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Nevada Nuclear Waste Storage Investigations Project

Thermal Analysis of Spent Fuel Disposal in Vertical Emplacement Boreholes in a Welded Tuff Repository

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THERMAL ANALYSIS OF SPENT FUEL DISPOSAL IN VERTICAL EMPLACEMENT BOREHOES IN A WELDED TUFF REPOSITORY

by

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ABSTRACT

Two- and three-dimensional heat transfer analyses were conducted to determine temperatures in the vicinity of a waste canister and an emplacement drift. The effect of emplacement of canisters containing Boiling Water Reactor (BWR) spent fuel in vertical boreholes was simulated for the cases of an emplacement drift either fully ventilated or sealed immediately after canister emplacement. Analyses were undertaken using two nodal-point integration (or finite volume) codes, PORFLOW and THERM3D, that respectively solve the two- and three-dimensional forms of the diffusion equation. In the unventilated case, the effect of radiation was approximated by defining an equivalent radiation thermal conductivity. Analyses were also performed using a simple code, TEMP3D, that is based on the closed form solutions for constant and decaying heat sources. The calculations indicate that the temperature at the canister borehole wall will peak at about 215°C if the drift is ventilated and about 240°C if it is unventilated. The peak temperature occurs sooner in the ventilated case; after 3 to 4 years, as opposed to 9 years. For a point 1 m from the wall of the emplacement borehole, the corresponding peak temperatures are 150°C for the ventilated case and 185°C for the unventilated case and occur approximately 5 and 17 years after canister emplacement. In the calculations reported here, it was assumed that the effect of drift ventilation would be to maintain a uniform temperature of 30°C at the drift perimeter. If the drift is unventilated the wall rock temperature peaks some 75-100 years after waste emplacement; reaching approximately 125°C at the mid-height of the drift wall. Comparisons between the results of the three-dimensional analyses performed using TEMP3D and THERM3D indicated that the simpler modeling technique, based on application of the closed form solutions for point heat sources, provided a good estimate of temperatures in the immediate vicinity of the canister for both the ventilated and unventilated cases. Comparisons of the results of two- and three-dimensional analyses performed using the PORFLOW and THERM3D codes indicated that the two-dimensional approximation is excellent, except in the immediate vicinity of the canister.

*Currently with J.F.T. Agapito & Associates.

FOREWORD

This "scoping" study was done to determine the most appropriate physical model for calculating borehole wall and drift temperatures. As such, it is an initial effort in the model verification and validation process. The study's purpose was to test models, not to predict temperatures accurately. The models examined included two- and three-dimensional geometric representations and closed-form solution and finite-element predictions of heat conduction.

The study was initiated before NNWSI project baseline data was established by Nimick and others*, and many parameters used herein are not current. The best data available at the time of the study were used. In general, except as noted in the text, the conclusions drawn from this study are not sensitive to the data used.

While the temperatures predicted herein and the data used are indicative of current design work on the prospective welded tuff repository, they should not be used in lieu of project baseline data.

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October 1985

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*Nimick, F. B., S. J. Bauer, and J.R. Tillerson, "Recommended Matrix and Rock-Mass Bulk, Mechanical and Thermal Properties for Thermomechanical Stratigraphy of Yucca Mountain," Keystone Document 6310-85-1, Sandia National Laboratories, Albuquerque, 1984.

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1. INTRODUCTION

1.1 Purpose and Justification

The work described in this report was performed for Sandia National Laboratories as a part of the Nevada Nuclear Waste Storage Investigations (NNWSI) project. Sandia is one of the principal organizations participating in the project, which is managed by the U.S. Department of Energy's Nevada Operations Office. The project is part of the Department of Energy's program to develop methods to safely dispose of the radioactive waste from nuclear power plants.

The Department of Energy has determined that the safest and most feasible method currently known for the disposal of such wastes is to emplace them in mined geologic repositories. The NNWSI project is conducting detailed studies of an area on and adjacent to the Nevada Test Site (NTS) in southern Nevada to determine the feasibility of developing a repository.

This report documents the results of a numerical investigation of the temperature in the vicinity of a typical spent fuel canister emplaced below the drift floor. The motivation for the work described here was to investigate the adequacy of alternative methods of computing the transient thermal response within a few meters of waste emplacement canisters. The results are pertinent to the particular case of vertical emplacement of canisters containing Boiling Water Reactor (BWR) spent fuel. Other cases could be analyzed in the manner described.

1.2 Approach

In all, three different methods of analysis were used in this study. First, several three-dimensional analyses were performed using a computer code based on the closed form solutions for constant and exponentially decaying point heat sources. Second, a three-dimensional nodal point integration (finite volume) model of the canister and emplacement drift was prepared; conductive heat transfer calculations were performed for the cases of ventilated and unventilated drifts. Third, a two-dimensional finite volume model approximating the three-dimensional geometry was developed by assuming that the heat from the canisters was uniformly distributed in a slot beneath the floor of the emplacement drift.

Again, conductive heat transfer calculations were performed for the cases of ventilated and unventilated drifts.

1.3 Assumptions

In all cases the computer codes used in this study considered only conductive heat transfer; however, for the analyses involving unventilated drifts, the radiative heat transfer within the excavation was approximated by ascribing equivalent conductive properties to the air. For the rock mass, it was assumed that nonlinear effects, including pore water migration and evaporation, could be ignored. In practice, nonlinear effects and the specific configuration of the canister, canister hole, and any backfilling material would strongly influence very near field conditions. For the excavations, it was assumed that either the ventilating air maintained an isothermal boundary condition at the excavation wall or that the excavation was sealed and unventilated.

2. PROBLEM DEFINITION

Data for the analyses of vertical emplacement of BWR spent fuel was derived from three sources. The emplacement drift geometry was obtained from the engineering drawing, prepared by Dravo Engineers for Sandia National Laboratories (Dravo, 1983), which is reproduced in Figure 1. The power decay characteristics of 10-year BWR spent fuel waste were assumed to be described by the following normalized function, defined in Keystone memorandum 6310-83-2 (Shirley, 1983):

$$Y(t) = 0.7614 \exp(-0.02626t) + 0.2007 \exp(-0.002068t) + 0.02415 \exp(-0.00005222t) \qquad (1)$$

in which the unit of time t is years. The remaining data were supplied in a task memorandum dated February 23, 1984 (Mansure, 1984). These data comprised:

Canister hole diameter	0.71 m
Canister length	4.5 m
Canister standoff distance	3.05 m
Centerline spacing between drifts	45.8 m
Canister hole pitch	4.0 m

Heat capacity (ρc) of the rock	2.17 MJ/m^3K
Thermal conductivity (K) of the rock	1.8 W/mK
Initial rock temperature	26.°C
Initial canister output	3. kW

For the cases of ventilated drifts, it was assumed that the emplacement drift perimeter would be maintained at a constant temperature of 30^oC. Several alternative assumptions were made concerning the equivalent conductive properties of the air in the cases of unventilated drifts. These assumptions are discussed in the context of the results of the analyses.

3. ANALYSIS METHODS

The solution methods used in this study are described briefly below.

3.1 Closed-Form Solution

The computer code TEMP3D (Christianson, 1979), which was used in this study, is based on the analytical solutions for exponentially decaying and constant-strength-point sources in an infinite region. Distributed heat sources, such as canisters, can be represented approximately by an equivalent distribution of point sources. The code treats the problem of the semi-infinite region using the method of images, allowing the free surface to be either isothermal or adiabatic. This method of handling boundaries cannot treat more general problems of planes of symmetry, so a simple means of modeling a repeated geometry, such as parallel emplacement drifts, is not available. Instead, it is necessary to explicitly represent all heat sources that would influence the temperature of any particular sample point during the simulated period. The region of influence of any source can be deduced from the closed form solution on which the computer code is based.

The temperature change (ΔT) at a distance R from a decaying point source of initial strength Q_o is given by (Christianson, 1979):

$$\Delta T = \frac{Q_o}{\pi^{3/2}} \exp(-At) \frac{\sqrt{\pi}}{4\kappa R} \exp\left(-\frac{R^2}{4\kappa t}\right) \mathrm{Re}\left\{ w\left(\sqrt{(At)} + \frac{iR}{\sqrt{(4\kappa t)}}\right)\right\} \qquad (2)$$

in which A is a decay constant, κ is the thermal diffusivity, and t is the time elapsed since emplacement of the source. The term Re{w(z)} represents the real part of the complex error function of the complex argument z.

From Eq. (2) it is clear that the temperature increase decays approximately in proportion to the expression $\exp(-R^2/4\kappa t)$. Accordingly, for $(R^2/4\kappa t) > 4.$, the temperature change will be small ($\exp(-4.) = 0.018$). To determine the number of sources within an infinite array that must be explicitly represented, it is sufficient to ensure that any sources within a distance $(4\sqrt{(\kappa t)})$ of the sample are included. (This condition is more stringent than using the time constant ($t_c = R^2/k$), as proposed by Montan and Patrick (1981)). In the present instance, since the thermal diffusivity of the medium is 26.18 m^2/year, this implies that the effect of the temperature at one canister on that of another more than 65 m distant will be insignificant for the first 10 years after emplacement.

Input to the analytical solution requires definition of the initial strength (Q_o) of the heat source. For an initial power (P_o) of 3 kW and the material properties defined above, the initial strength is:

$$Q_o = \frac{P_o}{\rho c} = 43.63 \times 10^3 \ {}^oC \ m^3/yr$$

For TEMP3D analyses this strength must be presented as one or more point sources. In the present instance, nine point sources were distributed uniformly along the axis of the canister. The choice of the number of sources is governed by the requirement that the concentration of the source should not influence the temperature at points at which it is calculated. It is, therefore, a function of the spacing of the point sources and the distance to the point at which the temperature is calculated. The choice of nine points is considered conservative for the calculations reported here and more than satisfies the empirical criterion developed by Montan and Patrick (1981).

Based on considerations described above, a distribution of heat sources appropriate to conduct 10- to 15-year simulations of the emplacement of BWR spent fuel was developed. That distribution is illustrated schematically in Figure 2. The adequacy of the idealization was confirmed by performing a series of analyses in which the number of canisters represented was progressively increased. Selected results of the sensitivity studies are reproduced in Table 1.

Figure 2 also identifies the unit cell that was used in the three-dimensional finite volume calculations discussed below. Four sample points, within that unit cell and in a horizontal plane at mid-height of the canister, were selected to provide reference points for presentation of the results of analyses. Those points, which are identified in Figure 3, are located on the canister hole wall and one meter into the rock mass. Points 2 and 4 will experience the highest temperatures of any points at the same radial distances from the canister axis, so their temperature histories are of particular interest when comparing the results of three-dimensional analyses conducted using different models.

3.2 Numerical Solutions

The numerical results presented in this report were obtained using two computer codes developed by Analytic and Computational Research, Inc.: PORFLOW for two-dimensional analyses and THERM3D for three-dimensional analyses. Both codes are based on the finite volume method that uses the nodal-point integration (NPI) technique. Both provide solutions to the diffusion equation that are second order in time and space. PORFLOW solves the diffusion equation using the Alternating-Direction-Implicit technique (Runchal and Hocking, 1981; Runchal, 1985) and allows definition of arbitrary geometries using nonuniform and nonrectangular elements. Detailed verification of PORFLOW, including benchmarking against the SWENT code, was recently performed by Battelle Pacific Northwest Laboratories (Eyler and Budder, 1984). THERM3D allows the user to choose between a fully explicit solution strategy and an implicit strategy based on the method of fractional steps (Yanenko, 1971). Zones can be nonuniform but must be rectangular prisms.

Since the objective of the analyses was to examine three-dimensional effects, we first consider the three-dimensional model developed using the THERM3D code. The unit cell modeled is represented schematically in Figure 4. All exterior boundaries were assumed to be insulated, with upper and lower boundaries removed sufficiently to ensure minimal effects during 20-year simulations.

A total of 2856 prismatic zones were used for the three-dimensional representation. A corresponding two-dimensional model was also developed using THERM3D, by defining zero flux boundary conditions for a cross section one zone thick, so that a detailed comparison of the THERM3D and the PORFLOW codes could be performed.

Since the THERM3D code does not allow definition of arbitrary prismatic volumes, approximations had to be made when defining the geometry of the canister and the emplacement drift. For the canister, the volume was preserved by substituting a cross section 0.6292 m square for the circular cross section. In fact, details of the canister and the canister hole were not considered in this study. Instead, heat generation was assumed to be uniform within the emplacement hole volume, which was ascribed the same thermal properties as the surrounding rock. For the drift, the actual shape of the excavation was replaced by a rectangular section 5 m wide and 7.62 m high. Those dimensions preserve the cross-sectional area and closely approximate the actual shape of the drift.

The idealizations developed for the THERM3D calculations were originally adopted for the two-dimensional analyses using the PORFLOW code. A portion of the model cross section, showing the zoning in the vicinity of the canister and drift, is illustrated in Figure 5. The model is 14 zones wide and 34 zones high and extends 50 m above and below the mid-height of the canister. Following the discussion presented in Section 3.1, it is evident that these upper and lower boundaries will begin to have some influence after approximately six years. However, any significant effect on near-canister temperatures can be expected to occur much later because the rate of heat transfer from the canister will be controlled by the steep temperature gradients in the immediate vicinity of the canister. Accordingly, boundaries at 50 m were considered acceptable for simulations of the first 20 years after canister emplacement. Subsequent results of simulations in which the boundary conditions were changed from isothermal to adiabatic confirmed this model size to be adequate. A larger PORFLOW mesh, comprising 644 zones and extending 187.5 m above and below the mid height of the canister, was used for simulations of longer periods.

Since the results of numerical simulations can be sensitive to the numerical idealization and solution strategy used, a number of sensitivity studies were performed with the THERM3D and PORFLOW codes. The results of several two-dimensional analyses performed using both codes are summarized in Table 2. It may be observed that the results obtained using the two codes are in good agreement and appear to be relatively insensitive to changes in either mesh refinement or the step size used in the time integration. This finding is particularly encouraging since the two codes solve the diffusion equation in quite different manners, and the period over which the comparison was made is one characterized by very high spatial and temporal temperature gradients.

4. ANALYSIS RESULTS

The results of analyses are presented through a series of tables and figures. To simplify this presentation, the analytical tasks are divided into two groups. The first group is concerned with application of the closed-form solution (TEMP3D) to estimate the near canister temperatures. The second is concerned with finite volume modeling (PORFLOW and THERM3D) to determine the temperature in the vicinity of the canister and around the perimeter of the drift.

4.1 Application of the Closed-Form Solution

As noted earlier, TEMP3D allows the user to simulate the placement of heat sources in either an infinite or a semi-infinite region. In the latter case, the half-space boundary may be either isothermal or adiabatic. For the first of the analyses based on the closed-form solution, it was assumed that the drift would have no influence on the temperature field in the vicinity of the canister; the sources were placed in an infinite region. Results of analyses conducted on that basis are illustrated in Figure 6, which consists of isotherms in the horizontal plane at mid-height of the canister. The figure illustrates that three-dimensional effects are relatively unimportant since the temperature will be invariant along any line parallel to the drift axis, except within one or two meters of the canister. This condition occurs particularly quickly because the canisters are very closely spaced in the case analyzed.

Several additional analyses were performed with the objective of investigating different means of approximating the influence of drift ventilation. In the first of these, the emplacement drift was approximated by treating the problem as a semi-infinite region with an isothermal surface at the base of the drift. This approximation should provide a lower bound on the temperatures in the vicinity of the canister when the drift is ventilated, while the infinite region solution should provide an upper bound, for both ventilated and unventilated cases.

The lower and upper bound temperature histories for point 4, which is located 1 m from the canister hole wall, are plotted in Figure 7. The two other histories on that figure are the result of using two alternative methods of approximating the effect of drift ventilation. In one approximation, an image sink was added immediately above the central canister, while in the other approximation image sinks were added along the entire length of the drift. In both cases the computed temperatures lie somewhere between the infinite and semi-infinite region solutions. Although either case may be a better approximation to the ventilated drift case than are the infinite or semi-infinite region solutions, they are of little value since neither is based on a rational estimate of the heat loss to the ventilating air. It is possible to conceive of a means to approximate the true boundary conditions for the drift by defining one or more time-varying heat sinks, but such an approach would, at best, be cumbersome. Also, such development does not appear justified when numerical models, such as the PORFLOW and THERM3D models discussed in this report, can be used to solve the same problem economically.

4.2 Application of the Numerical Models

The initial objectives of the analyses performed with the PORFLOW and THERM3D codes were to obtain an estimate of the peak temperatures in the immediate vicinity of the canister and to provide a basis for evaluating the adequacy of simpler models based on the application of closed form solutions. Because the results reported in the previous section indicated that peak temperatures would occur within a few years of canister emplacement, 20 years was selected as an appropriate period for the three-dimensional simulations conducted with the THERM3D model. These simulations were first performed for the case of a ventilated drift, and the results of those calculation were later verified by performing analogous two-dimensional analyses using the PORFLOW model.

