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SENSITIVITY CALCULATIONS FOR LOW-HEAT GENERATING
DEFENSE WASTE REPOSITORY TEMPERATURES

by

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DEFENSE WASTE REPOSITORY TEMPERATURES*

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ABSTRACT

Repository temperatures were calculated for Savannah River wastes by using both two- and three- dimensional numerical schemes. The error introduced by using the simpler and more efficient two- dimensional models is less than the present uncertainties introduced by waste power generation and host rock properties. Waste canister temperatures were found to be relatively insensitive to geometric asymmetry and model detail.

* The information contained in this article was developed during the course of work under Contract No. DE-AC09-76SR00001 with the U.S. Department of Energy.

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ABSTRACT

One alternative for the ultimate disposal of radioactive waste is to immobilize the waste through vitrification, or an equivalent process, and to bury it in an underground repository. Leachability of the waste form is strongly influenced by the surface temperature of the waste. Leachability is one of the most important factors in a multibarrier approach to ensure immobility of the radionuclides.

Calculation of the waste form surface temperature is a transient, three-dimensional conduction heat transfer problem with time-dependent heat sources, temperature-dependent properties, and mixed boundary conditions. Although closed-form solutions are not available, the problem yields to numerical solution. Only the moderate complexity of the geometry, as well as large core and central processing unit (CPU)

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requirements, complicates the calculation. In particular, the cost of a calculation requiring up to 3 hours of CPU on an IBM 360-195 can be burdensome.

Current practice is to use detailed cylindrical three-dimensional unit cell computer models. This approach has the advantage of providing information useful to repository designers interested in mine stability, water migration, and design refinements.

For those primarily interested in the integrity of the waste form, it was desirable to determine if simpler computer models could be used to calculate waste form temperatures and to evaluate the uncertainty of the results. Since there appears to be no rigorous way to generalize, a specific case typical of defense waste repositories was examined. Five-year-old Savannah River waste buried on 6.1-m (20-ft) centers in a salt repository was used as the base case. Power generation, host rock thermal conductivity, and geometrical asymmetry of waste canister spacings were varied. Both two- and three-dimensional computer models were used. The rectangular three-dimensional models considered details such as the existence of a disposal room, the disposal room's contents, and a shielding plug.

By using a two-dimensional model only, power generation and thermal conductivity were varied. For low-heat generating Savannah River wastes (nominally 1 kW/waste canister at burial), there may exist an uncertainty in power of +0 to -40% due to the

uncertainties in future reactor operation and separation schemes. These uncertainties in power cause peak waste form temperatures (nominally 426°K) to vary from +0 to -12%. For uncertainties in host rock thermal conductivity of $\pm 50\%$, peak waste form temperature varied from -5 to +13%. (While salt alone has an uncertainty of 15% in thermal conductivity, bedded salt has been shown to exhibit a fourfold variation in thermal conductivity at a single site.)

Two- and three-dimensional models were compared. The two-dimensional model used half the CPU time and 15% less core than the three-dimensional model. For a symmetry ratio (disposal room spacing/waste canister spacing) equal to one, the two-dimensional model gave peak waste temperatures that were 7% higher than those of the three-dimensional model. The two-dimensional model gives higher temperatures because the area associated with a waste canister in the two-dimensional model is smaller than that in the three-dimensional model by a factor of $\pi/4$. If the two-dimensional calculation is made such that the areal power loading is equal to that of the three-dimensional model, the discrepancy is less than 1%.

For the three-dimensional model, symmetry ratios less than 7 gave peak waste temperatures that were within 0.5% of those for a ratio of one. For a symmetry ratio of 25, the results were about 2% higher than those for a ratio of one, although the peak was observed to occur nearly 14 years earlier. Additions of shielding

plugs and disposal room with stagnant air or dry crushed host rock changed peak waste temperatures less than 3% for a symmetry ratio of one.

