30
9-3-86 ST (2)   12 cy to vault   I-27782   Dr. 1916-1

UCID-20780

THERMAL CALCULATIONS PERTAINING TO EXPERIMENTS IN THE YUCCA MOUNTAIN EXPLORATORY SHAFT

D. N. Montan

March 1986

Lawrence Livermore National Laboratory

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

Nuclear Waste Management Projects

UCID--20780

DE86 015154

MASTER

TABLE OF CONTENTS

1.0. INTRODUCTION

Waste Package Environment Tests are being planned for the NNWSI Exploratory Shaft to provide information about the near field hydrological, thermal, and mechanical environment of the waste package for use in assessing the expected performance of the waste package subsystem. The rationale of the tests is driven by the need for this information, but is constrained by the measurement capabilities that can be applied in situ, and by the ability of analytical and numerical models to use the data obtained with the measurements. A secondary purpose of the tests is to provide the option of testing certain components that may be part of the engineered barrier system.

The reference horizon for a candidate repository at Yucca Mountain is the densely welded, devitrified portion of the Topopah Spring Member of the Paintbrush tuff (Vieth, 1982). The water table at Yucca Mountain is more than 500 m below the central portion of the mountain; as a result, the Topopah Spring Member lies entirely within the unsaturated zone. The matrix porosity of the welded tuff is approximately 13 percent, and the rock has a fracture frequency of 0.8 to 3.9 fractures per meter (Dudley and Erdal, 1982).

The Waste Package Environment Tests will be located in drifts at a depth of about 310 m (1020 ft) in the Exploratory Shaft. The tests will be separated from one another by at least 6.1 m (20 ft) based on the need to avoid interaction of the individual tests. This planned minimum separation will be refined as scoping and design calculations proceed. The actual test locations within the access drift will be dependent on local geology.

The Waste Package Environment Tests will include measurements of several parameters as a function of location and time in the near field environment. The tests include an accelerated thermal cycle to examine the cooling side of the thermal pulse. The parameters to be measured or derived include temperature, moisture content, pore water pressure, rock mass deformation, and rock mass stress changes. Temperatures and pore pressures will be used directly with the moisture content data to define the spatial distribution of liquid water with time around the emplacement hole. Rock mass deformation and stress changes will be used with conceptual models of discontinuity stiffness (Goodman, 1980) to indirectly evaluate average fracture aperture changes;

fracture closure may force fluid migration to occur primarily as flow in the porous matrix. This information may be used in fracture flow models where fracture flow mechanisms are dominant. Rock core samples will be obtained before and after the tests to allow laboratory determination of index properties such as porosity, permeability, fracture stiffness, and elastic modulus. Such index properties are needed to facilitate integration of Waste Package Environment Test results with the results of other Exploratory Shaft tests.

Electrical resistance heaters will be used to simulate the heat produced by radioactive decay. Preliminary calculations indicate that with a heat loading of approximately 5 kW, the 100°C isotherm will reach a radial position about 1 m into the surrounding rock in approximately three months (Yow, 1985). This thermal loading is higher than that of the reference PWR spent fuel package (O'Neal et al., 1984). A stepped cooldown period of approximately six to nine months may be used to allow the entire rock volume surrounding the heater to drop below 100°C. More refined calculations and modeling will be completed prior to testing to determine the expected time-temperature fields around the heaters. Actual heater power levels will be varied in order to achieve desired temperature profiles; this manipulation will be based on pretest calculations and the temperatures observed in the rock mass as each test progresses. Field confirmation of temperature profiles will provide confidence that simulations of the near-field environment are based on realistic conditions.

Instruments will be installed in the rock mass around the heaters to measure temperature, moisture content, pore pressure, stress change, and displacement as a function of time and location. High-frequency electromagnetic (HFEM) measurements and other geophysical probes will be used to indirectly measure the moisture content in the rock before, during, and after thermal cycling. Preliminary calculations using the best available estimates for material properties are needed in order to anticipate the range of rock mass conditions to be experienced by the instruments.

2.0 DESIRED CALCULATIONS

While several heated tests are planned, they involve only two basic configurations as far as the heat source is concerned. In one configuration a 5 kW heater, 6 m in length, is placed in the deepest 6 m of a 12 m long, 0.30 m diameter horizontal hole. In the other configuration a 4.25 kW, 4.5 m long heater is located in the bottom 4.5 m of a 6 m deep vertical hole 0.30 m in diameter. In both cases the full power (5 or 4.25 kW) is intended to be applied for approximately 13 weeks and then gradually decreased to zero over the next 26 weeks.

The desired calculational results are temperature vs time histories and thermal contours. The temperature history locations (see Fig. 1) are the hole wall and points 0.5, 1.0 and 1.5 m from the hole wall radially outward from the heater center. The thermal contours were desired in a plane containing the heater and at the time of maximum temperature in the near field (13 weeks).

We used thermal properties for the tuff unit II-NL with 80% saturation, as given in SNL Keystone Document 6310-85-1 (Nimick et al. 1984). The values used were:

ρ	2340.0 (kg/m^3)
k	2.07 - 1.91 (W/m·K)
ρC	$2.25 \times 10^6 - 1.88 \times 10^6$ (J/m^3·K)
ΔH_v	82418.0 (J/kg)

with the water vaporization range specified as 100°C to 125°C. For k and ρC the first value of the pair is for below the vaporization range and the second is for above.

For some of the calculations only single values of k and ρC were used. These were approximately average values: 2 W/m·K and 2×10^6 J/m^3·K.

The ambient temperature used in all calculations was 25°C.