Following completion of the ventilated drift case, analyses were performed for the case of an unventilated drift. Both three- and two-dimensional analyses were again undertaken, although in this case the two-dimensional simulations were continued for a period of 100 years so that peak drift wall temperatures could be determined.

4.2.1 Analyses with a Ventilated Drift

For the ventilated drift analyses, the drift perimeter was maintained at a constant temperature of 30°C. Representative results for the three-dimensional analyses performed using THERM3D are reproduced in Figure 8. The canister hole wall appears to peak at approximately 215°C after three to four years, while the temperature at a point one meter into the rock mass peaks at approximately 150°C some two years later. Additional data on the short term, near canister temperature is provided in Figure 9, in which the temperature histories for the four sample points identified in Figure 3 are presented. These predictions of very near-field behavior should be used with caution because the model is a very simple idealization of the real situation. Short-term, near-field response might be quite different from that predicted by such a simple model because of local nonlinear behavior. On the other hand, simple models can be expected to provide quite acceptable predictions away from the immediate vicinity of the canister, particularly at later times when transient effects are less pronounced.

Temperature distributions in the horizontal plane at the mid-height of the canisters (z = 0.0 m) are illustrated in Figure 10. Detailed comparison of this figure with Figure 6 is not appropriate since the latter is based on the assumption that there is no heat loss to the drift. However, it is immediately apparent that the results are qualitatively similar and both show a rapid decay of three-dimensional effects.

The corresponding time varying distribution of temperature in a vertical plane midway between canisters is illustrated in Figure 11. The sequence of plots in that figure clearly illustrates the influence of the drift; the temperature in the immediate vicinity of the drift is depressed to maintain a steady value of 30°C. One consequence of this depression is that there are very steep temperature gradients immediately above the canister, implying high heat flux through the floor of the drift.

Total heat flux from the rock into the drift can be calculated from the temperature gradients perpendicular to the drift perimeter. Since the accuracy of this calculation depends strongly on the accuracy of the temperature gradient, the effects of mesh refinement and time step size were again assessed by performing sensitivity studies. In this case comparisons were made of two- and three-dimensional calculations performed with THERM3D and two-dimensional calculations performed with PORFLOW. As recorded in Table 3, the results proved to be insensitive to the code used, the mesh size, and the time step size. Accordingly, the heat flow history for two-dimensional case, given in Figure 12, can be considered as representative. The history indicates that the peak heat loss to the ventilating air occurs between 10 and 15 years after canister emplacement and has a value of approximately 360 W/m of drift. As illustrated in Figure 12, the output of the canisters will have decayed to some 75 percent of its emplacement value of 750 W/m of the drift after 15 years. This indicates that the peak load on the ventilation system corresponds to approximately 60 percent of the instantaneous output of the waste.

It is interesting to note that the flow to the drift was insensitive to whether the analysis was performed using a two-dimensional or a three-dimensional geometry. This finding implies that, in the particular set of circumstances investigated, the drift conditions are relatively uninfluenced by the details of the spatial distribution of the canisters. Further support for this observation is provided by comparing the temperature distributions in the drift cross-section for the two-dimensional case (Figure 13) with those already presented for the three-dimensional case (Figure 11). There are obvious differences at very early times. These differences are in large part due to the fact that the isotherms are plotted for a plane that lies midway between two canisters in the three-dimensional case, while in the two-dimensional case the location of the sample plane is unimportant since the heat source is distributed uniformly along the drift. These differences quickly fade, indicating that two-dimensional analyses are appropriate for performing thermal calculations of the drift.

4.2.2 Analyses with an Unventilated Drift

The objective of the second set of numerical calculations was to assess the consequences of sealing, but not backfilling, the emplacement drifts after canister emplacement. Since it is clear from the results presented above that ventilating air removes a substantial proportion of the heat generated by the emplaced waste, the temperatures of the canister and the surrounding rock mass should be significantly higher in the unventilated case. Also, under static air conditions there will be a vertical temperature gradient across the drift that was absent in the ventilated case. The tendency for that gradient to exist under unventilated conditions will be offset by conduction, radiation and free convection in the drift. Since the THERM3D and PORFLOW codes solve only the diffusion equation, approximate methods of accounting for the effects of radiation and convection were sought.

Several investigators have evaluated the contribution of free convection to heat transfer in a drift by conducting analyses using computer models in which both convection and radiation were included. Calculations reported by Montan and Patrick (1981) indicated that radiation was more important than convection, and that the influence of both was to cause drift temperature to be more uniform. George (1980) concluded that radiation is an order of magnitude more important than free convection. Based on these findings, it was not considered necessary to specifically consider possible effects of convection.

Approximate methods of accounting for radiation through use of an equivalent conductive medium have been considered by several investigators. For example, Butkovich and Montan (1980) derived the following equation for the equivalent effective radiation thermal conductivity (K_e) by equating the estimated radiative transport with the equivalent conductive heat flow:

$$K_e = 4\sigma T^3 L \ , \qquad (3)$$

in which σ is the Steffan Boltzman constant, T the absolute temperature, and L the average path length. A similar relationship was derived by Sundberg and Eaton (1982) by considering the excavation as two parallel plates with radiative heat transfer between them. Substitution of representative values for the quantities in Eq. (3) yield estimates of the effective conductivity in the range of 40 W/mK to 100 W/mK, where the lower value corresponds to initial conditions and the upper to conditions several years after canister emplacement. Ideally, the equivalent thermal conductivity should be defined in the computer models as a function of temperature. However, calculations reported by George (1980) and by Butkovich and Montan (1980) have indicated that excellent results are obtained even when a fixed value is used.

Although the investigators referenced above appear to have taken trouble to develop estimates of the equivalent thermal conductivity, little consideration was given to the other properties of the air. Butkovich and Montan apparently used a low, but unspecified, value for the thermal capacitance of the air. George states that the thermal capacitance of the air was assumed to be zero. The implication of such an assumption can be illustrated by noting that with zero capacitance the diffusion equation reduces to:

$$K \nabla^2 T = 0. \tag{4}$$

Under such conditions the temperature distribution is independent of the thermal conductivity. Also, when considering heat flow from one medium to another, the rate is determined by the harmonic mean of the conductivities of the two materials. For widely differing values of the thermal conductivity, the harmonic mean value approaches twice the smaller value. Hence, if the effective thermal conductivity of the air is much higher than the thermal conductivity of the rock, the actual value for the air should be relatively unimportant. Such insensitivity was observed in the present investigation and also by during analyses performed George (1984).

A number of analyses were performed to confirm the insensitivity of the results to the assumed properties of the air in the drift. Specifically, PORFLOW simulations were performed with diffusivities of 50 m^2/yr, 1000 m^2/yr, and 10^6 m^2/yr. (This last value is approximately equal to the thermal diffusivity calculated from the equivalent radiation thermal conductivity and the heat capacity of the air for the initial conditions in the drift). Selected results of these analyses are presented in the discussion that follows, and here we note only that the temperature in the vicinity of the canister varied only a few degrees despite such a large variation, while the drift temperatures were slightly more sensitive. Based on these findings and the computational advantage of using a lower diffusivity, the three-dimensional analyses were conducted using a diffusivity of 50 m^2/yr. Longer term simulations were then performed using a two-dimensional idealization. In those analyses, diffusivities of 50 m^2/yr and 1000 m^2/yr were considered.

The effect of variations in the assumed properties of the drift are illustrated by Figure 14, for which results were derived from two-dimensional simulations performed using PORFLOW. From Figure 14, which consists of temperature histories for selected points in the drift, it is clear that the effect of increasing the diffusivity is to decrease the vertical temperature gradient. However, the temperature at mid-height of the drift is virtually unaffected. This implies that use of the lower value of diffusivity will give a good estimate of the mean air temperature and a conservative estimate of the drift floor temperature. As illustrated by Figure 15, the choice of the lower diffusivity will also result in a conservative estimate of the canister and near-canister temperatures. In view of the number of assumptions made in the analyses, this measure of conservatism seems appropriate.

Results presented in Figure 15 were for the two-dimensional idealization of the canister and drift and should, therefore, be considered as average values. The peak near canister temperatures must be calculated using a three-dimensional model. Results of such calculations, in which a diffusivity of 50 m^2/yr was assumed, are presented in Figure 16. In that figure the temperature at the canister hole wall can be seen to peak at approximately 240°C some nine years after emplacement. One meter into the rock, the temperature peaks at 185°C after 17 years. Additional information on the three-dimensional temperature field is provided in Figures 17 and 18, which consist of isotherms in a horizontal plane at the mid-height of the canister and in a vertical plane mid-way between canisters. These figures may be compared to the corresponding figures (10 and 11) for the ventilated case.

As in the ventilated case, results of two-dimensional analyses are also presented. Temperature histories for the drift and canister were given in

Figures 14 and 15. The corresponding distribution of temperature in a vertical plane is given in Figures 19 and 20, for thermal diffusivities of 50 m^2/yr and 1000 m^2/yr, respectively. Again, these may be compared with the results for the ventilated case, which were presented in Figure 13. In this case, however, the simulations were extended to 100 years after waste emplacement so that the peak drift temperatures could be determined. From Figure 14, the peak temperature at the mid-height of the drift is approximately 125°C and occurs about 75 years after emplacement. There is no corresponding value for the ventilated drift, which was assumed to be maintained at a constant temperature of 30°C.

Review of the results of both two- and three-dimensional analyses of the unventilated drift indicates that the temperatures are higher than in the ventilated case. However, they will not be as high as if the excavation were absent or perfectly insulated because the effect of the relatively conductive air is to quickly distribute heat across the drift. Heat transfer within the drift diminishes the temperature differential between the floor and the roof of the drift. This effect is more pronounced if higher equivalent thermal conductivity is assumed for the air.

5. CONCLUSIONS

Two sets of conclusions result from the series of analyses reported here. The first is concerned with the predicted temperature field in the vicinity of a spent fuel canister and waste emplacement drift and with the heat load to a ventilation system. The second is concerned with the adequacy of the several models used in the investigation.

With respect to heat transfer calculations for the canister and the drift, it is concluded:

- The predicted temperature field is relatively sensitive to the assumed conditions in the drift.

- For the case of continuous ventilation that maintains a constant wall rock temperature of 30°C, the temperature close to the canister peaks within a few years of canister emplacement. For example, the temperature at the canister hole wall peaks at approximately 215°C after 3 to 4 years, and the temperature at a point 1 m into the rock mass peaks at approximately 150°C after 5 years.

- For the case of an unventilated drift, the temperature close to the canister peaks somewhat later and is higher than in the ventilated case. For example, the temperature at the canister hole wall peaks at approximately 240°C after 9 years, and the temperature at a point 1 m into the rock mass peaks at approximately 185°C after about 17 years.

- The rock mass adjacent to the canister is subjected to very high temperature gradients immediately after canister emplacement. Accurate simulation of the early temperature history required the use of extremely small time steps. This suggests that the early temperature history of points close to the canister may be influenced by the specific configuration of the emplacement scheme. Also, non-linear effects, including local dehydration of the tuff, may influence the temperature field. Accordingly, any predictions of the near-field temperatures field must be regarded as approximate unless the geometry and material properties are modeled precisely. Such refinements will not be required if the present approach is demonstrated to result in conservative (i.e. higher than actual) predictions.

- In the case of vertical emplacement of closely spaced canisters, three-dimensional effects appear to be important only to prediction of very near-field, short-term temperatures. Within a few diameters of the canisters, the temperature is relatively invariant along the length of the emplacement drift. Accordingly, two-dimensional analysis should be adequate for prediction of the temperature field adjacent to the drift, providing canisters are emplaced relatively closely. This assertion is supported by the close agreement between the two- and three-dimensional predictions of heat load air in the ventilated drift.

- The peak heat pickup by the air in a ventilated drift was estimated to be approximately 360 W per m of drift. The peak occurs 10 to 15 years after waste emplacement, at which time the ventilation system is removing as much as of 60 percent of the instantaneous thermal output of the waste (or 48 percent of the initial thermal output). The peak heat load to a repository ventilation system may be estimated from the total length of drifts and the waste emplacement. However, such an estimation would be likely to be unduly conservative since it is unlikely that it will be necessary to ventilate the entire repository adequately to maintain uniform drift wall temperature of 30°C. Also, the calculations reported here have ignored any cooling effect associated with vaporization of water present in the rock mass.

With respect to the analysis alternatives, it was concluded:

- Simple models based on the computer code TEMP3D, which utilizes the closed-form solutions for point heat sources, provided a convenient and effective means to estimate the three-dimensional temperature field in the vicinity of the canister. As illustrated in Figure 21, the quality of the predictions appears excellent, with the infinite and semi-infinite region solutions appearing to be good upper and lower bounds on the results predicted using the three-dimensional finite volume code, THERM3D. Hence, application of simple, analytically based models can be recommended for scoping calculations of near canister temperatures.

- Three-dimensional analysis is required to predict transient temperatures in the immediate vicinity of a waste canister and the emplacement drift. In all probability, simplified methods of approximating the heat loss to ventilated or unventilated drifts could be developed. However, such methods would be likely to be problem specific and the computational effort involved in numerical model studies, such as reported here, is already quite modest. Hence, refinement of current simplified modeling procedures is not recommended.

- The two-dimensional finite volume model provided results that differed little from those obtained using a three-dimensional model, except in the immediate vicinity of the canister. Predicted heat loads to the ventilating air were not influenced by whether two- or three-dimensional geometries were considered. Hence two-dimensional analyses can be recommended for room scale calculations, providing the waste canisters are relatively closely spaced.

Since the above conclusions draw attention to the measure of agreement between the various models, it is important to reiterate that these conclusions may be peculiar to the particular set of conditions for which the analyses were performed. The agreement between the numerical and closed form solutions might not have been as good if the numerical solutions had incorporated the real geometry of the canister and the emplacement hole, or accounted for material non-linearity and coupled thermo-hydrologic effects. Also, the close spacing of the canisters in the case analyzed undoubtedly contributed to the rapid disappearance of three-dimensional effects, and thereby to the excellent agreement between the two- and three-dimensional simulations.

6. ACKNOWLEDGEMENT

The finite volume calculations, using the PORFLOW and THERM3D codes, were performed by A. K. Runchal of Analytic and Computational Research, Inc. A. J. Mansure, of Sandia National Laboratories, was project technical monitor and contributed significantly to both analysis and report preparation through peer review, constructive criticism,and suggestion. Brian Ehgartner was also a peer reviewer.