From these results, it may be concluded that:

- 1) The uncertainty in waste form temperature calculations is presently dominated by uncertainties in waste power and host rock properties. Model detail is of secondary importance.
- 2) A two-dimensional computer model gives conservatively high waste form temperature results.
- 3) A two-dimensional computer model gives peak waste form temperatures within 1% of the three-dimensional computer model by using the same areal loading.
- 4) Waste form temperatures calculated for a symmetry ratio of one can be extrapolated to symmetry ratios of 25 with less than 3% error for low-heat generating wastes.

INTRODUCTION

One alternative for the ultimate disposal of radioactive waste is to immobilize the waste through vitrification, or an equivalent process, and to bury it in an underground repository. Leachability of the waste form is strongly influenced by the surface temperature of the waste. Leachability is one of the most important factors in a multibarrier approach to ensure immobility of the radionuclides.

The waste form surface temperature can be calculated by a straightforward process. Mathematically, it is a transient, three-dimensional conduction heat transfer problem with time-dependent heat sources, temperature-dependent properties, and mixed boundary conditions. Although closed-form solutions are not available, the problem yields to numerical solution. Only the moderate complexity of the geometry, as well as large core and central processing unit (CPU) requirements, complicates the calculation. In particular, the cost of a calculation requiring up to 3 hours of CPU on an IBM 360-195 can be burdensome.

Current practice is to use detailed three-dimensional unit cell computer models. This approach has the advantage of providing information useful to repository designers interested in mine stability, water migration, and design refinements.

For those primarily interested in the integrity of the waste form, it is desirable to determine if simpler computer models can be used to calculate waste form temperatures and

to evaluate the uncertainty of the results. Since there appears to be no rigorous way to generalize, a specific case, typical of defense waste repositories, was examined. Five-year-old Savannah River waste buried on 6.1-m (20-ft) centers in a salt repository was used as the base case. Power generation, host rock properties, and geometric asymmetry of waste canister spacings were varied. Both two- and three-dimensional models were used. The three-dimensional models considered details such as the existence of a disposal room, the disposal room's contents, and a shielding plug.

MATHEMATICAL MODELS

Both two- and three-dimensional models were used for this study. Figures 1 and 2 show schematics of the two models. Material properties and stratigraphy are given in Table 1. Solutions were obtained with HEATING5¹ by using an implicit, transient, finite difference scheme.

The cylindrical, two-dimensional model² extends from the earth's surface to a depth of 1220 m axially and from the center-line of the waste canister to a distance equal to half the canister spacing radially. The radial boundary is adiabatic. An initial geothermal temperature gradient equal to 36°C for every 1000-m depth is imposed. The temperature at the lower boundary is fixed, and the upper boundary is allowed convection to a 16°C environment. The waste canister is represented as a uniform heat source 61 cm in diameter and 2.27 m high and is buried 610 m below the

earth's surface. The power generated for each waste canister is given in Figure 3.

The rectangular three-dimensional model is very similar to the two-dimensional model. Depth, boundary conditions, stratigraphy, and initial temperature gradients are the same. For uniform spacing of waste canisters, the case represented by the two-dimensional model, adiabatic boundaries in the X and Y directions are each placed at a distance equal to half the canister spacing. Since uniform spacing is not realistic, the three-dimensional model allows for variation of the symmetry ratio, \emptyset , defined as the disposal room spacing divided by the waste canister spacing. The disposal room is assumed to be a tunnel 5.5 m high and 5.5 m wide. Between the floor of the disposal room and the top of the waste canister is a shielding plug (61 cm x 61 cm x 3.05 m). The waste canister is represented as a uniform heat source of rectangular geometry (61 cm x 61 cm x 2.27 m).

Neither the two- nor three-dimensional model considered insulating annuli such as overpacks and backfilled annuli in the immediate vicinity of the waste canister. Although an important element in the calculation of waste canister temperatures, the temperature rises across these annuli may be independently calculated by using simple, one-dimensional, quasi-steady state techniques.