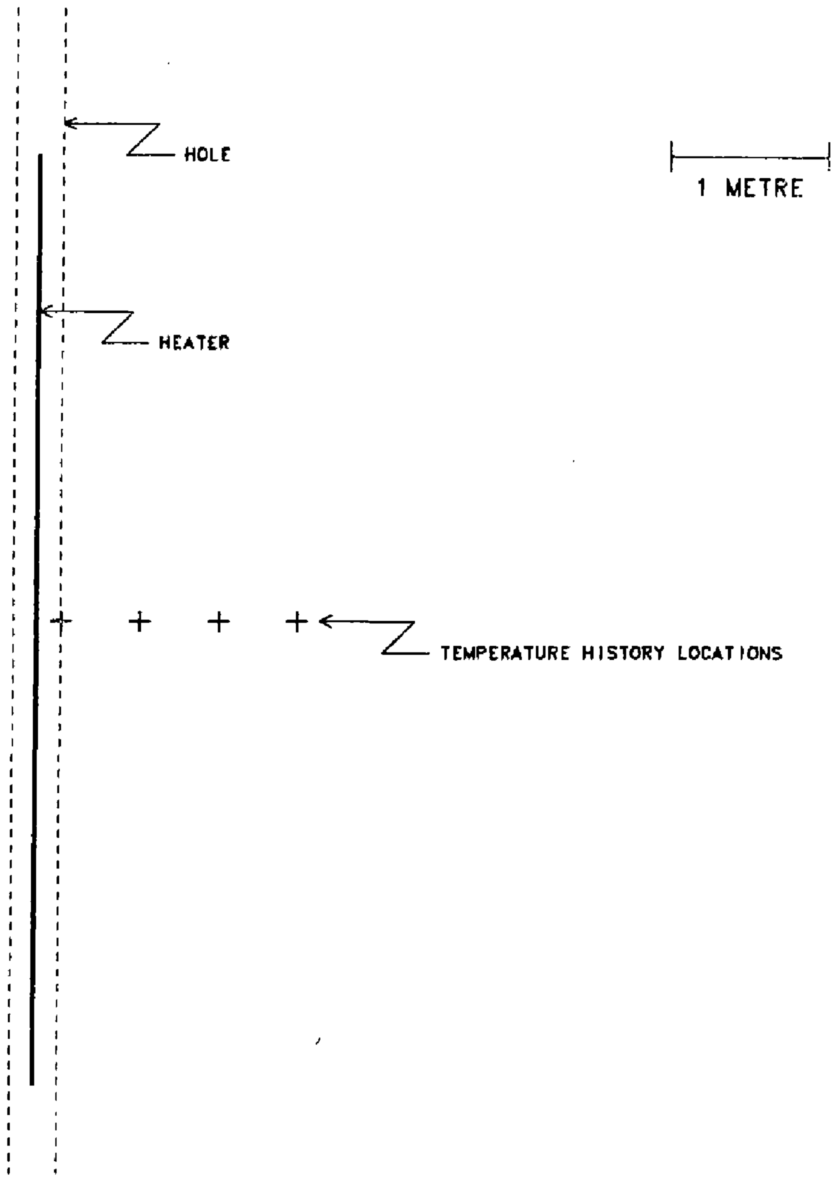

Figure 1. Geometry for the 6 m heater calculations.

3.0 CALCULATIONAL METHODS

A variety of techniques are available to handle the desired calculations. They range from simple analytical solutions of tne diffusion equation to relatively complex computer programs using finite element or finite difference techniques. We have chosen two methods, one from each end of the spectrum.

The first approach uses simple analytical solutions for the finite length line source as embodied in the PLUS Family (Montan, 1986). In these programs the source (heater) is represented by a line emplaced in an infinite, homogeneous, isotropic medium with constant thermal properties. Thus the heater hole is not considered, nor is the latent heat of vaporization and the accompanying change of thermal properties.

A more accurate modeling of the situation requires a more complex program and we have chosen to use the finite difference thermal program TRUMP (Edwards, 1972). The use of such a program requires a calculational mesh. The mesh used was a two dimensional cylindrical R-Z mesh with the heater emplacement hole along the Z axis. The mesh used for the 6 m heater calculation is shown in Figure 2, and an expanded view of the portion nearest the heater is given in Figure 3. There were 21 nodal positions in the R direction, giving an outer boundary of 17.6 m, and 15 nodal positions in the Z direction with an outer boundary at 19.3 m. All boundaries were adiabatic, with the outer boundaries being far enough removed from the place where the temperatures were desired that the boundary condition did not affect the results. The boundary at Z = 0 is a plane of symmetry; only one half the problem need be considered. The thermal flux from the heater was applied to the nodal points of 7 zones comprising the 3 m half length of the heater. The mesh for the 4.5 m heater was very similar. It was shrunk ~ 5% in the Z direction, giving an outer boundary of 18.4 m and 6 zones comprising the 2.25 m half length.

In the analytical type calculations, using members of the PLUS family, i.e., TWIGS for the temperature histories and its companion DAYLITE for the thermal contours, the power was input as a constant for the first 13 weeks and then decreased in twelve 2-week long steps to zero at 37 weeks. In the TRUMP

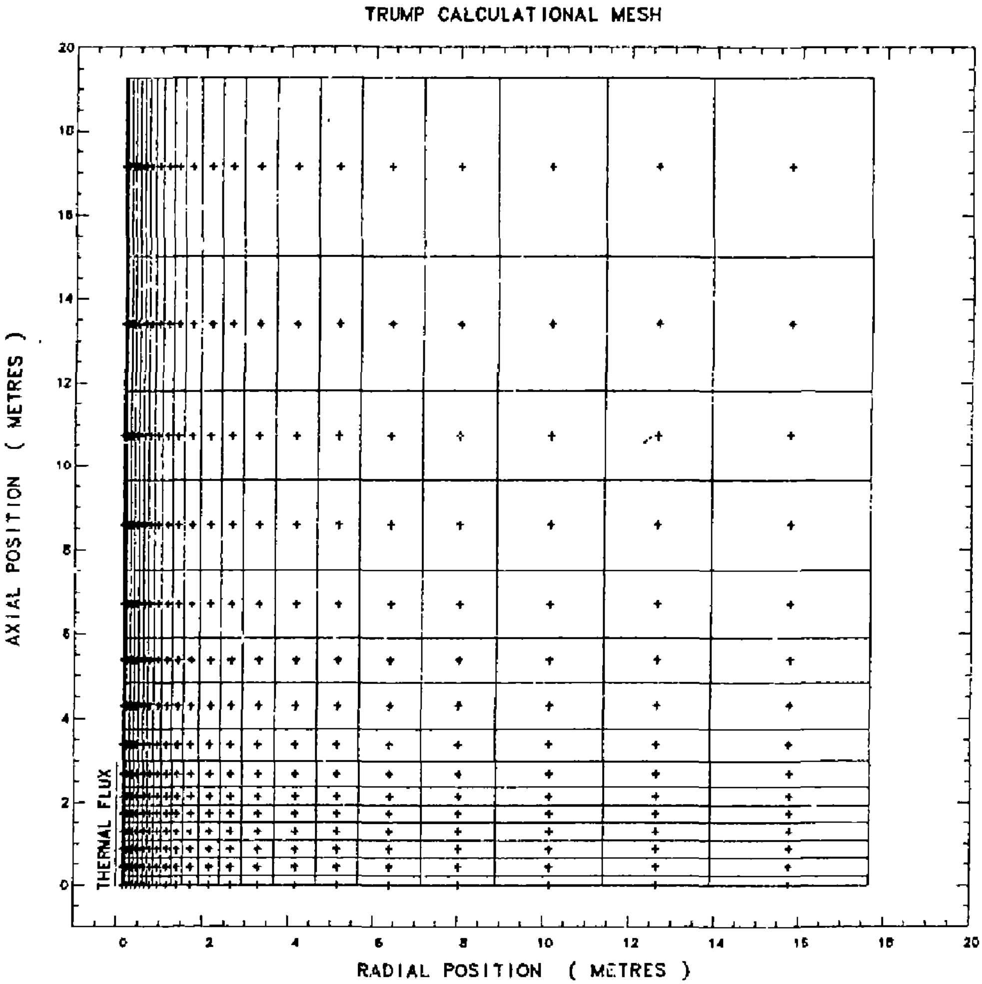

Figure 2. The calculational mesh used with TRUMP for the 6 m heater.