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TABLE 1

TEMPERATURES COMPUTED FOR POINT 4 ($x = 0.0$, $y = 1.355$ m)
FOR A FINITE RANGE OF SOURCES IN INFINITE REGION
AT AN INITIAL TEMPERATURE OF 26^{o}C

	Range of Heat Sources		
Time Years	36 m	65 m	104 m
	Temperature ^{o}C		
1	138.35	138.35	138.35
2	158.22	158.22	158.22
3	168.55	168.57	168.57
4	174.89	175.02	175.02
5	179.00	179.39	179.39
6	181.67	182.51	182.51
7	183.35	184.82	184.82
8	184.30	186.56	186.58
9	184.77	187.90	187.93
10	184.70	188.92	188.98

TABLE 2

COMPARISON OF RESULTS OF TWO-DIMENSIONAL ANALYSES USING THE THERM3D AND PORFLOW CODES

	Canister Centerline Temperature °C				
Code: Grid: Time Step:	THERM3D Standard[1] 0.001	THERM3D Fine[2] 0.0005	PROFLOW Standard 0.001	PROFLOW Standard 0.005	PORFLOW Fine 0.0025
Time (yrs)					
0.5	75.7	75.9	75.5	-	-
0.10	94.0	94.2	93.7	93.7	94.0
0.15	105.6	105.9	105.4	-	-
0.20	114.2	114.5	113.9	113.9	114.2
0.25	120.9	121.2	120.5	-	-
0.3	126.5	126.8	126.0	126.0	126.3
0.4	135.1	135.4	134.4	134.4	134.8
0.5	141.7	141.9	140.7	140.7	141.1

Note: 1 Standard Grid: 15 zones x 35 zones;
Domain: 22.9 x 100 m; Typical Resolution 0.5 m x 0.5 m
Note: 2 Fine Grid: 22 zones x 45 zones;
Domain: 22.9 x 50 m; Typical Resolution 0.3 m x 0.3 m

TABLE 3

COMPARISON OF HEAT FLUX TO THE VENTILATION AIR CALCULATED USING THE THERM3D AND PORFLOW CODES

	Heat Loss: watts/meter of drift		
Code: Grid: Time Step:	THERM3D Standard[1] 0.001 yr	PORFLOW Standard 0.005 yr	PORFLOW Fine[2] 0.0025 yr
Time (yrs)			
0.1	-3.1	-45.9	-44.2
0.2	11.2	13.3	16.0
0.3	51.5	55.4	60.7
0.4	82.6	89.0	94.8
0.5	107.5	115.8	121.8
1.0	184.0	196.7	202.6
2.0	253.1	266.0	272.0
3.0	288.9	298.4	304.6
4.0	312.6	315.9	323.9
5.0	330.4	328.7	336.9

Note 1: Standard Grid - 15 zones x 35 zones
Note 2: Fine Grid - 22 zones x 45 zones

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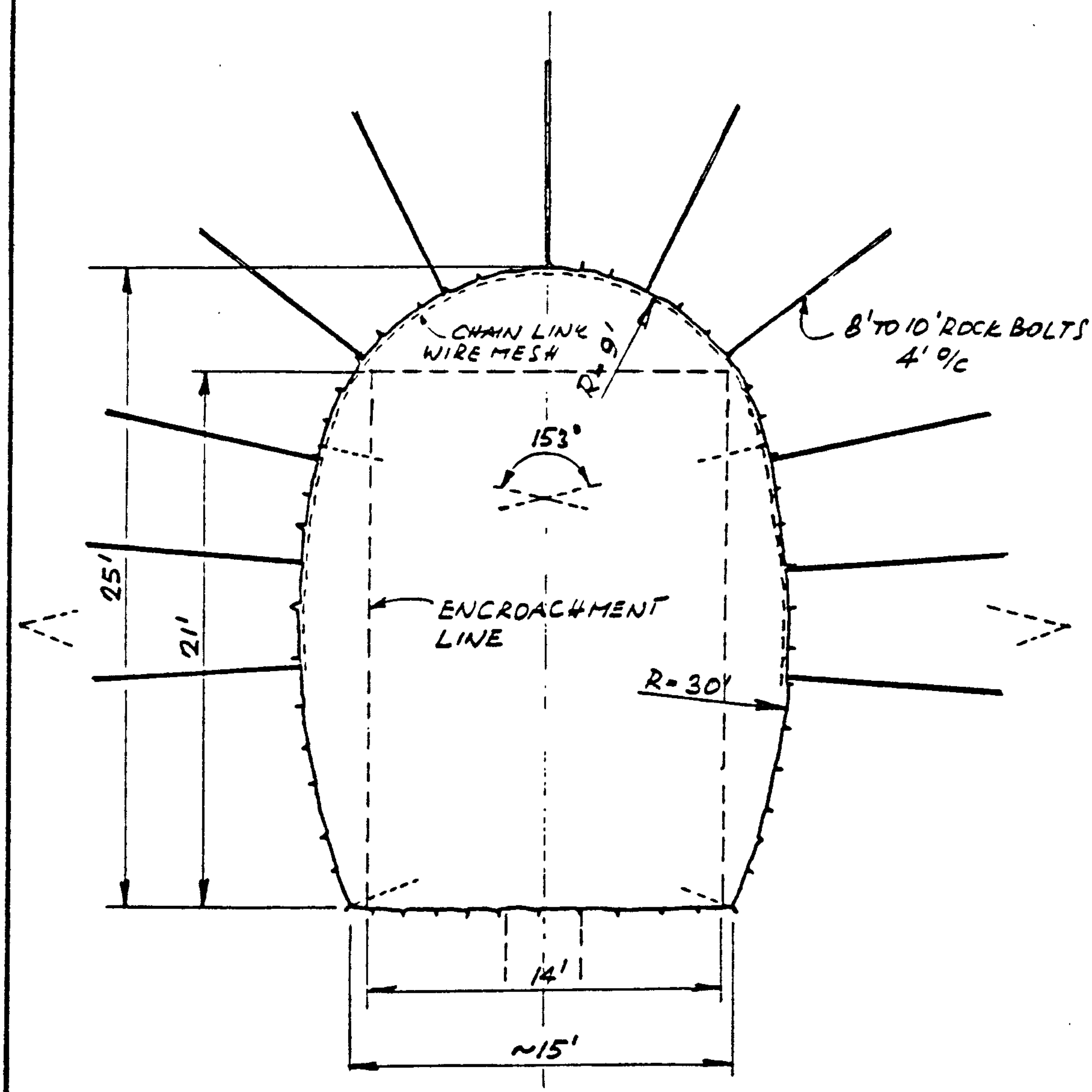
DESCRIPTION STORAGE DRIFT FOR VERT. EMPLACEMENT

DATE 11-7-83
DR I.L. CH ____
REF ____



STORAGE DRIFT FOR VERT. EMPLACEMENT

NOTE: THE GROUND SUPPORT SHOWN IS PROPOSED FOR GOOD GROUND CONDITIONS (Q = 10 TO 40)

SHEET NO. 4/5

Figure 1. Geometry of Emplacement Drift - BWR - Spent Fuel

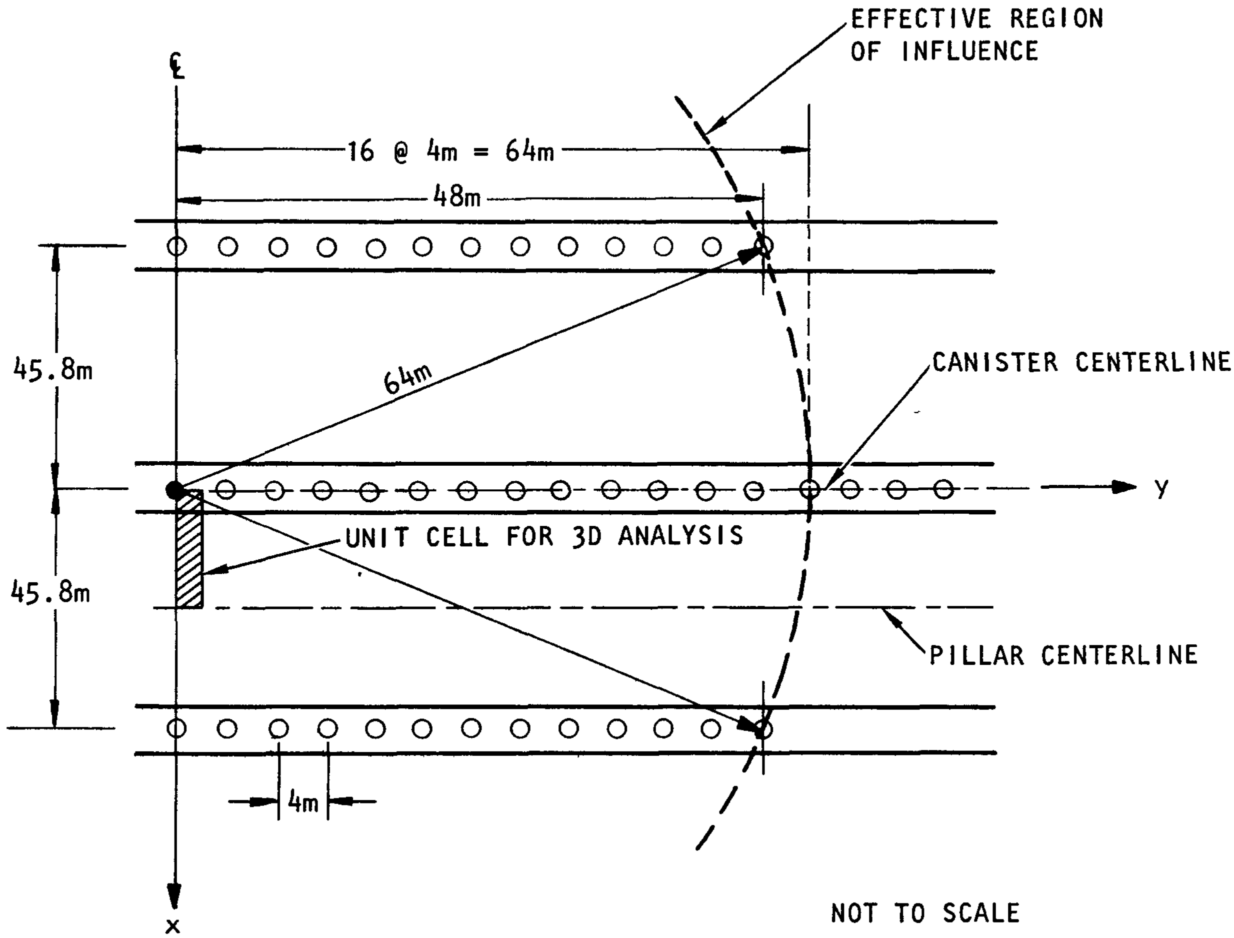
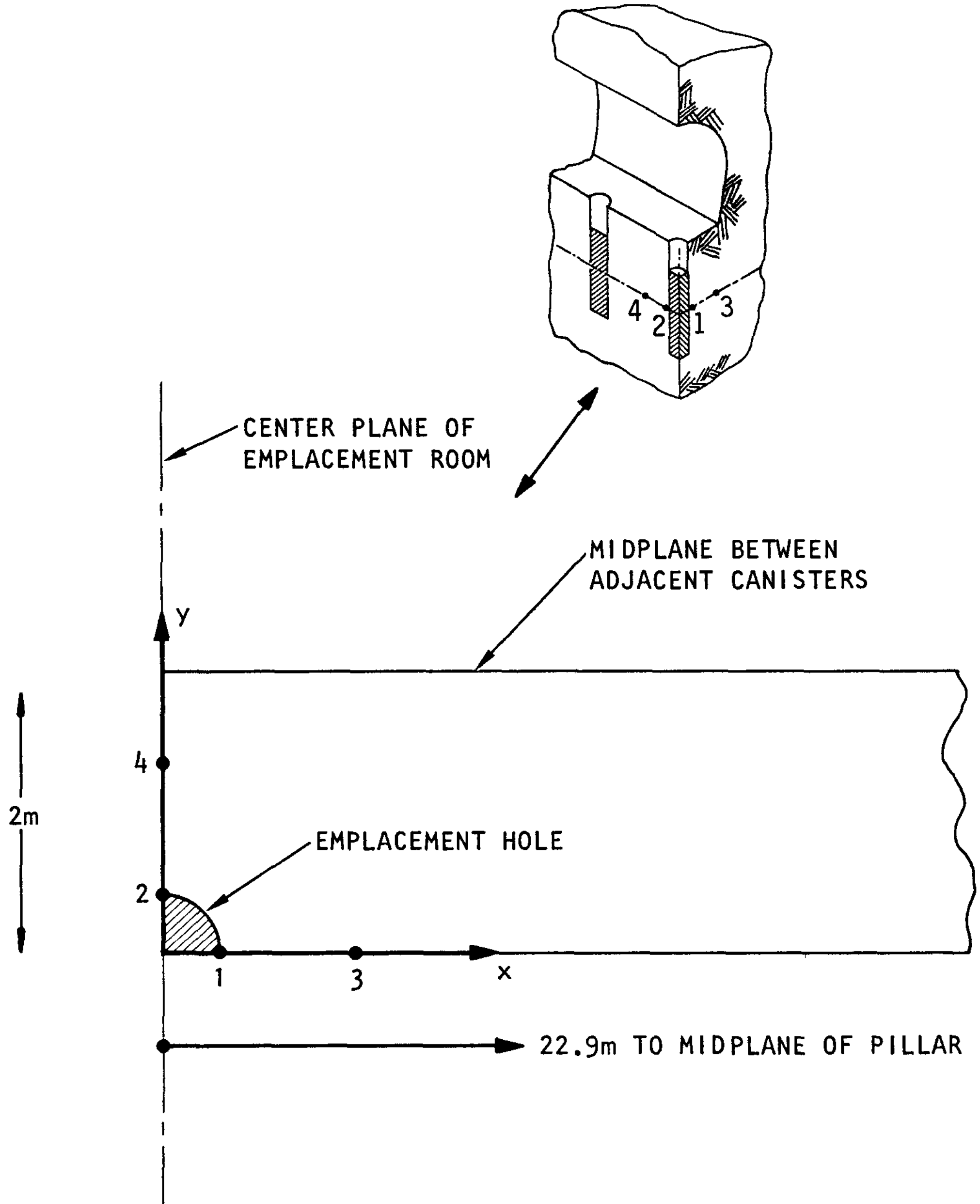


Figure 2. Schematic of Layout of Heat Sources for Analyses Using the TEMP3D Code



POINT	COORDINATES	
1	x = 0.355m	y = 0.m
2	x = 0.m	y = 0.355m
3	x = 1.355m	y = 0.m
4	x = 0.m	y = 1.355m

Figure 3. Location of Sample Points at Midplane of Canister Used For Both Closed-Form and Finite-Difference Models

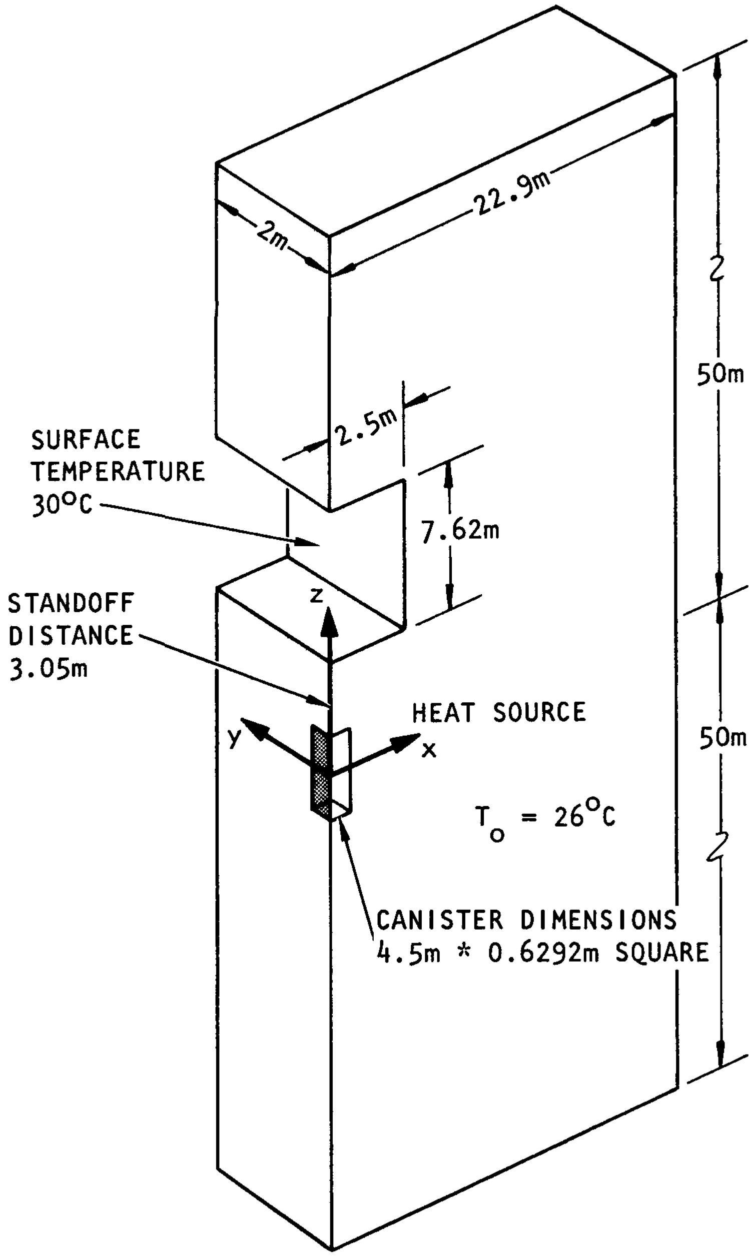


Figure 4. Schematic of the Three-Dimensional Geometry Modeled Using the THERM3D Code. The Interior Boundary Condition is for the Case of a Ventilated Drift