RESULTS AND DISCUSSION

Waste canister temperatures calculated for various canister spacings by using the two-dimensional model are shown in Figure 4. For 6.1-m (20-ft) spacings, the model predicts the waste canister temperature will peak at 153°C, 42 years after burial. Wider spacings result in earlier peaks and lower temperatures.

The 6.1-m (20-ft) spacing results of Figure 4 were used as a base. Waste canister power was varied as shown in Figure 5. For the low-heat generating Savannah River waste, there may exist an uncertainty in power of +0 to -40% due to uncertainties in future reactor operation and separation schemes. These uncertainties in power cause peak waste canister temperatures to vary from +0 to -12% (based on absolute temperature).

The uncertainty in thermal conductivity of salt alone is $\pm 15\%$; however, bedded salt has been shown to exhibit a four-fold variation in thermal conductivity at a single site. Other host rocks such as granite, shale, basalt, and tuff exhibit equal or greater uncertainties in their thermal conductivity. Generic values for thermal conductivity, therefore, may be significantly different from those for a specific site. As shown in Figure 6, a moderate variation of $\pm 50\%$ in thermal conductivity results in peak waste canister temperature variation of -5 to +13%.

The uncertainties in the thermal capacitance of the host rock (density x specific heat) appear to be relatively

small when compared to thermal conductivity. As shown in Figure 7, an expected variation of $\pm 10\%$ in thermal capacitance results in peak waste canister temperature variations of about $\pm 2\%$.

For a symmetry ratio equal to one, the two-dimensional model gave peak waste temperatures that were 7% higher than those of the three-dimensional model (see Figure 8). The two-dimensional model gave higher temperatures because the area associated with the waste canister in the two-dimensional model was smaller than that in the three-dimensional model by a factor of $\pi/4$. If the two-dimensional calculation is corrected so that the areal power loading is equal to that of the three-dimensional model, the discrepancy is less than 1%.

The three-dimensional results are shown in Figures 9 and 10. Symmetry ratios less than 7 gave peak temperatures within 0.5% of those for a symmetry ratio of one. For a symmetry ratio of 25, the results were about 2% higher than those for a ratio of one, although the peak was observed to occur nearly 14 years earlier. As shown in Figure 10, the addition of a shielding plug and disposal room with stagnant air or dry crushed salt changed peak temperatures less than 3% for a symmetry ratio of one.

Finally, the two-dimensional model having 924 nodes used half the CPU time and 15% less core than the three-dimensional models having 1092 nodes. When the disposal room and shielding

plug were added to the three-dimensional model, 1344 nodes were required.

CONCLUSIONS

From the results of this study it may be concluded that:

- 1) The uncertainty in waste canister temperature calculations is presently dominated by uncertainties in waste power and host rock thermal conductivity. Model detail is of secondary importance.
- 2) A two-dimensional computer model gives peak waste canister temperatures within 1% of the three-dimensional computer model having the same areal power loading.
- 3) Waste canister temperatures calculated for a symmetry ratio of one can be extrapolated to symmetry ratios of 25 with less than a 3% error for low-heat generating wastes.

REFERENCES

1. W. D. Turner, D. C. Elrod, and I. I. Siman-Tov. HEATING5 - An IBM 360 Heat Conduction Code. Report ORNL/CSD/TM-15, Oak Ridge National Laboratory, Oak Ridge, TN (March 1977).
2. M. H. Tennant. "Temperature Generated by Underground Storage of Defense Waste Canisters." *Proceedings of the Symposium in the Scientific Basis for Nuclear Waste Management*. The Materials Research Society, Boston, MA (November 1979).