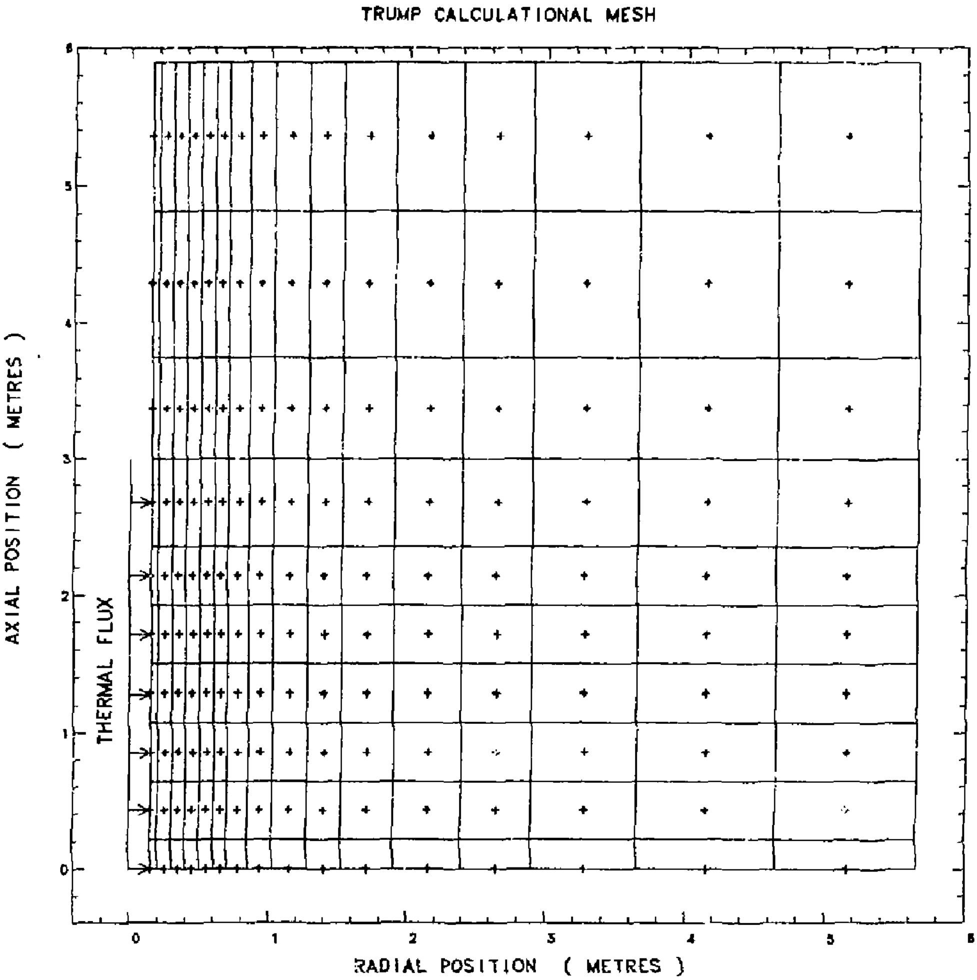

Figure 3. The inner portion of the calculational mesh used with TRUMP for the 6 m heater.

calculations the power was constant for 12 weeks and then decreased linearly to zero at 38 weeks. Both methods give the same total energy input. They were chosen partially for convenience, but also to show that it makes very little difference in the final results. The power input for the 6 m heater is shown in Figure 4. The power input for the 4.5 m heater is the same, but reduced by a factor of 0.85.

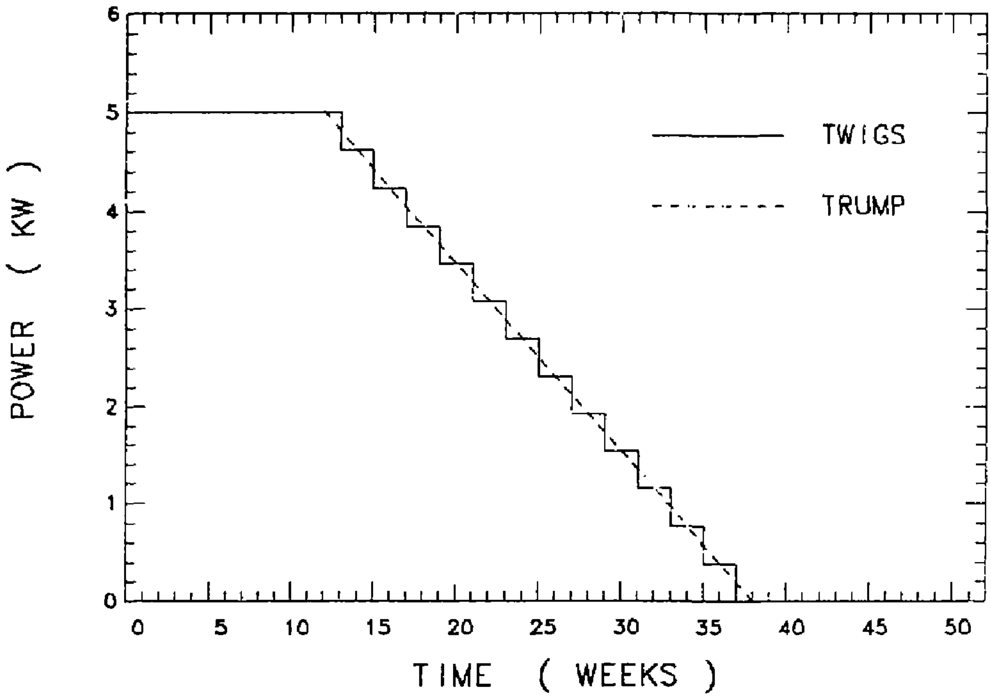

Figure 4. Power history used for the 6 m heater calculations.

4.0 INITIAL CALCULATIONS

Three pairs of calculations were made using the average thermal properties (2 W/m•K and 2 x 10^6 J/m^3•K) with TWIGS, TRUMP and DAYLITE. Each pair consisted of a 6 m heater calculation and a 4.5 m heater calculation.

The TWIGS and TRUMP results, shown in Figures 5 and 6, should differ only in the absence or presence of the heater emplacement hole. The excellent agreement of the two, quite different, calculational techniques shows at least two things:

a) The hole is not important.

b) The much more complex TRUMP input with its discretized calculational mesh, has been apparently specified correctly. This is a non-trivial consideration.