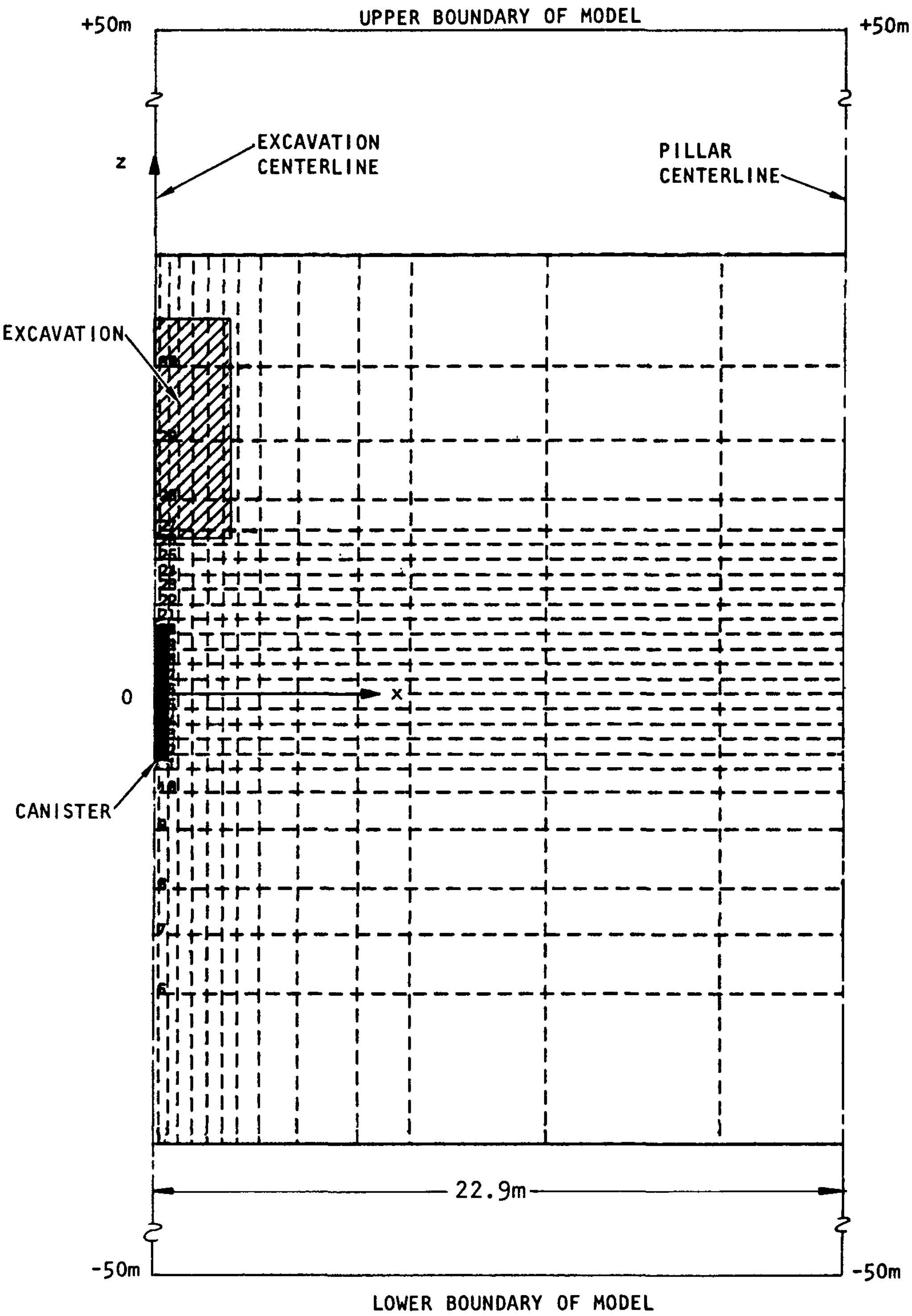


Figure 5. A Portion of the Finite-Difference Grid for PORFLOW Calculations Showing Canister and Drift Location in the Grid

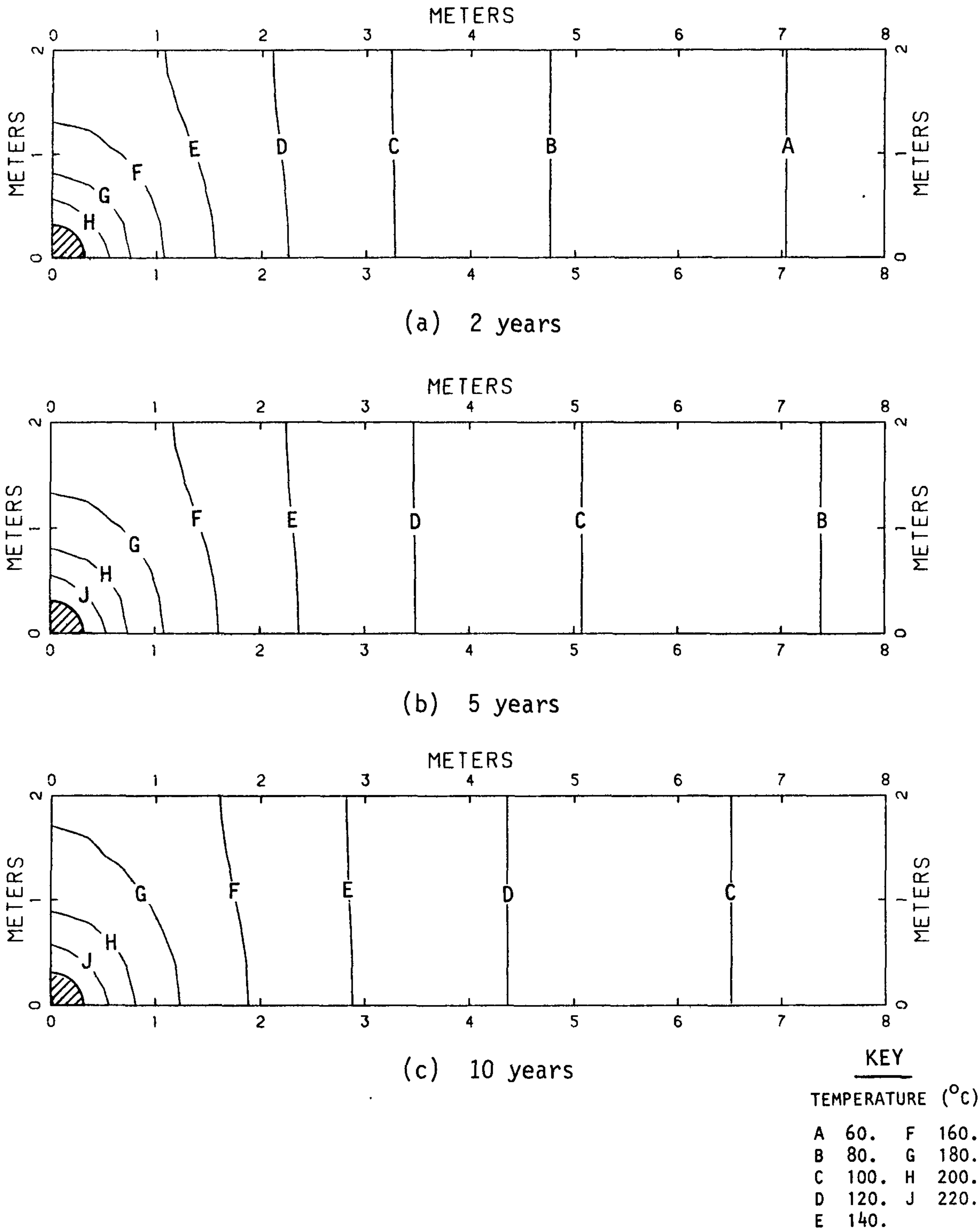


Figure 6. Temperature Contours at Canister Midplane 2, 5, and 10 Years After Emplacement. Closed-Form Solution for an Infinite Region

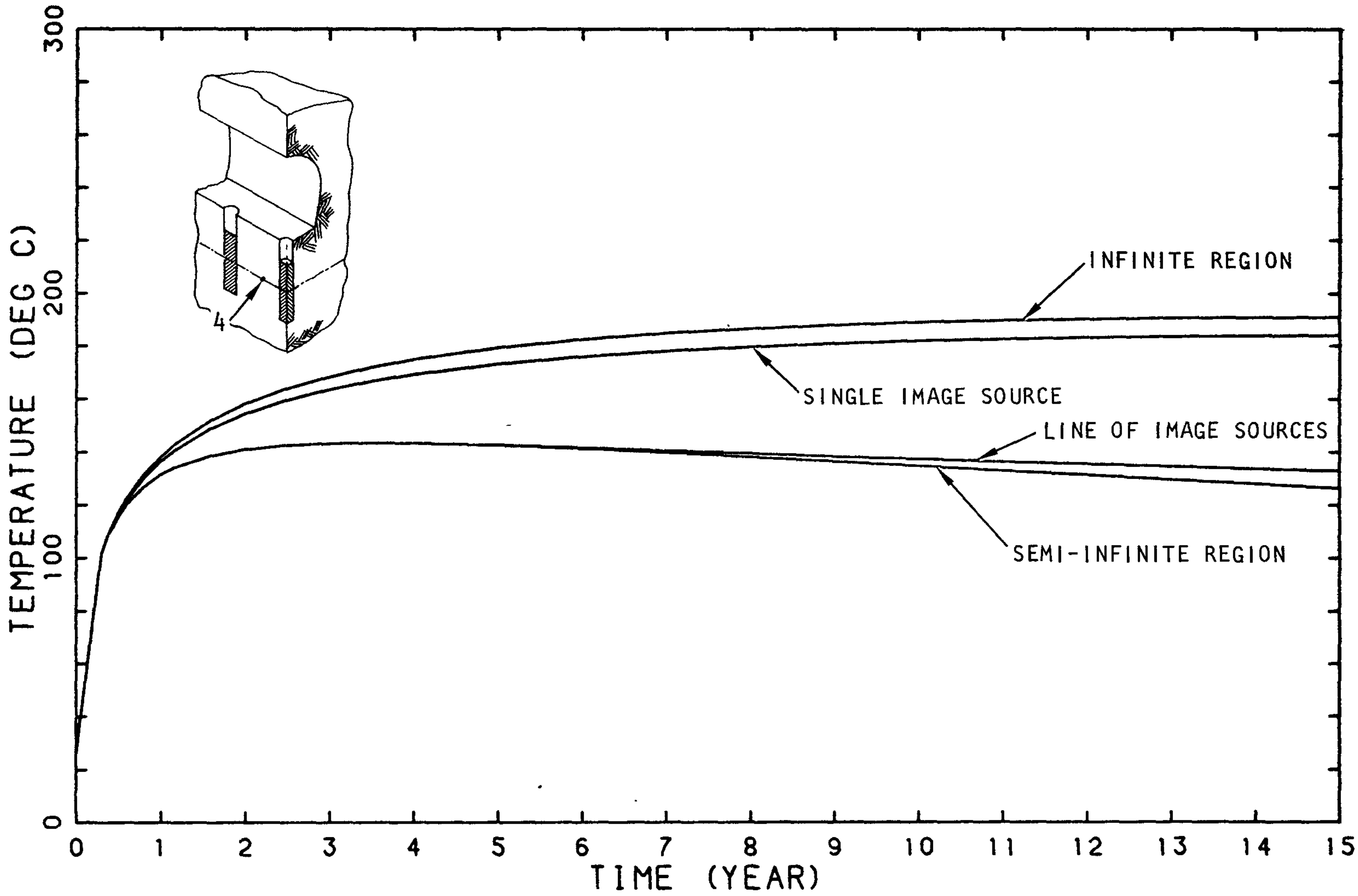


Figure 7. A Temperature History for Point 4 (x = 0.0, y = 1.355) in an Infinite Region. Computed for Four Boundary Conditions at the Excavation Floor

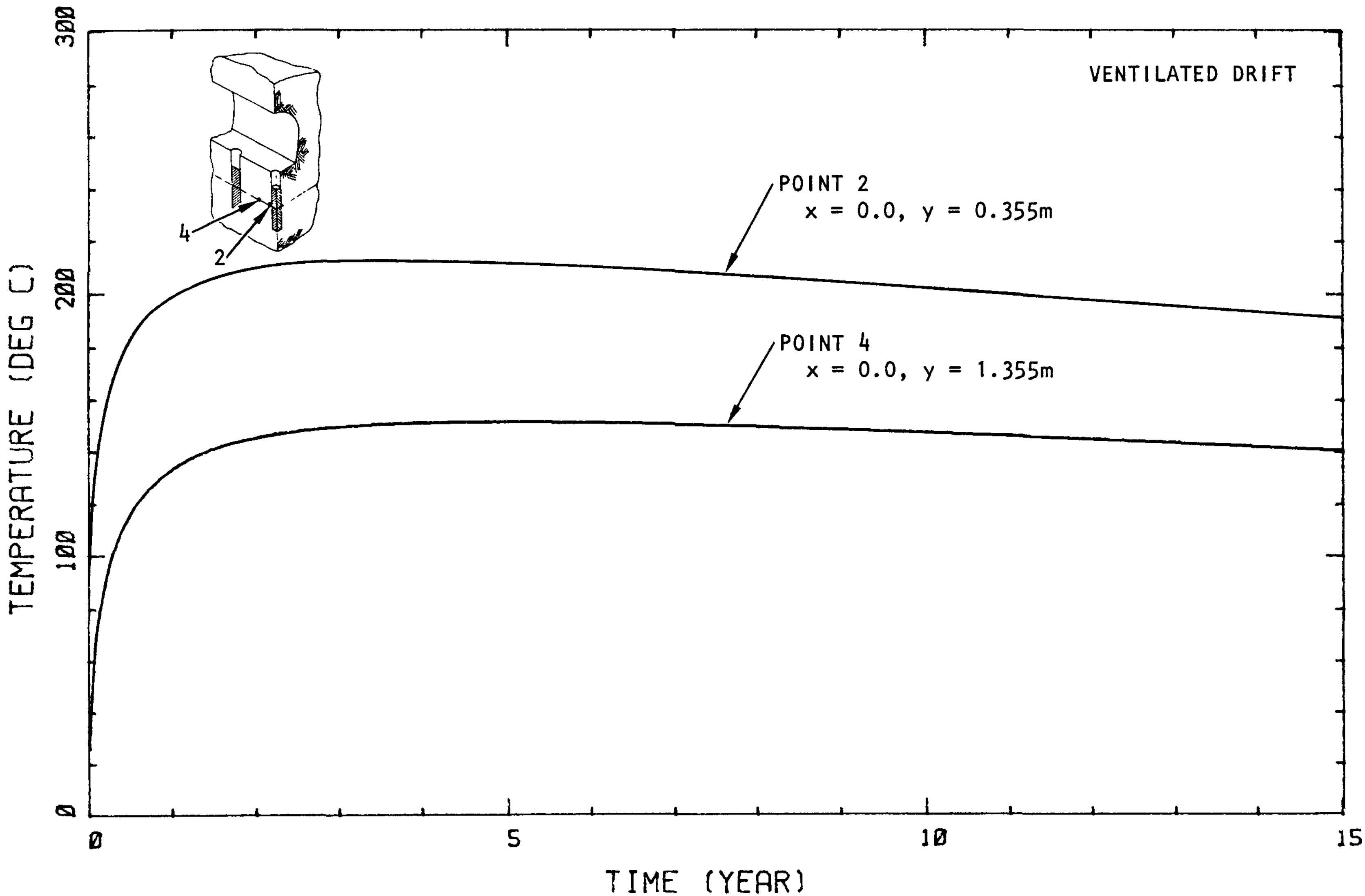


Figure 8. Temperature Histories for Sample Points 2 and 4 - Three-Dimensional THERM3D Solution, with Ventilated Drift