TABLE 1

Material Properties

Salt

<i>Temperature, °C</i>	<i>Thermal Conductivity, K_s watts/m - °K</i>
0	6.01
50	4.93
100	4.14
150	3.55
200	3.06

Repository

<i>Depth, m</i>	<i>Density, Kg/m³</i>	<i>Specific Heat, Cal/Kg - °K</i>	<i>Thermal Conductivity, watts/m - °K</i>
0 - 305	2403	0.22	0.4 K _s
305 - 556	2242	0.22	0.57 K _s
556 - 660	2162	0.22	K _s
660 - 914	2242	0.22	0.57 K _s
914 - 1220	2403	0.22	0.4 K _s

Disposal Room

	<i>Density, Kg/m³</i>	<i>Specific Heat, Cal/Kg - °K</i>	<i>Thermal Conductivity, K_s watts/m - °K</i>
Dry crushed salt	2162	0.22	0.26
Concrete	2306	0.20	0.94
Air*	1.1	0.24	0.033

* With air in disposal room, radiation was considered between the floor and ceiling with a grey body shape factor of 0.9.

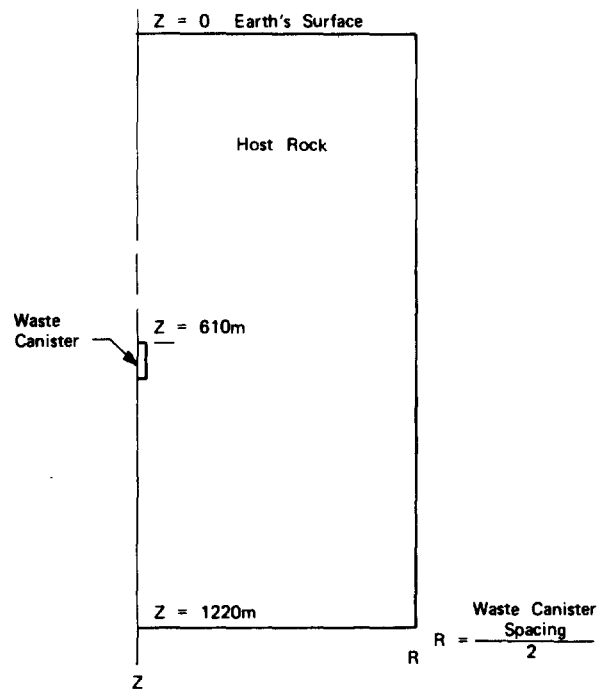


FIGURE 1. Two-dimensional Model