The thermal contours produced by DAYLITE shown in Figures 7 and 8 were produced from a 41 by 41 point array (0.15 m by 0.15 m spacing) whose origin is a heater center. The time chosen (13 weeks) is the time when the near field temperatures are at or very near their maximum.

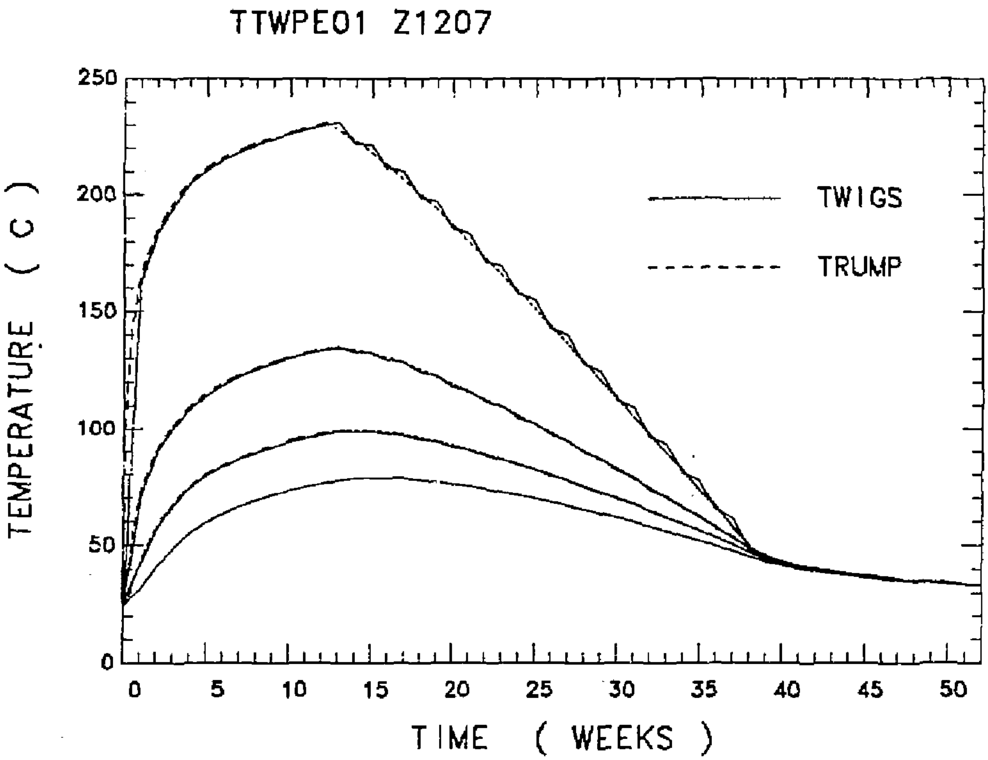

Figure 5. Comparison of TWIGS and TRUMP calculations for the 6 m heater. Average thermal properties used.

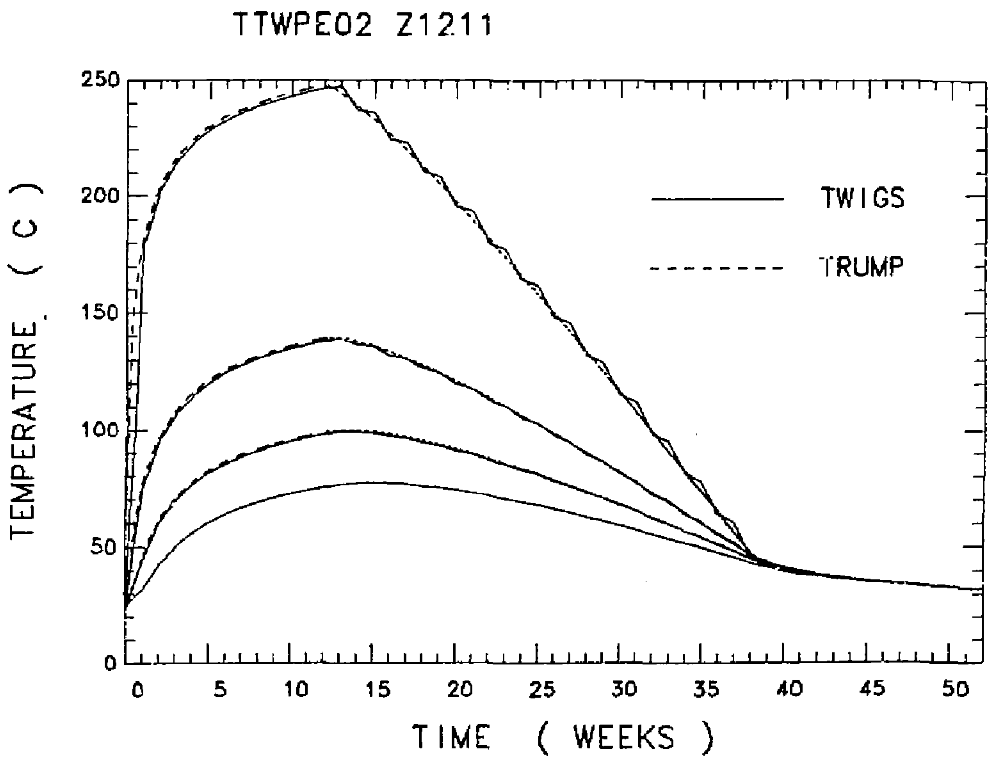

Figure 6. Comparison of TWIGS and TRUMP calculations for the 4.5 m heater. Average thermal properties used.