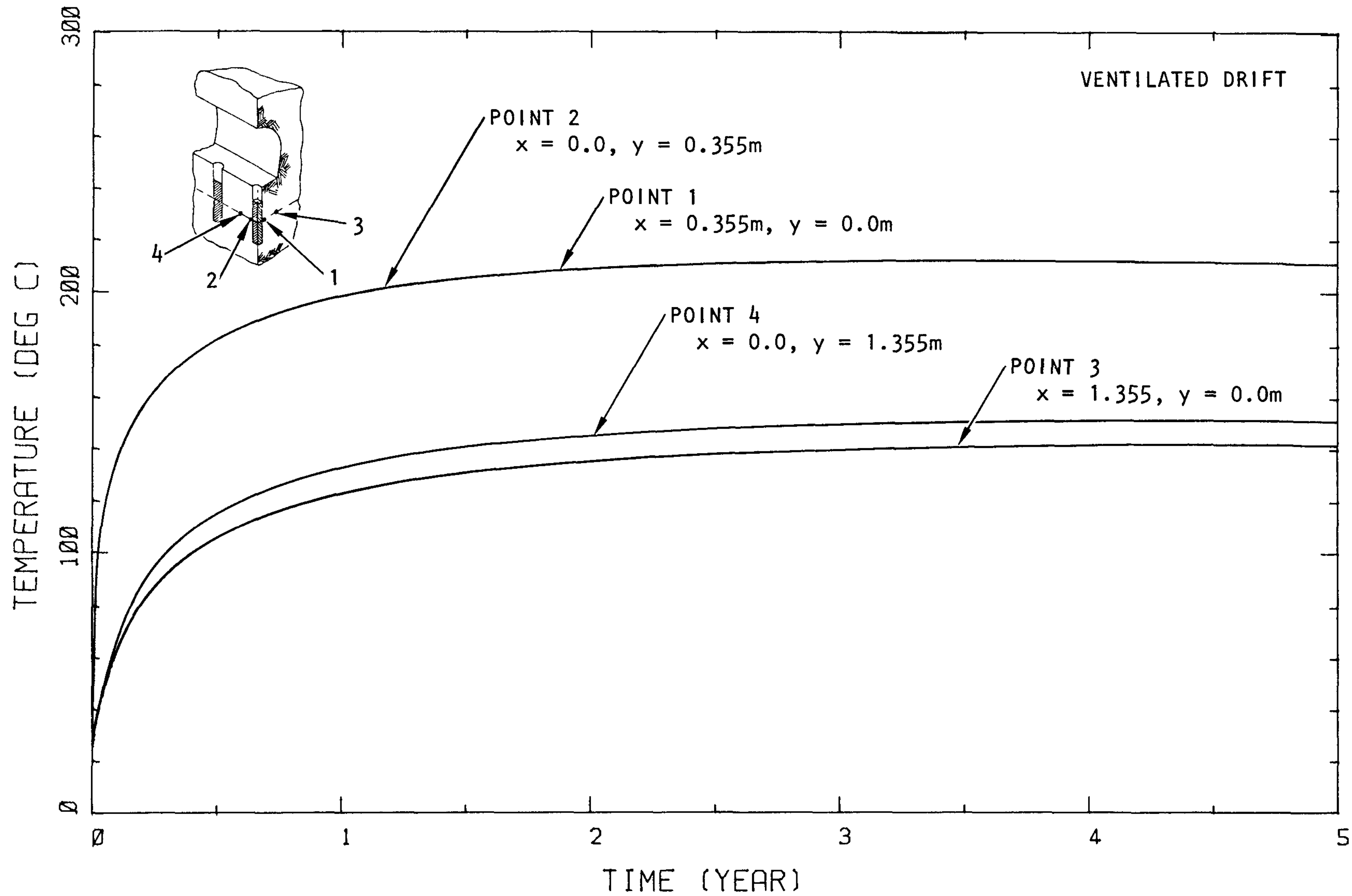
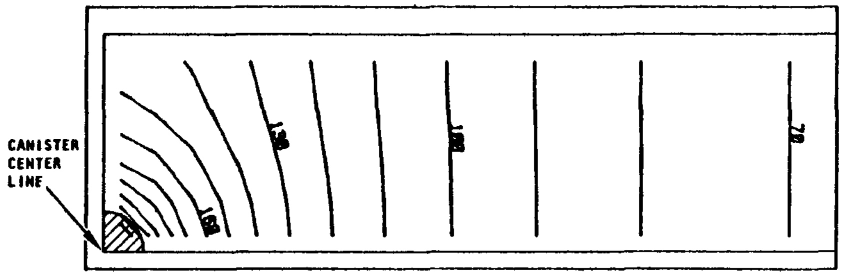
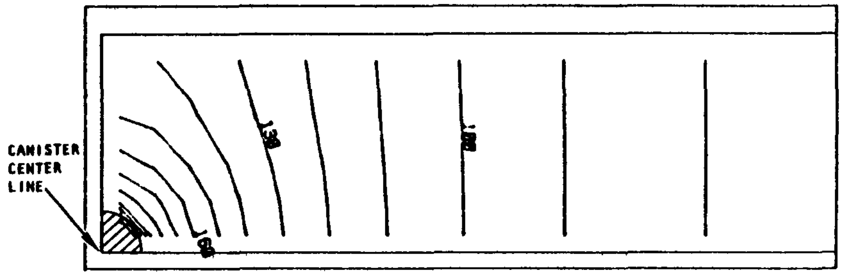


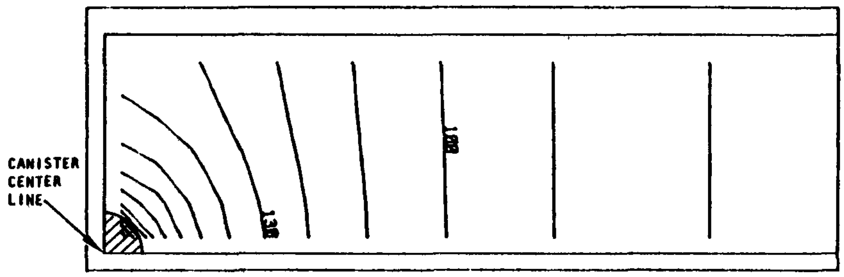
Figure 9. Temperature Histories for Sample Points 1 through 4 - Three-Dimensional THERM3D Solution, with Ventilated Drift



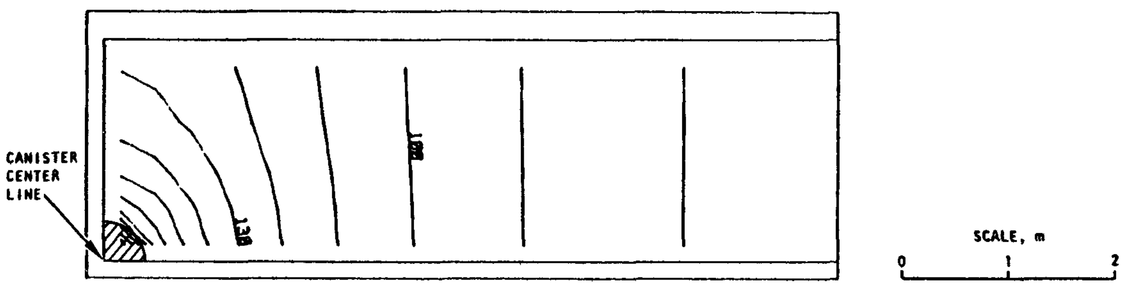
(a) 5 years



(b) 10 years

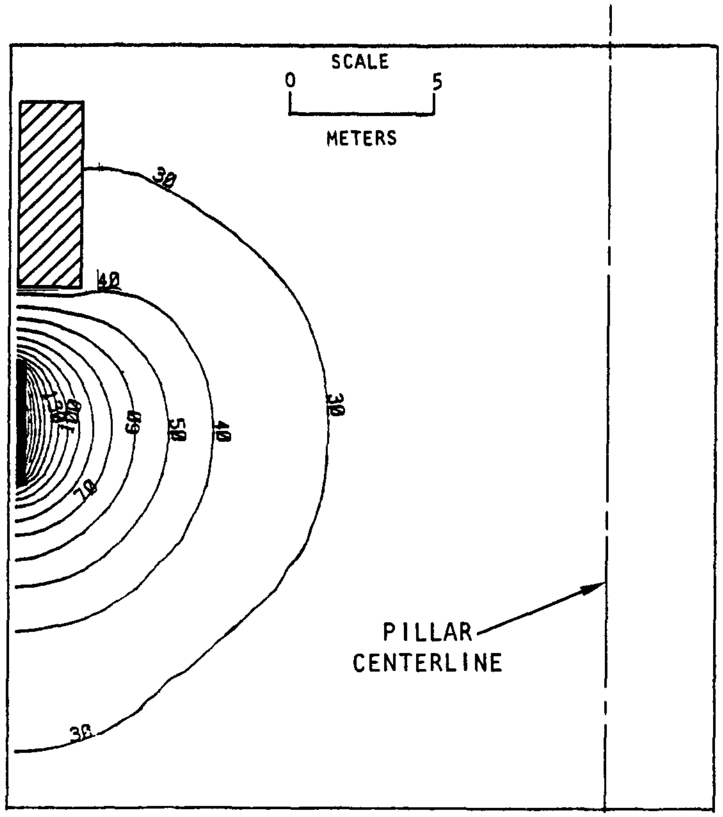


(c) 15 years

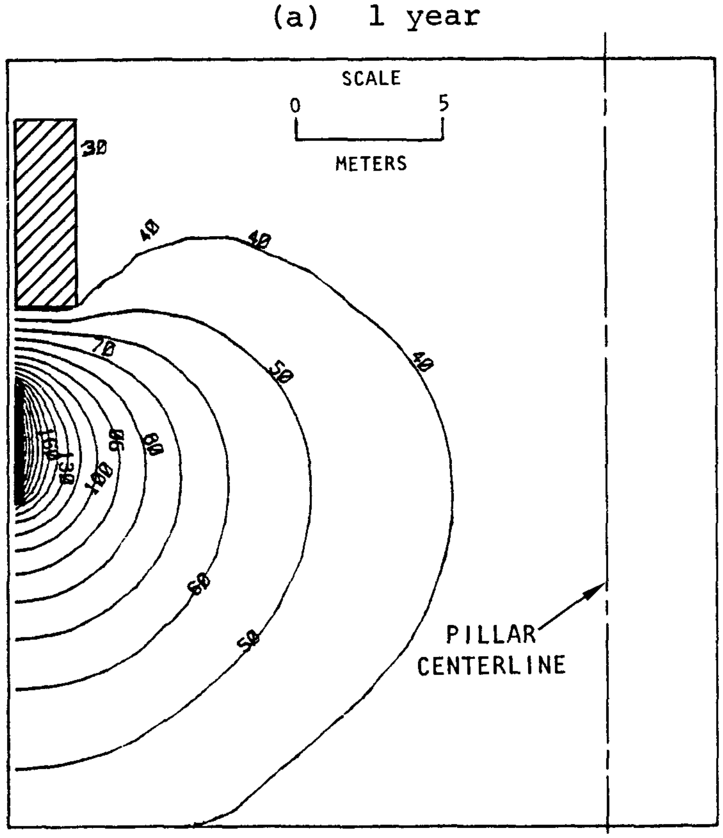


(d) 20 years

Figure 10. Temperature Distribution in a Horizontal Plane at the Midheight of the Canisters - Three-Dimensional THERM3D Solution, with Ventilated Drift

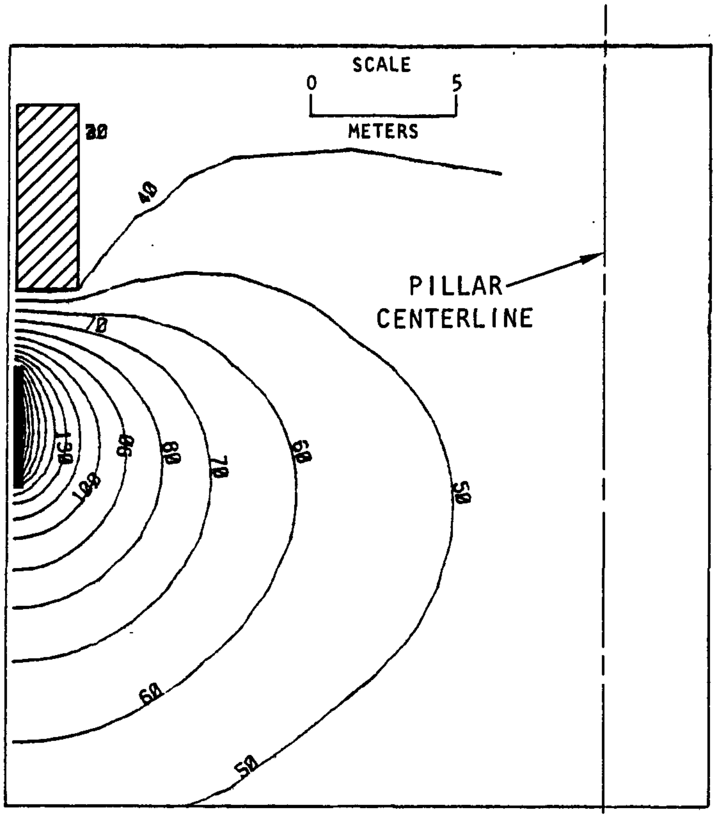


(a) 1 year

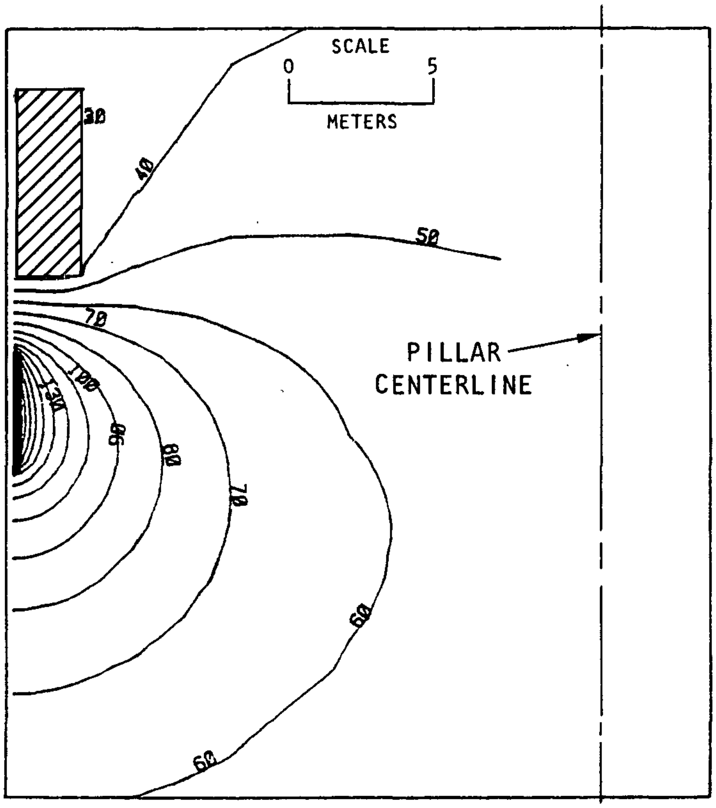


(b) 5 years

Figure 11. Temperature Distribution in a Vertical Plane Between Waste Canisters - Three-Dimensional THERM3D Solution, with Ventilated Drift



(c) 10 years



(d) 20 years

Figure 11. (Concluded)

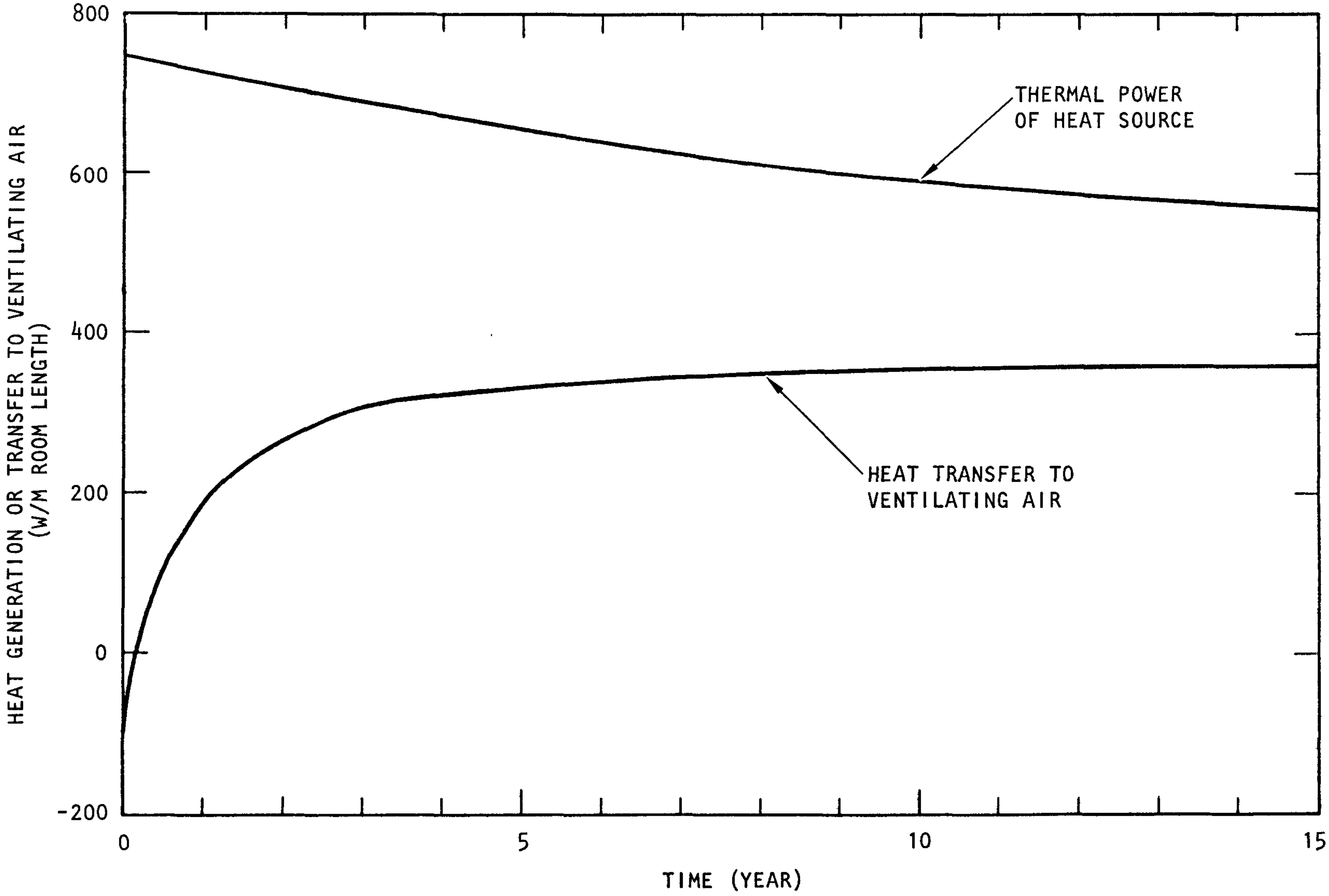
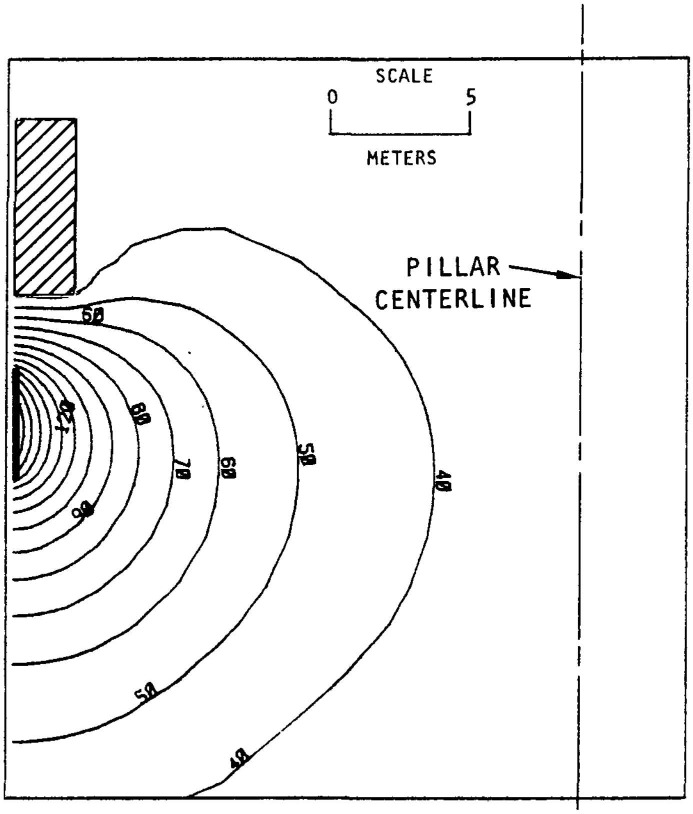
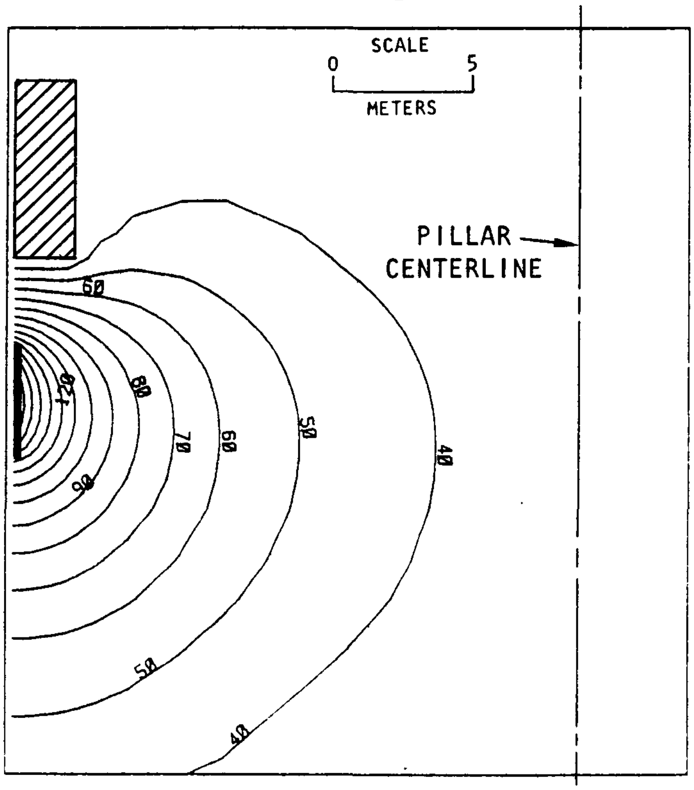