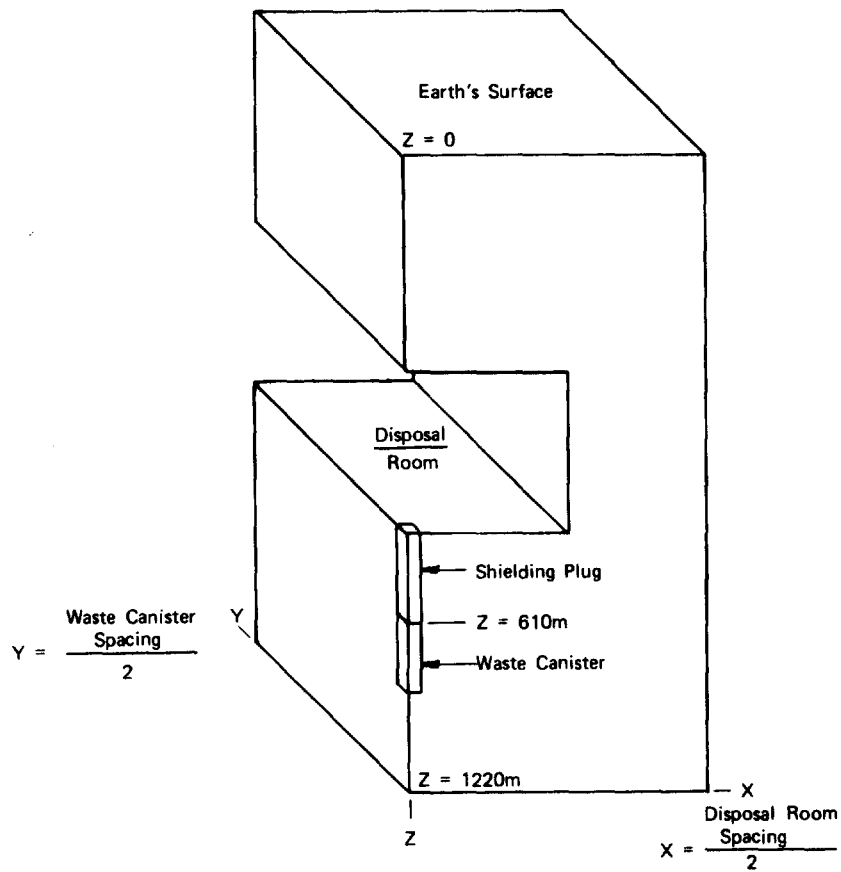


FIGURE 2. Three-dimensional Model

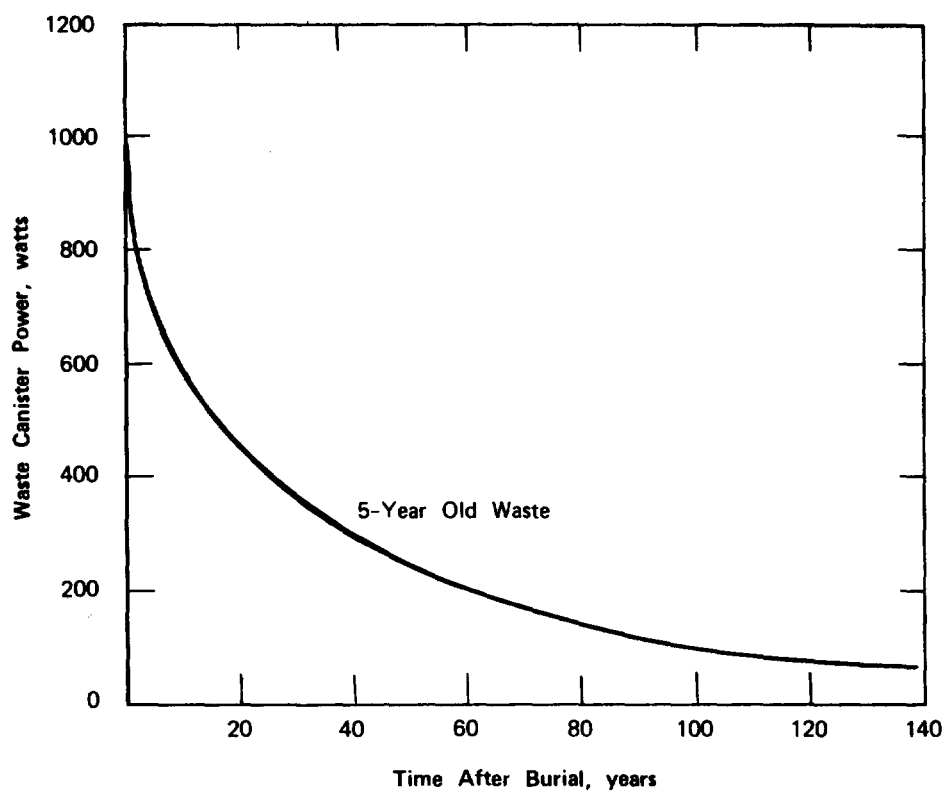


FIGURE 3. Waste Canister Power

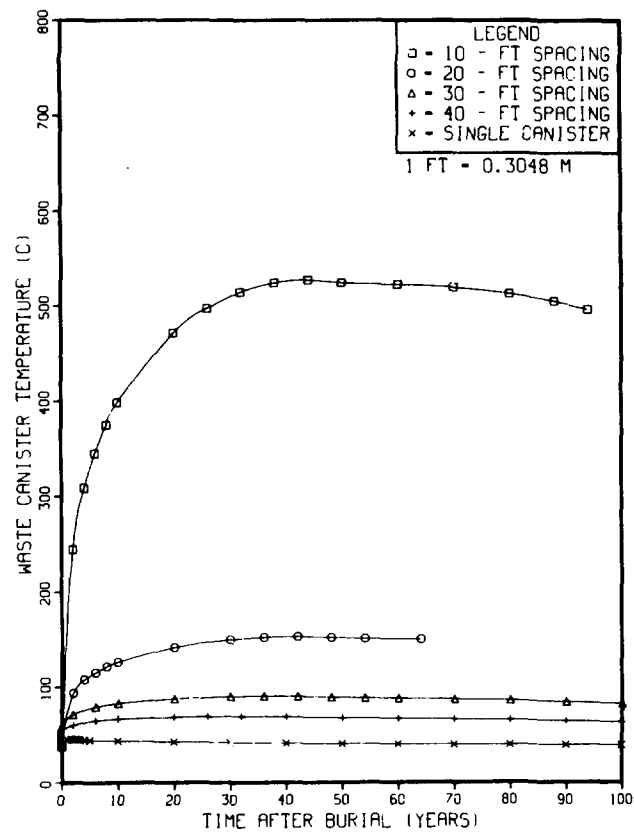


FIGURE 4. Waste Canister Temperature, Two-dimensional Model

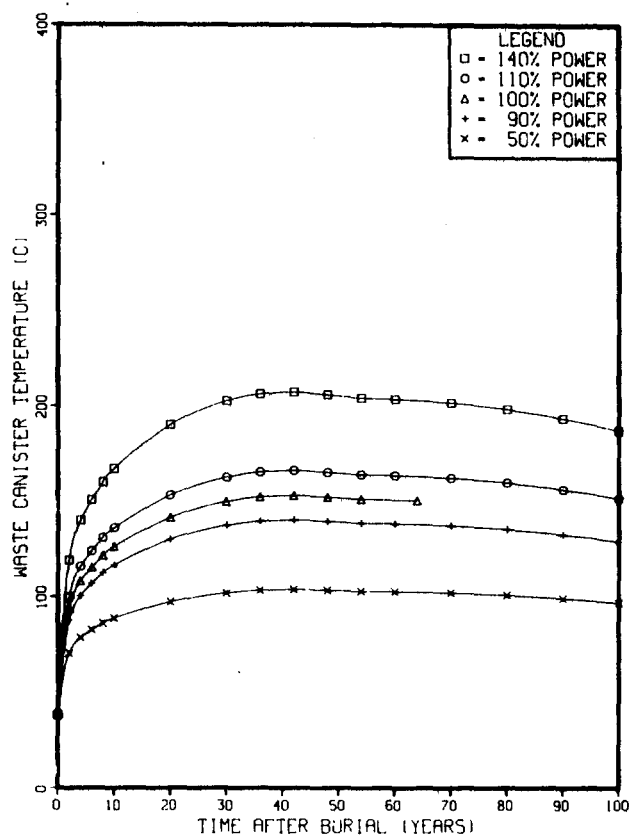


FIGURE 5. The Effect of Power Variation on Waste Canister Temperature, Two-dimensional Model