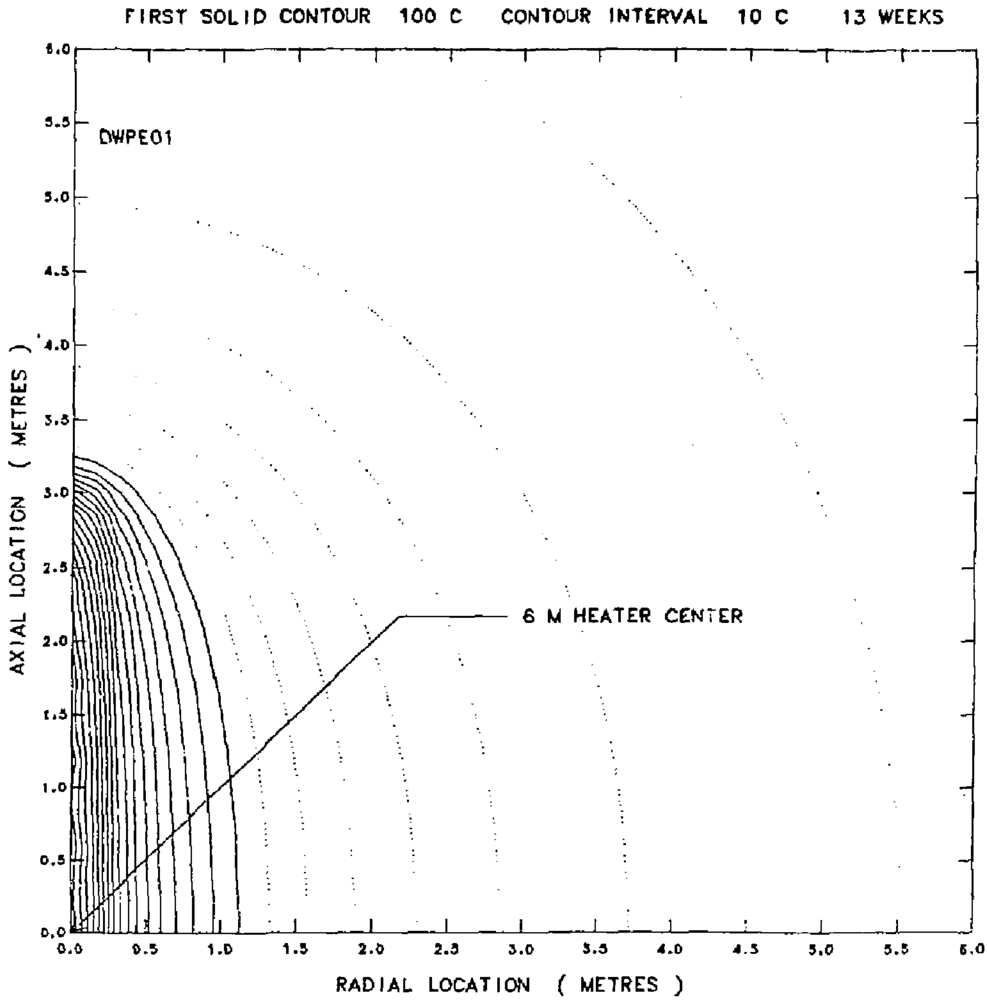

Figure 7. Thermal contours for the 6 m heater at 13 weeks.

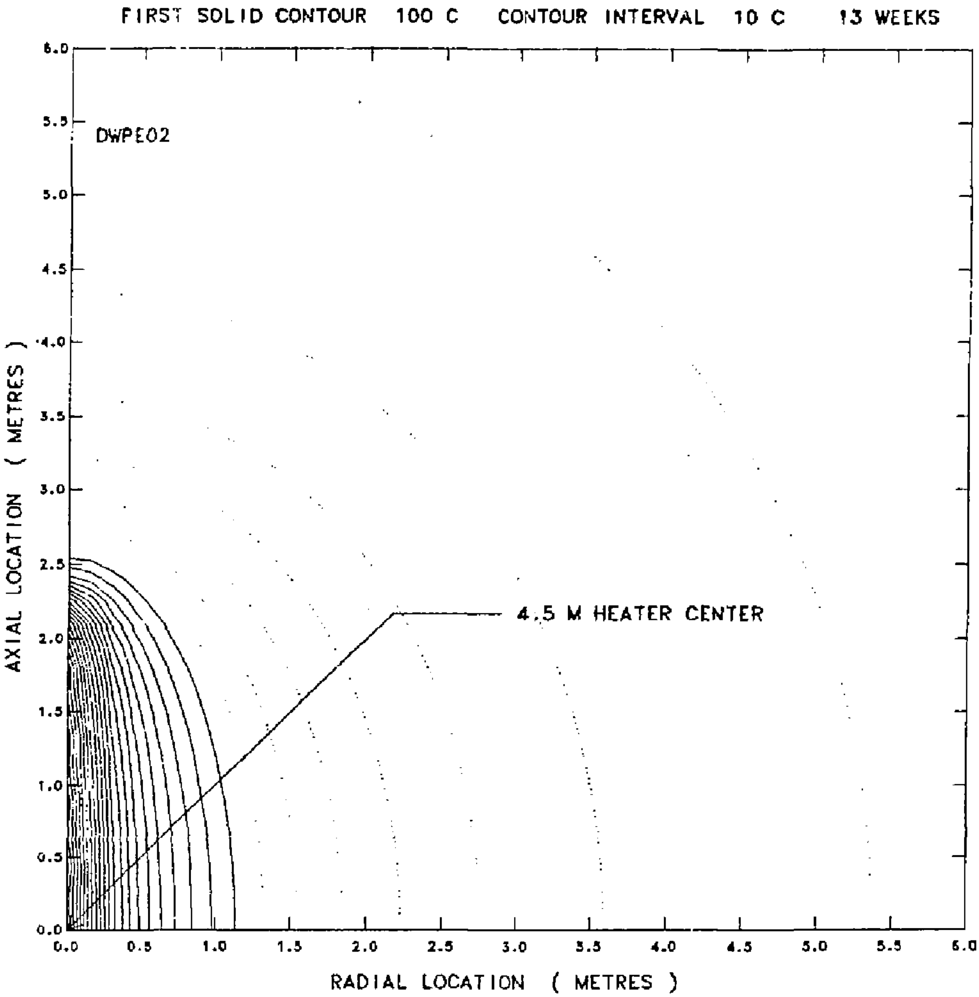

Figure 8. Thermal contours for the 4.5 m heater at 13 weeks.

5.0 CALCULATIONAL VARIATIONS

A series of calculations were made to examine the sensitivity of the results to variations in thermal properties and to the presence of surfaces and other sources in the experimental area. Most of the calculations could have been done using either TWIGS or TRUMP, but since the TWIGS calculations require only ~ 1/50 of the computer time, it was the obvious choice in most cases.

5..1 Variation of Thermal Conductivity

The thermal conductivity of the medium is the most important property. The calculated temperature changes are inversely proportional to it (sensitivity = - 1.0). This is illustrated in Figure 9 where two additional 6 m heater calculations with the conductivity varied by + and - 5% are compared with the original calculation. This ± 5% variation is approximately the spread in the recommended wet and dry conductivity about the average.

5.2 Variation of Thermal Diffusivity

The thermal diffusivity ($\kappa = k/\rho C$) is much less important than conductivity, but its effect varies with time and place. This is illustrated in Figure 10, where two additional calculations for the 6 m heater, with the diffusivity varied by + and - 10% are compared with the original calculation. At 12 weeks the sensitivity ranges from 0.09 at the hole wall to 0.34 at 1.5 m from the hole. The ± 10% variation is approximately the spread that would result if the conductivity were held constant, but the recommended wet and dry values of ρC were used.