Figure 12. Heat Transfer to the Ventilating Air - Two-Dimensional PORFLOW Solution with Drift Maintained at 30 C

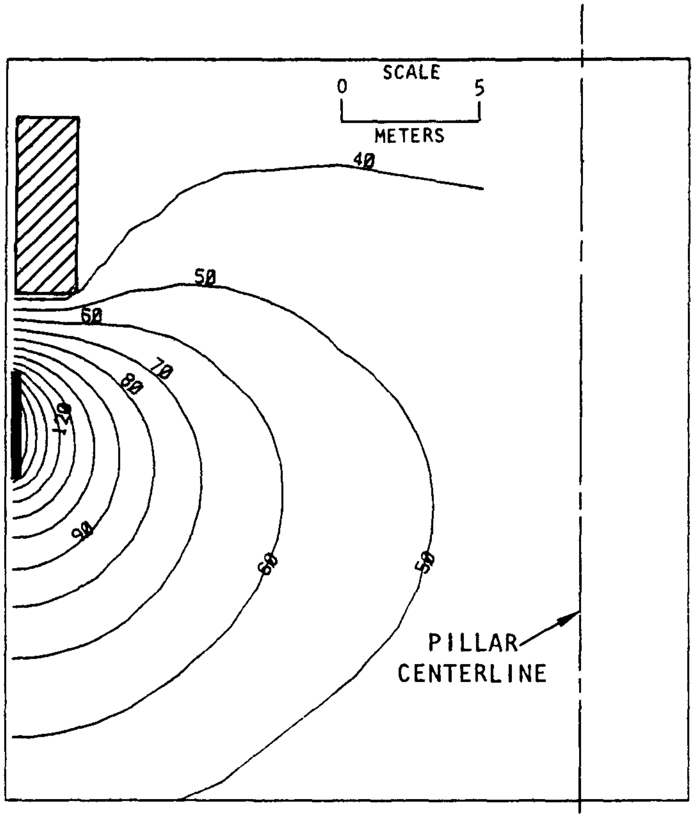


(a) 1 year

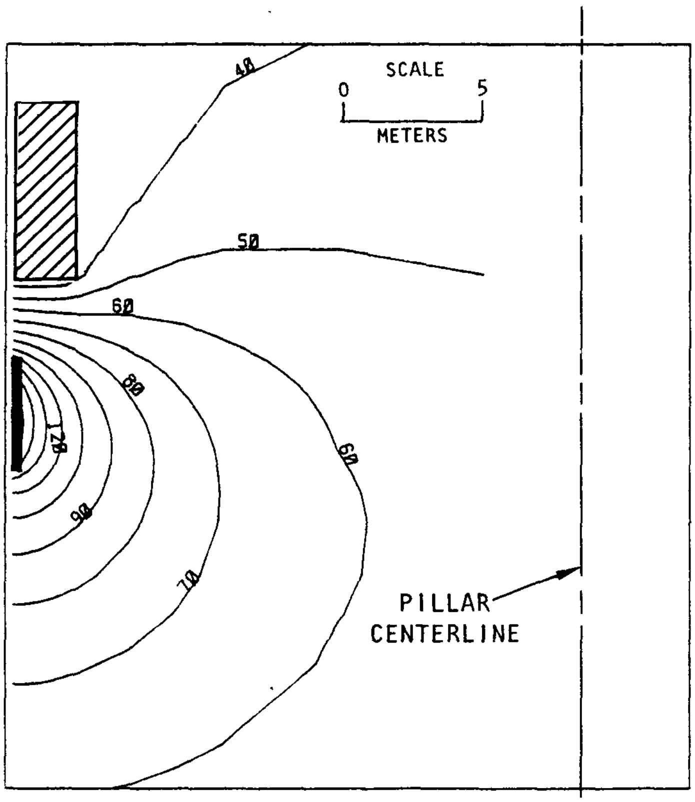


(b) 5 years

Figure 13. Temperature Distribution in a Vertical Plane - Two-Dimensional PORFLOW Solution, with Ventilated Drift



(c) 10 years



(d) 20 years

Figure 13. (Concluded)

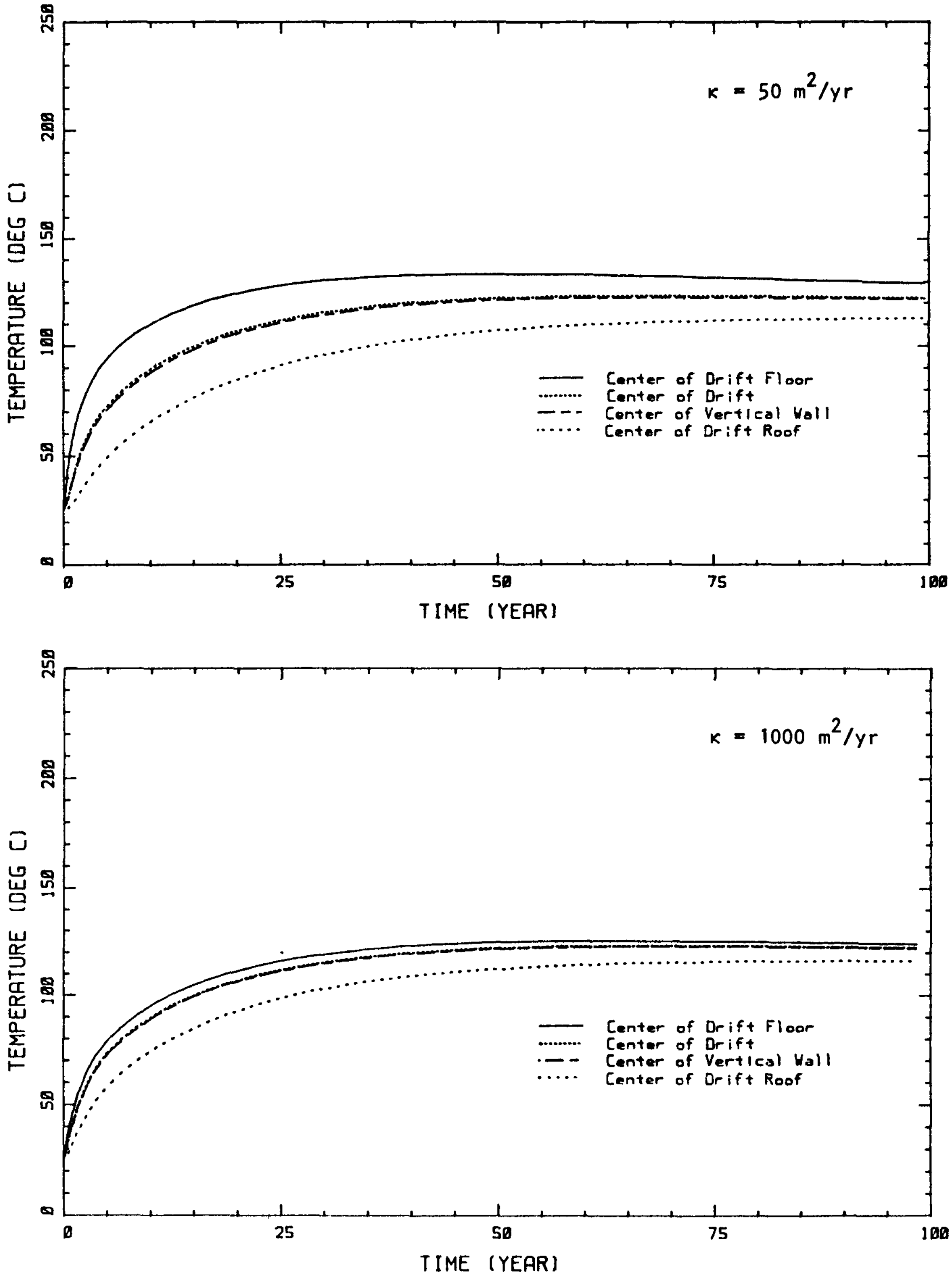


Figure 14. Temperature Histories for Alternative Equivalent Radiation Properties of Air in an Unventilated Drift - Two-Dimensional PORFLOW Calculations

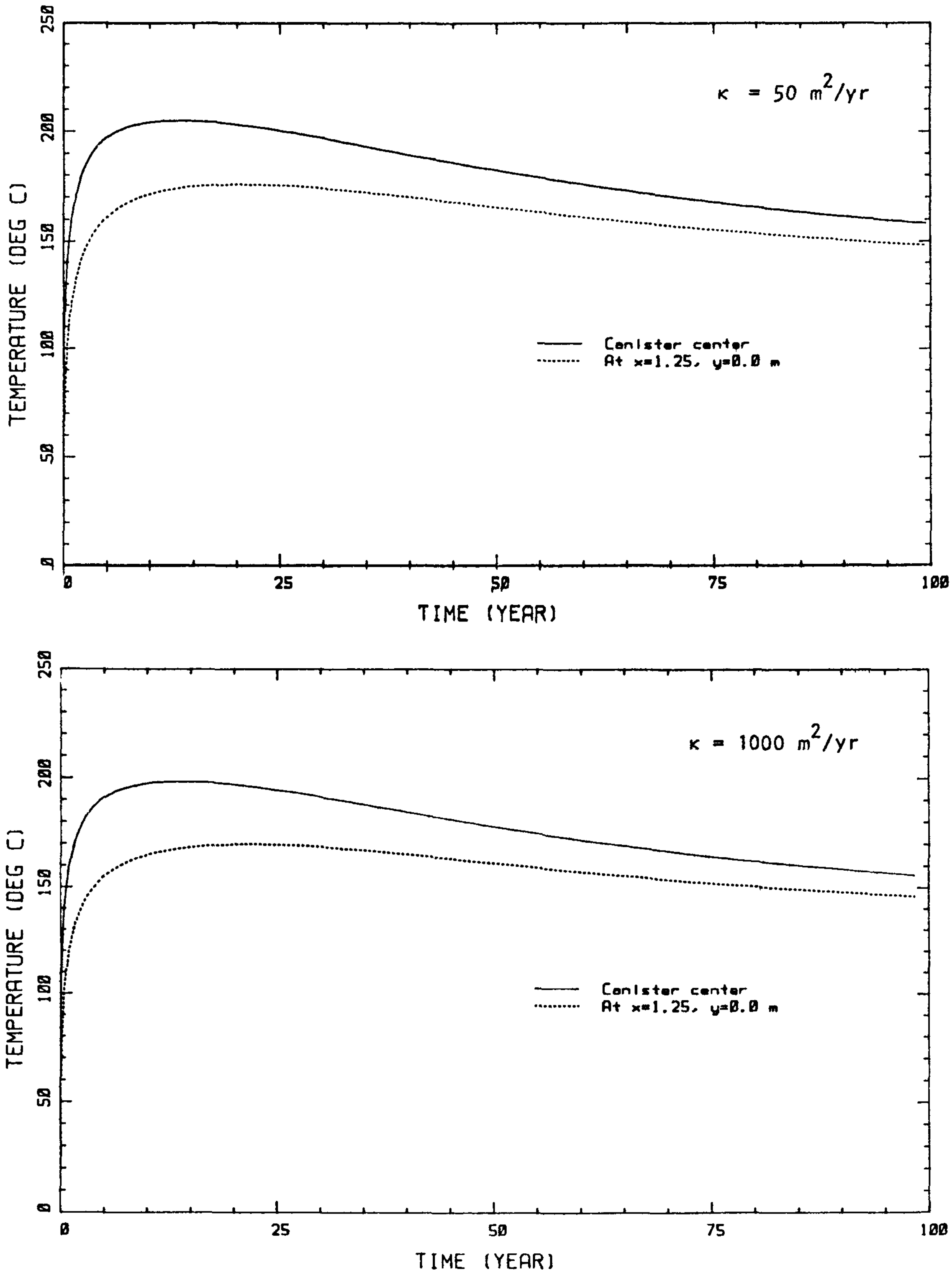


Figure 15. Near Field Temperature Histories for Alternative Equivalent Radiation Properties of Air in an Unventilated Drift - Two-Dimensional PORFLOW Calculations