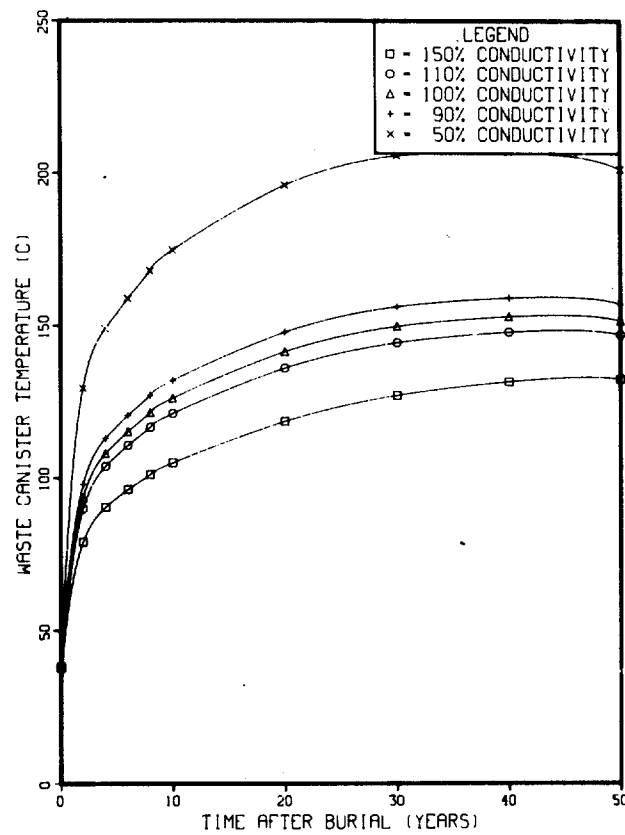


FIGURE 6. The Effect of Thermal Conductivity Variation on Waste Canister Temperature, Two-dimensional Model

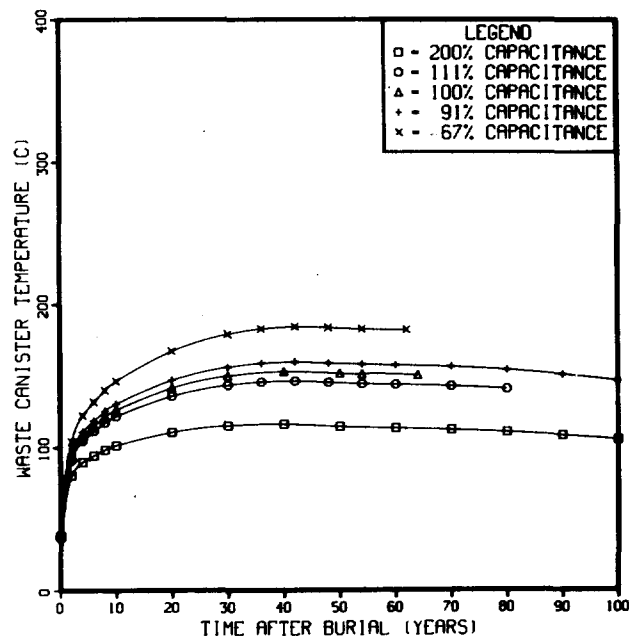


FIGURE 7. The Effect of Thermal Capacitance Variation on Waste Canister Temperature, Two-dimensional Model

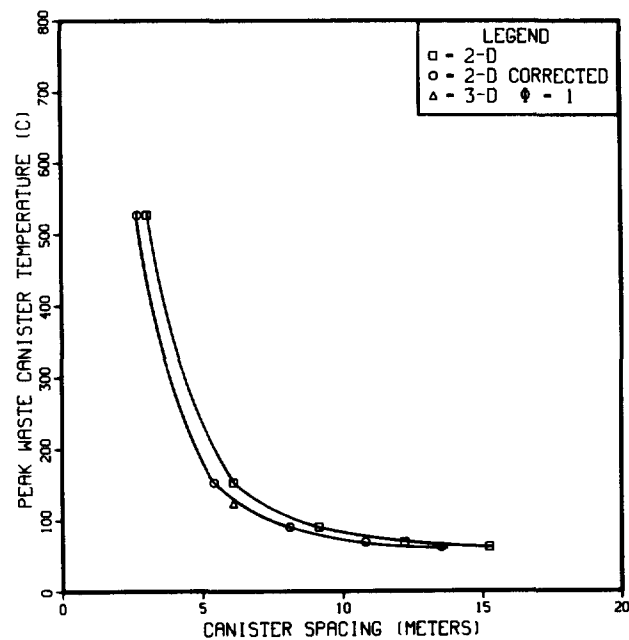


FIGURE 8. Comparison of Two- and Three-dimensional Peak Waste Canister Temperatures