5.3 Influence of a Nearby Surface

In the calculations described so far the medium has been of infinite extent. This comes with the analytical solutions used in the PLUS Family and was approximated by a suitably large mesh size in the TRUMP calculations. In the actual experimental area there will be a number of drifts from which the

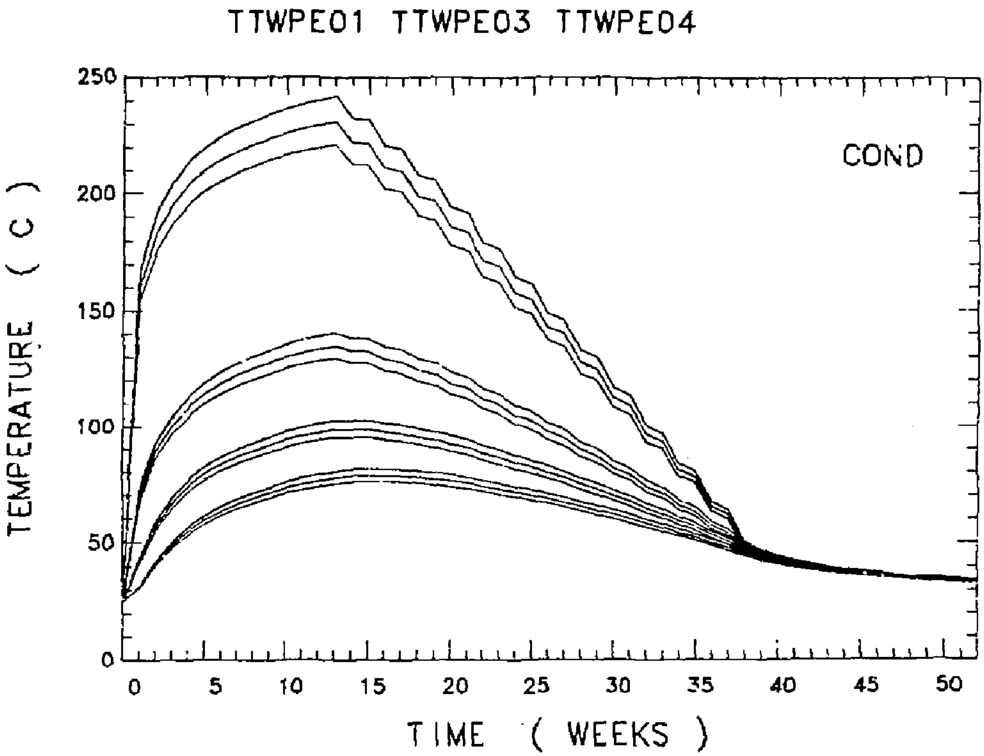

Figure 9. The effect of a ± 5% variation of thermal conductivity on the 6 m heater calculations.

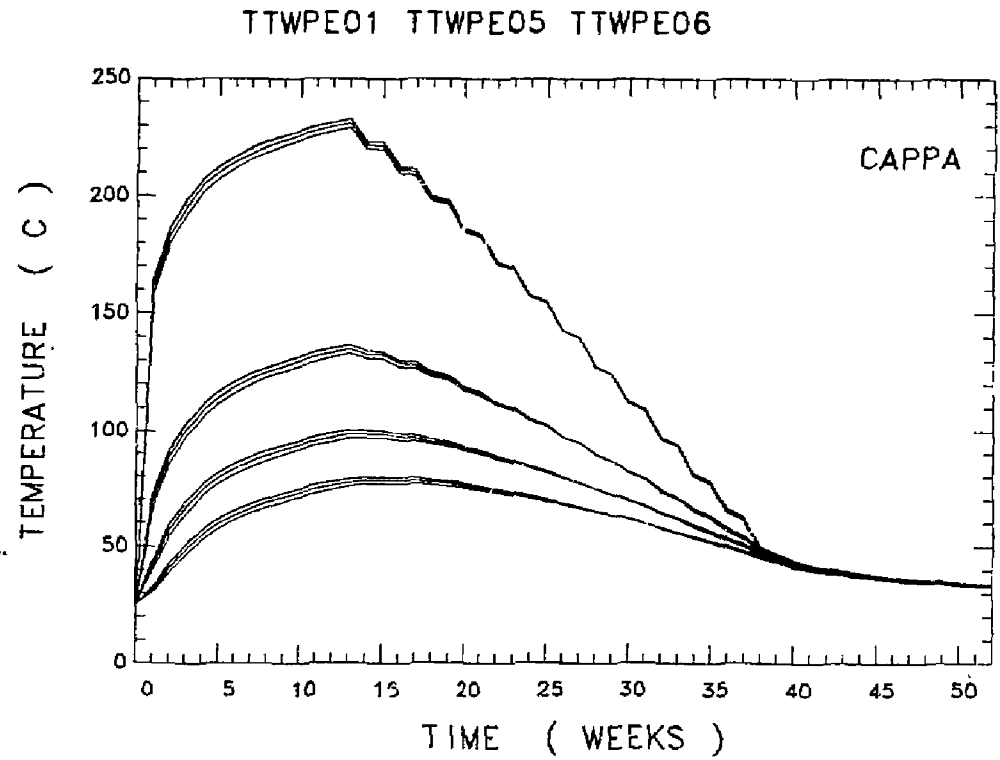

Figure 10. The effect of a ± 10% variation of thermal diffusivity on the 6 m heater calculations.

heater emplacement holes are drilled. The surfaces of these drifts will presumably be kept near the ambient temperature in the region by ventilation. Thus the effect of an isothermal surface at the end of the drill hole should be considered. For the 6 m heater in a 12 m hole the nearest distance of the source to wall is 6 m. However, the top of a 4.5 m heater in a 6 m hole is only 1.5 m from the floor. This situation has been investigated with TWIGS and DAYLITE using the "method of images" in which a negative "image" source is located symmetrically above the location of the desired isothermal surface. The results of TWIGS calculations at the hole wall, 0.5 m and 1.0 m from the wall are shown compared to the initial calculation in Figure 11. These calculations, in the plane of the heater center (3.75 m below the floor), show the small effect, mainly at late times. The effect is greater at locations nearer the floor. This may be seen in the contours produced by DAYLITE (Figure 12). From these contours the thermal gradient, near the floor and directly above the heater, may be estimated as ~ 30 K/m giving a flux of ~ 60 W/m^2.

5.4 Influence of Other Sources

In the introduction, we mention the intent to separate the various tests by some distance (initial estimate ~ 6 m) to minimize interaction between the tests. To assist in deciding on this distance the results of a pair of calculations of temperature histories in the 5-10 m range from a single heater is shown in Figure 13.

5.5 Vaporization of Water

The tuff in the experimental area may contain on the order of 10 percent water by volume. Thus, due to the high latent heat of vaporization of water, any calculation in a situation where the temperature is expected to exceed the boiling point should consider this phase change. Since the analytical solutions in the PLUS Family do not handle phase change, one might go directly to a more sophisticated program such as TRUMP in which phase change can be handled. However, the analytic solution technique may be employed in a relative simple manner to give an approximate upper bound to the phase transition effects.