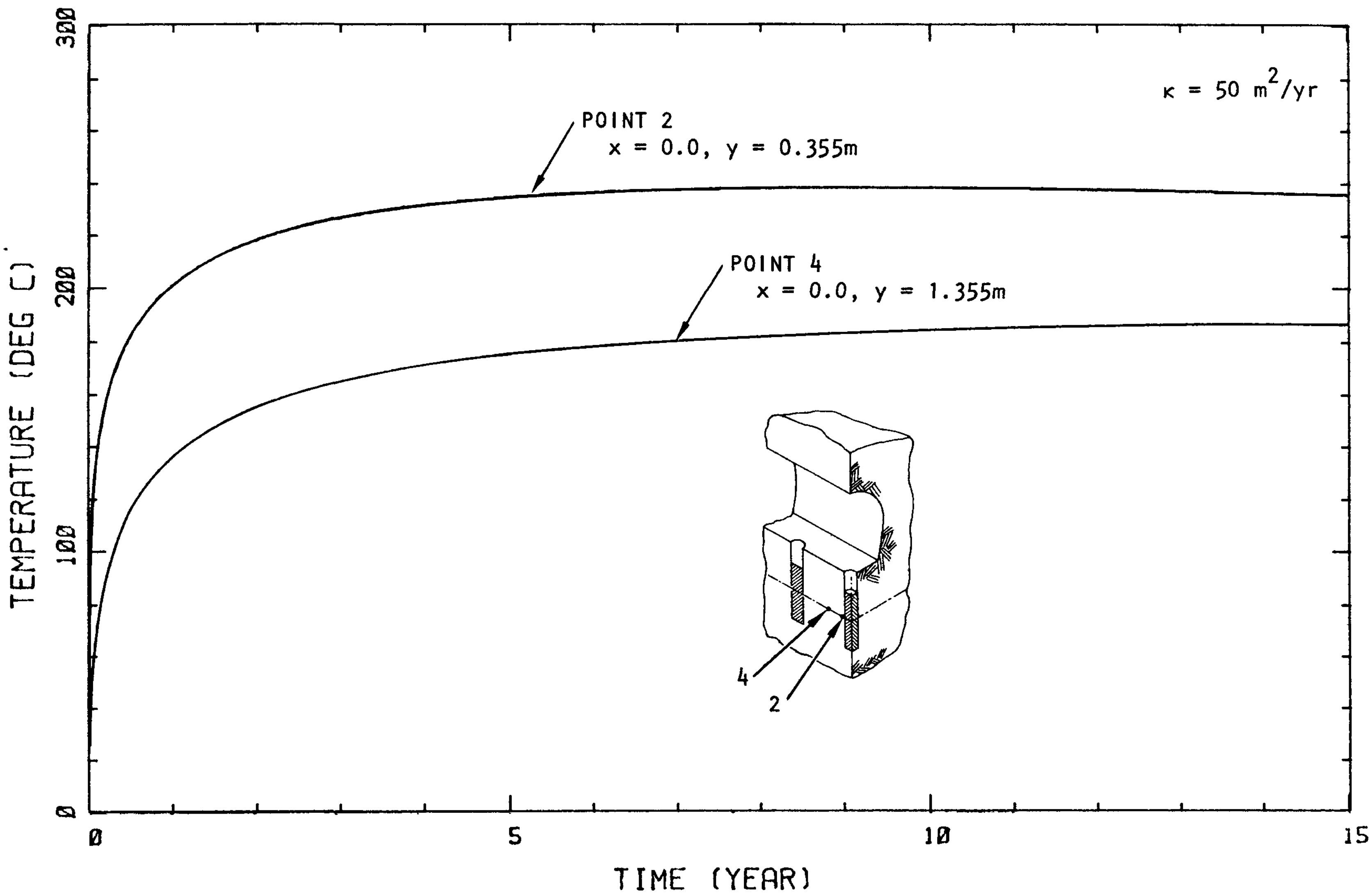
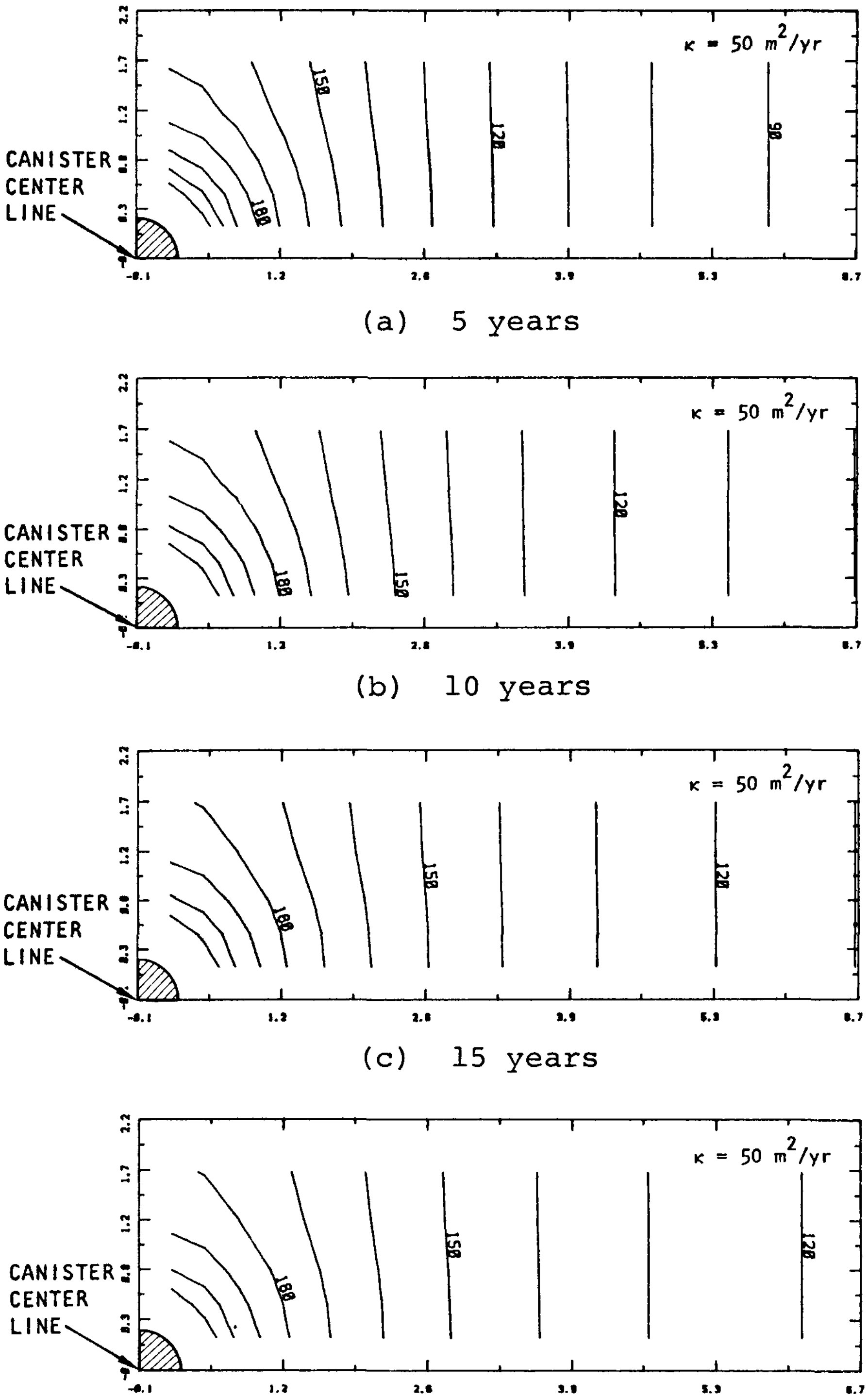


Figure 16. Temperature Histories for Sample Points 2 and 4 - Three-Dimensional THERM3D Solution, with Unventilated Drift



(a) 5 years

(b) 10 years

(c) 15 years

(d) 20 years

Figure 17. Temperature Distributions in a Horizontal Plane at the Midheight of the Canisters - Three-Dimensional THERM3D Solution, with Unventilated Drift

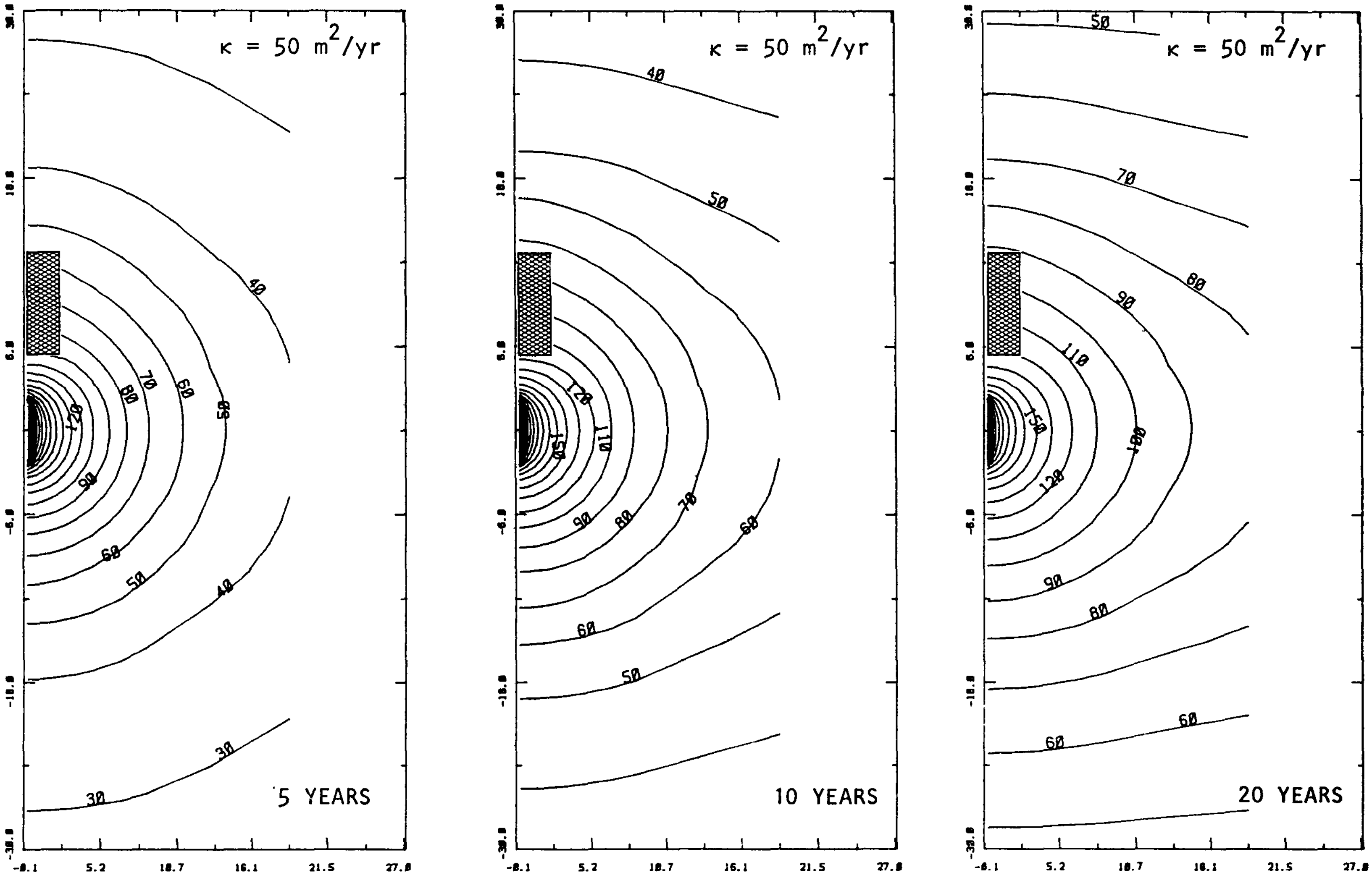


Figure 18. Temperature Distribution in a Vertical Plane Between Waste Canisters - Three-Dimensional THERM3D Solution with Unventilated Drift

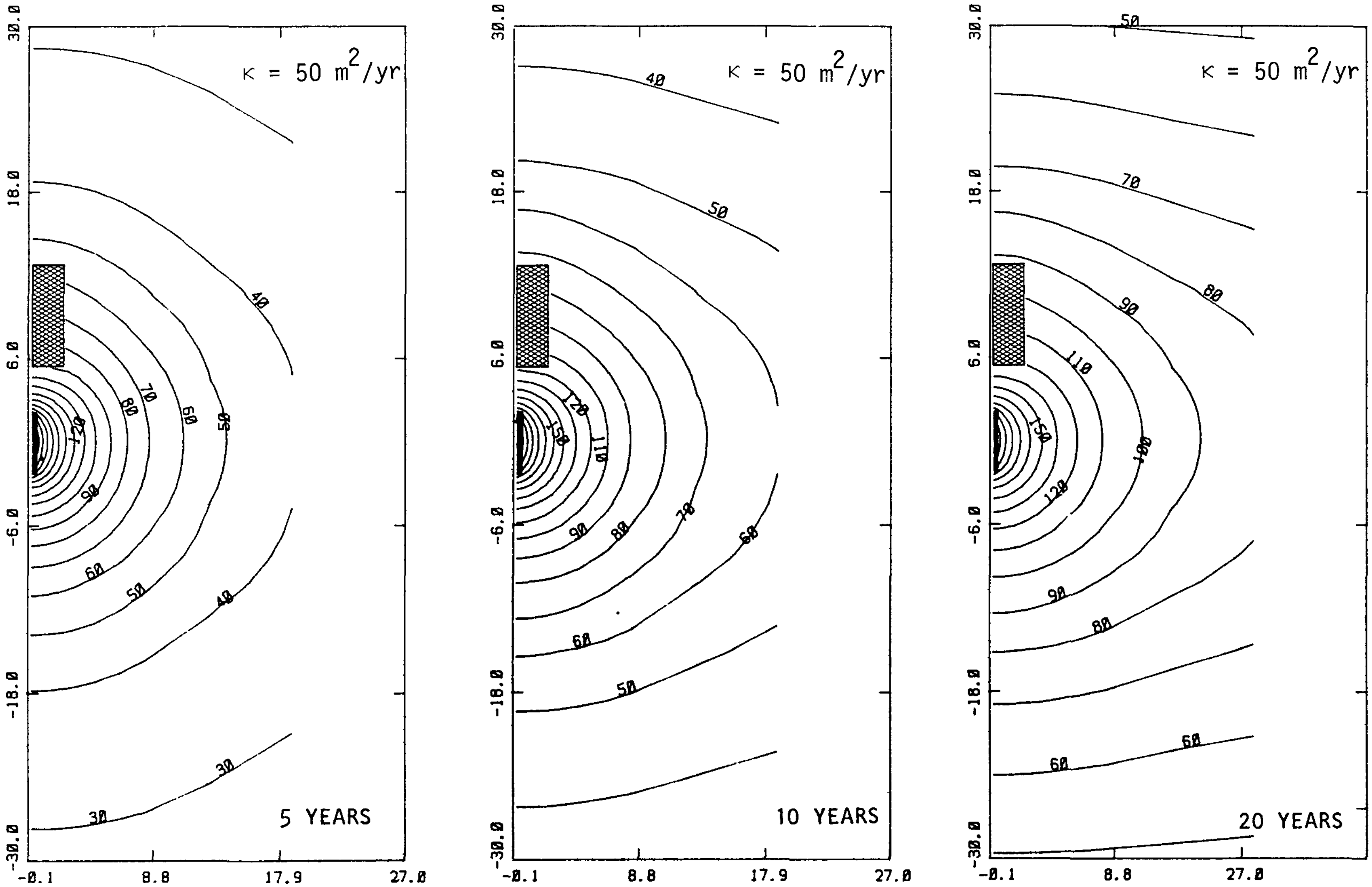


Figure 19. Temperature Distribution in a Vertical Plane - Two-Dimensional PORFLOW Solution with Low Diffusivity Approximation of Radiation (κ = 50 m^2/yr)

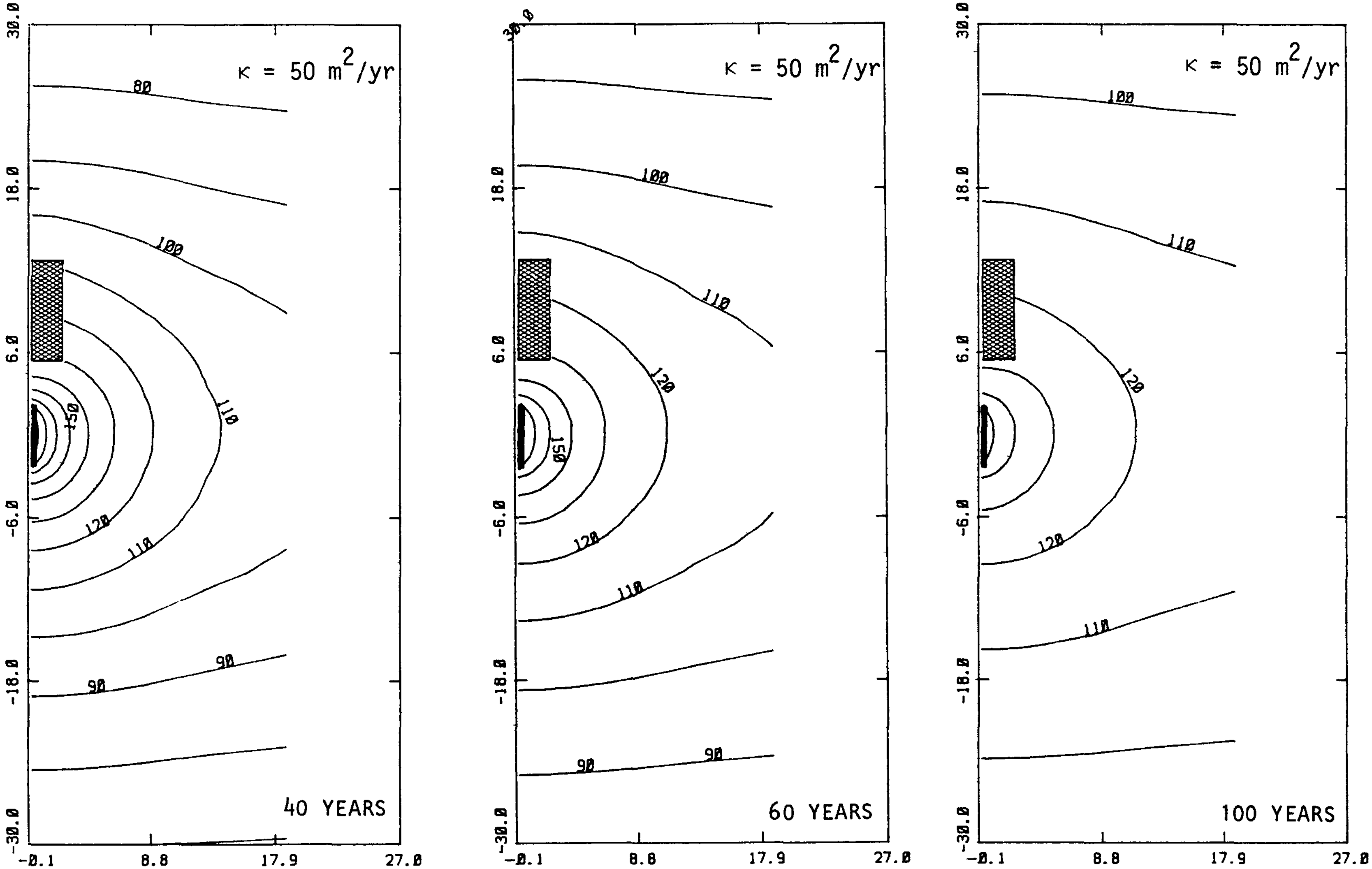


Figure 19. (Concluded)