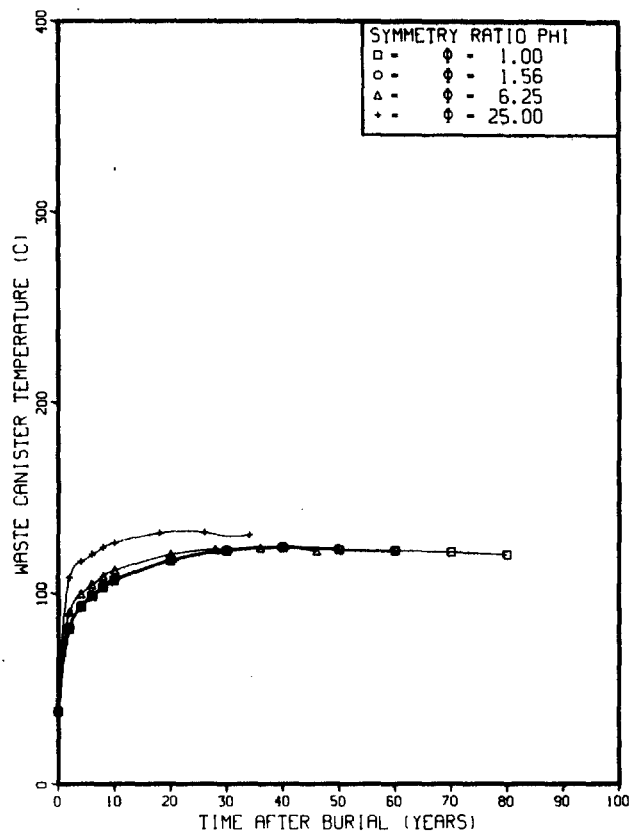


FIGURE 9. The Effect of Symmetry Ratio, ϕ , on Waste Canister Temperature, Three-dimensional Model

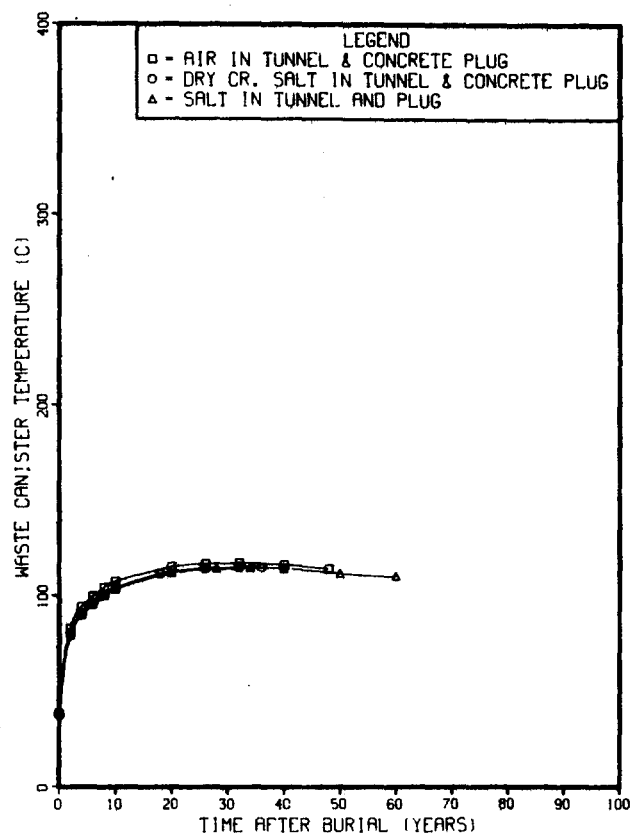


FIGURE 10. The Effect of Model Detail on Waste Canister Temperature, Three-dimensional Model $\phi=1$