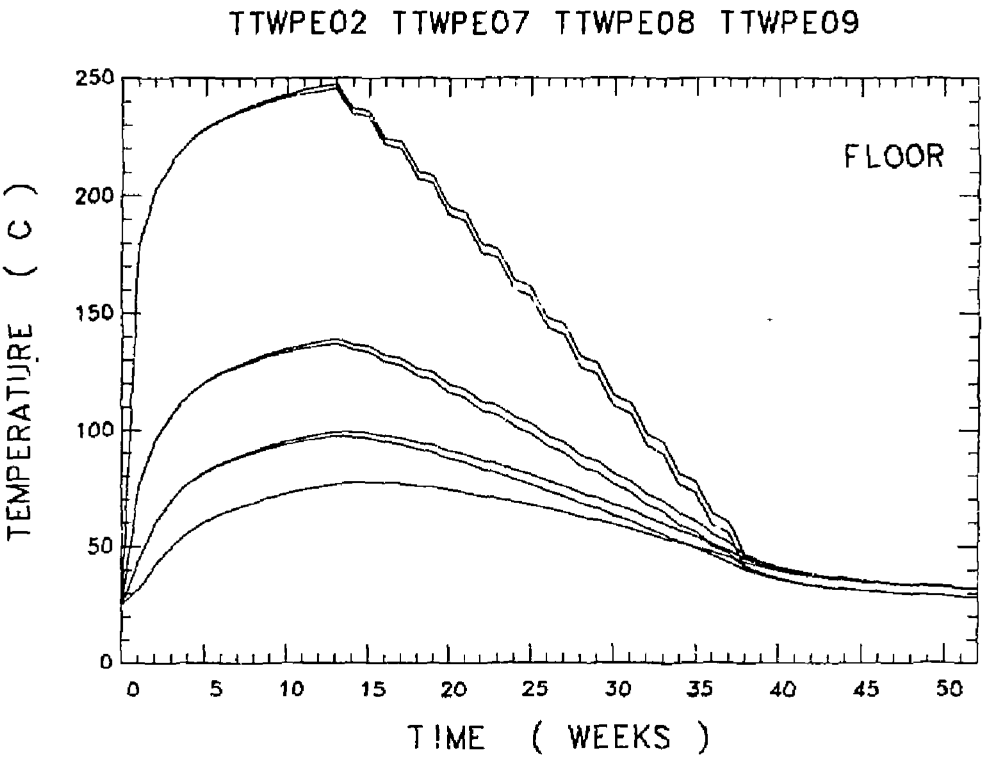

Figure 11. The influence of an isothermal surface 1.5 m from one end of a 4.5 m heater.

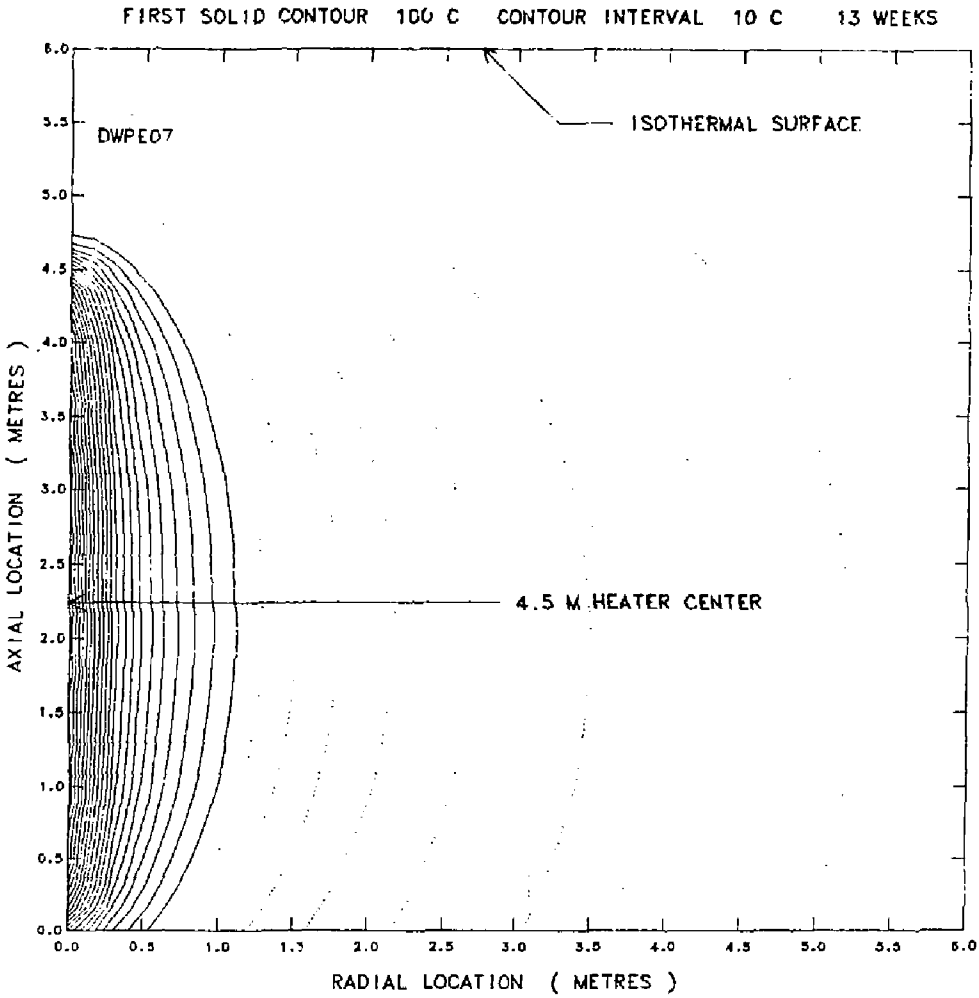

Figure 12. Thermal contours at 13 weeks with an isothermal surface 1.5 m above one end of a 4.5 m heater.