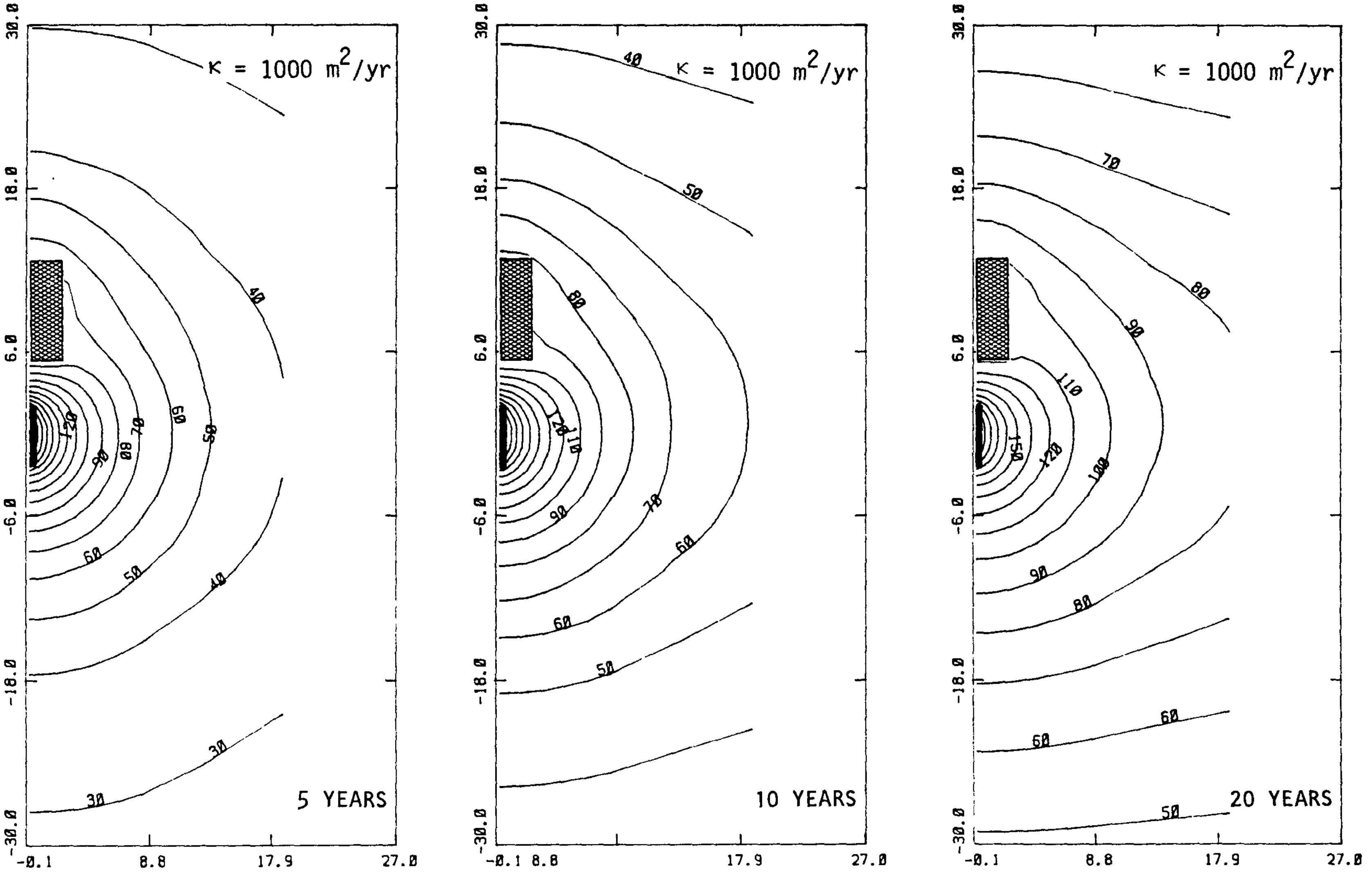


Figure 20. Temperature Distribution in a Vertical Plane - Two-Dimensional PORFLOW Solution with High Diffusivity Approximation of Radiation (κ = 1000 m^2/yr)

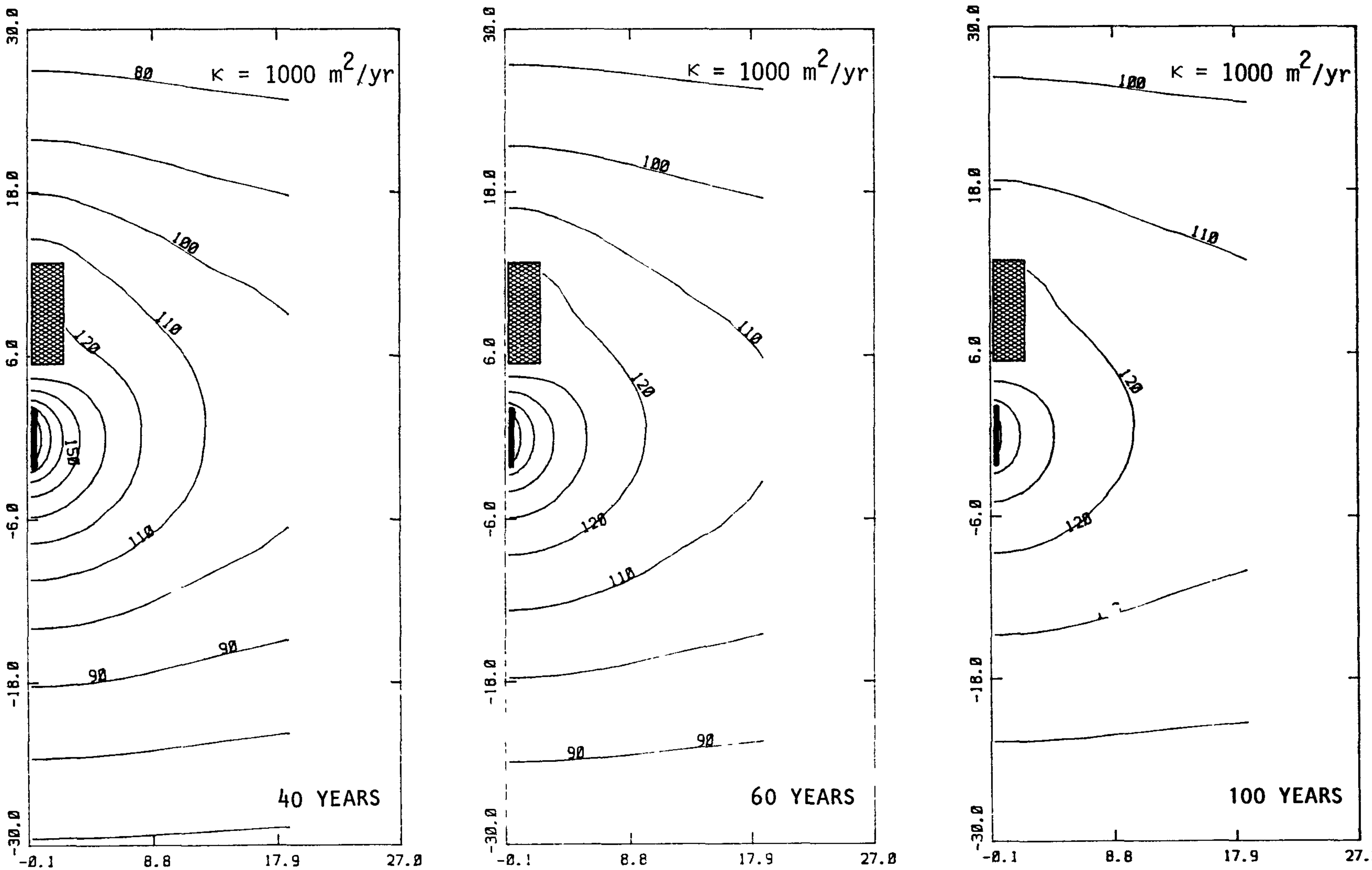


Figure 20. (Concluded)

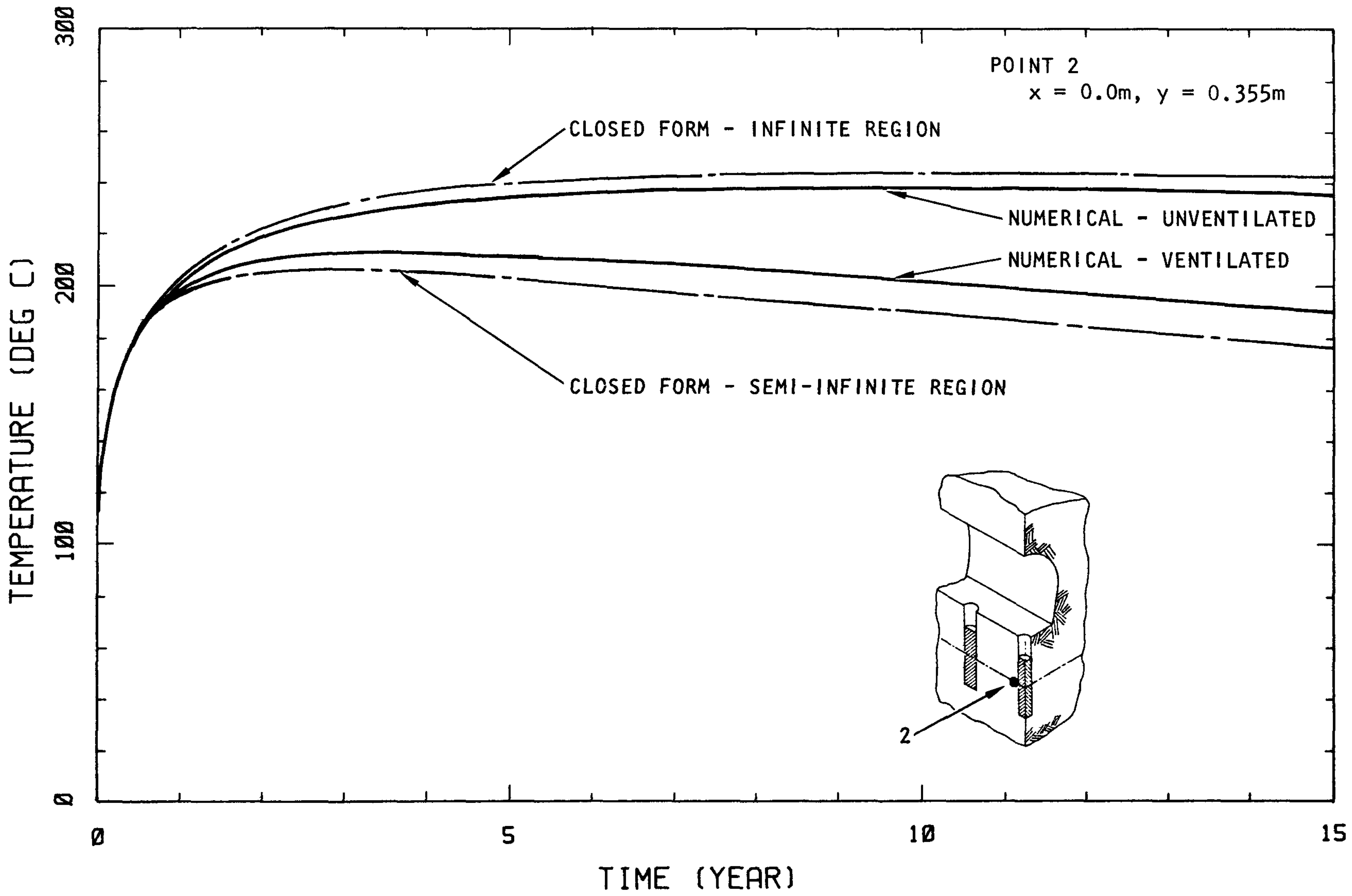


Figure 21. A Comparison of the Temperature History of Points at the Canister Wall (Point 2) and 1 m from the Canister Wall (Point 4). Results Obtained Using Several Different Three-Dimensional Models.

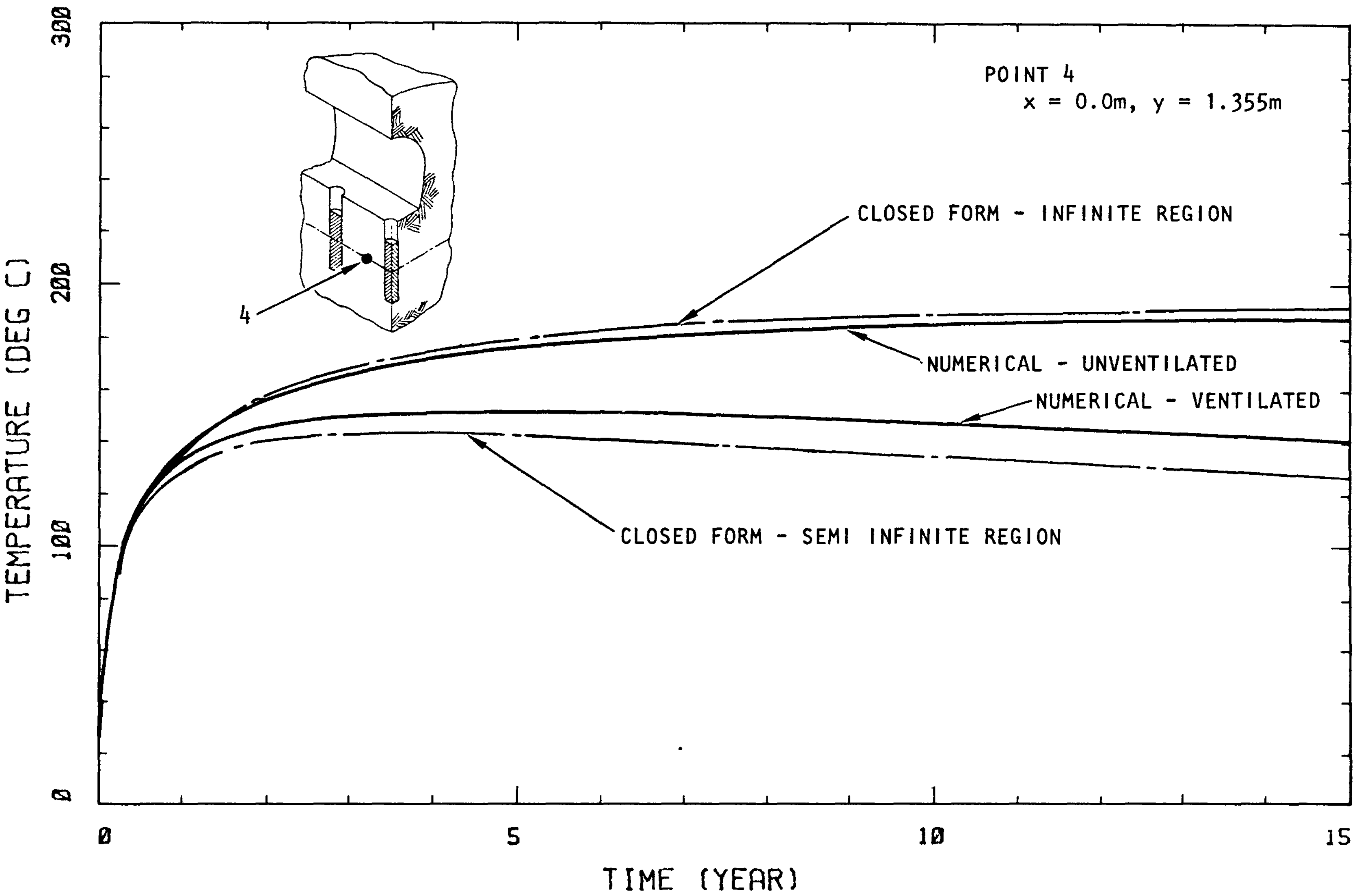


FIGURE 21. (Concluded)

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