. As shown in Figure 7, the regions of this underprediction are primarily centered over the central sections of central panels.

The reason for the degradation in agreement is straightforward. By virtue of its geometry, a plate source is a representation of a diffuse, uniform heat source. The waste packages in an actual emplacement panel, however, could be visualized at the next level of resolution as thin bands of heat-generating material within the panel. In the early times following emplacement, the source strengths are enough to mask the striated nature of an emplacement panel and make it behave much as the diffuse plate source. As time increases and source strengths decrease, the scale over which the heat-generating material in a given area is smeared becomes more important and the more concentrated bands of heat-generating material within the discrete-canister model begin to assert their thermal influence. This represents an important consideration for long-time far-field models, since there is no evidence to suggest that this trend would not continue beyond the modeled time frame.

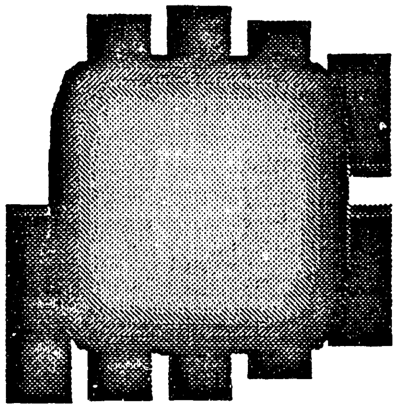

Figure 5. Plan View of 95°C Isotherm for Single-Plate Model 1,500 Years Following Emplacement

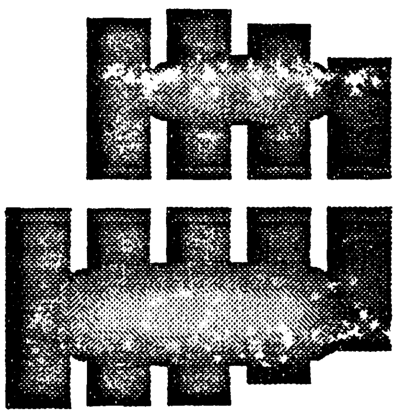

Figure 6. Plan View of 95°C Isotherm for Two-Plate Model 1,500 Years Following Emplacement

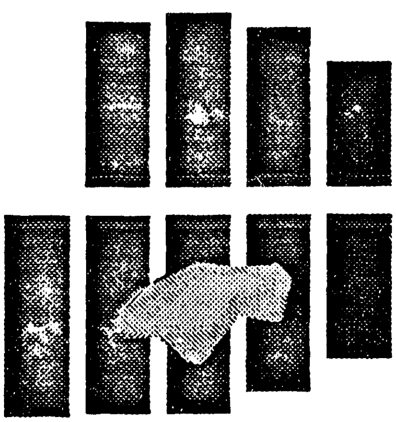

Figure 7. Plan View of 10°C Isosurface of Underprediction by Nine-Plate Model 2,000 Years Following Emplacement

CONCLUSIONS AND RECOMMENDATIONS

The use of a single plate representation of the potential repository's heat-generation appears inappropriate for far-field (distances greater than 10 m from the potential repository horizon) analyses that are meant to model layouts similar to the SCP-CDR. The inability of the single plate model to capture even the most basic geometric features of the potential repository layout causes it to overpredict the spatial extents and temporal durations of the isothermal surfaces. The benefits from going from a single plate to a two plate model are pronounced. By capturing the most thermally significant feature of the repository, the main drift corridor, the two plate model is able to account for some of the internal edge effects inherent in the general repository layout of the SCP-CDR. However, if one is pursuing a far-field thermal analysis based on the SCP-CDR design, the impacts of the panel access regions should not be ignored. A two plate model is incapable of capturing the delay in coalescence of isotherms across panels, and for this particular case, a nine-panel model is required. It is emphasized, however, that the nonuniform nature in which a panel is expected to be loaded makes the diffuse nature of a plate source result in solutions that diverge from the discrete-source solutions as the times of interest progress into the postclosure period.

It is recognized that the discrete modeling of each individual canister anticipated for emplacement is not always practical, or even possible, particularly in phenomenologically coupled models. However, as has been shown, the major geometric features of a given repository layout must be accounted for in the heat source definition if significant confidence is to be placed in the results.

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