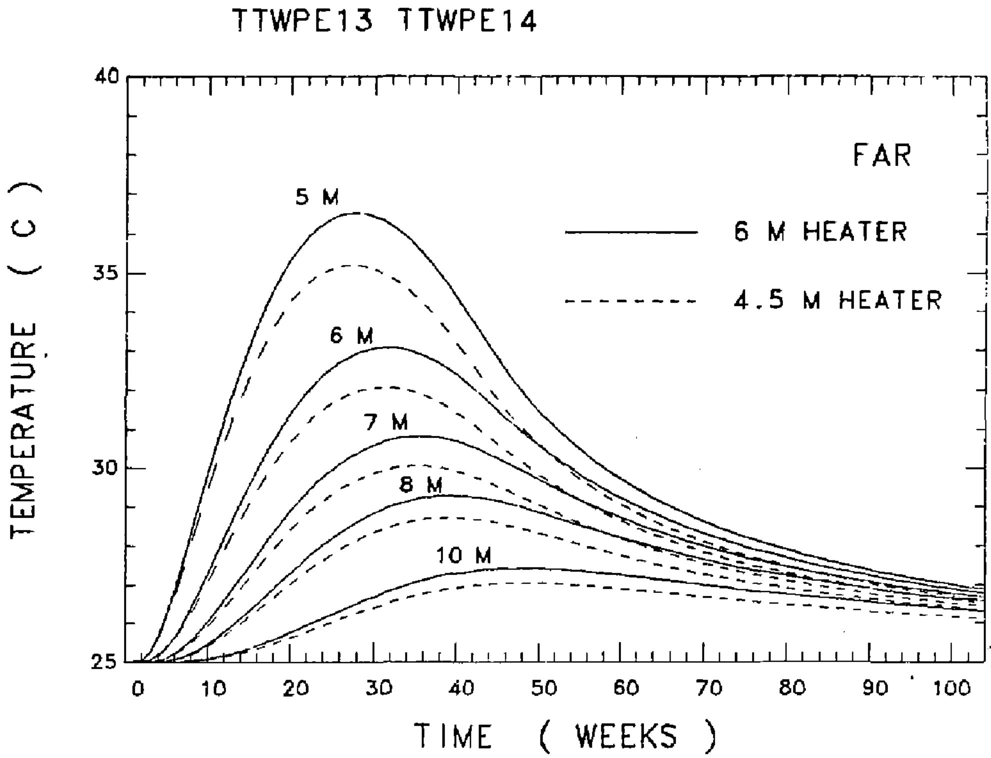

Figure 13. Temperatures in the 5-10 m range from the 6 and 4.5 m heaters.

In this approximation, the analytic solution is used to determine the volume of material that has exceeded the transition temperature and from this one calculates the heat of transition. This is then subtracted from the heat input and the volume recalculated. If the effect is not too large, a few iterations should give a stable result. This result should be expected to give a reasonable approximation at places near or below the transition temperature since at these places the heat removed by this approximation should indeed have been removed as the heat flowed through the hotter regions. At places closer to the heat source only part of the total vaporization will have occurred as the heat flux reaches these places and thus the approximation will remove too much heat and provide only an upper bound on the effect.

To implement this approximate method a simple means of volume calculation is desirable. At steady state the isothermal surfaces surrounding a constant power finite line source are a family of confocal prolate spheroids whose foci are the source ends. This suggests that an ellipse might be a useful approximation for an isotherm under nonsteady state conditions as well. To test this idea we used a large (20" x 20") version of Figure 7 and read from it the axial and radial extremes of the 100°C isotherm. Using these as semi-major and semi-minor axes, an ellipse can be calculated. This is shown in Figure 14 along with the isotherm. The agreement is quite good.

Using this ellipse the volume of the enclosed spheroid and the volume of rock may be calculated by subtracting the volume of the enclosed emplacement hole. From this the heat of vaporization is calculated, removed from the power input and the process repeated. Four DAYLITE calculations were involved with the following powers and ellipses.

Power (W)	Semi-major axis (m)	Semi-minor axis (m)
5000.0	3.23	1.12
4591.35	3.19	1.01
4631.5	3.19	1.02
4648.25	3.20	1.02

Thus it appears that for this case the vaporization of water will have a ~ 7% effect on power input (and hence temperature change). Using the final power

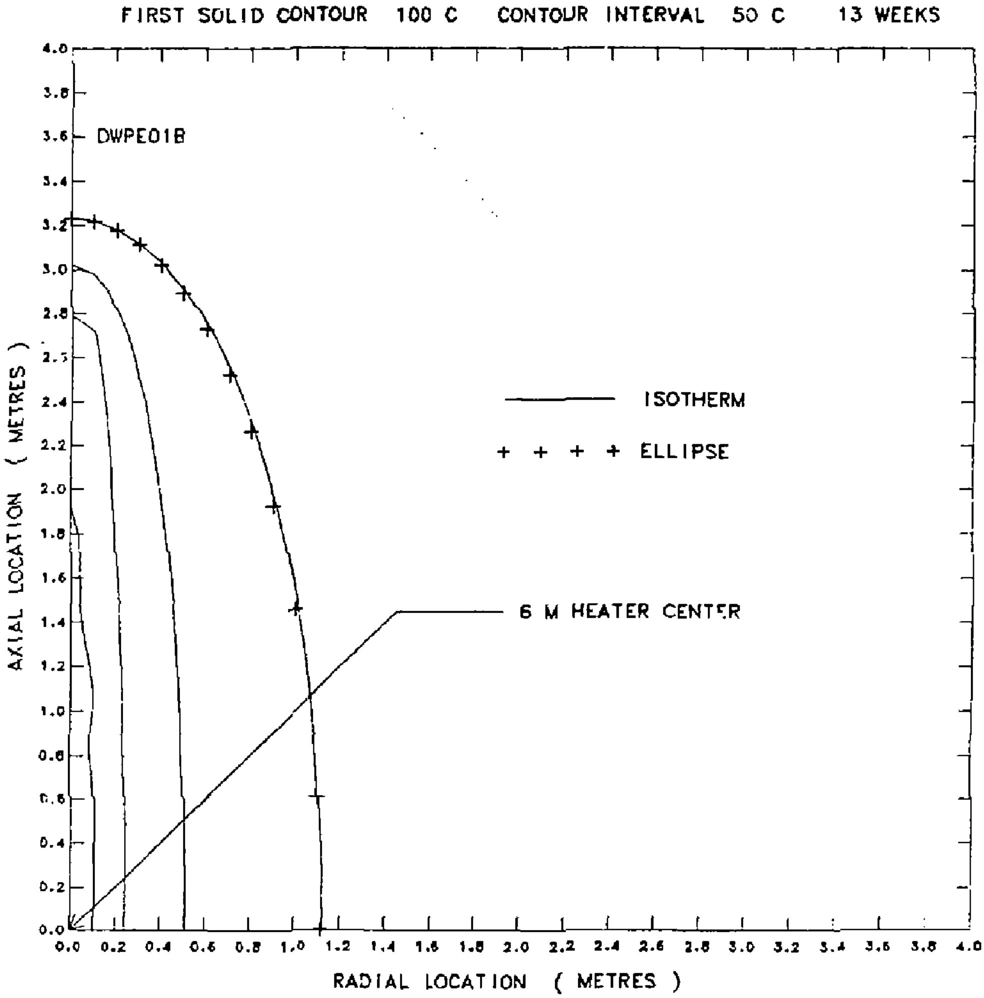

Figure 14. The approximation of an isotherm by an ellipse.

(for the first 13 weeks) a set of temperature histories were calculated using TWIGS. A comparison with the original (5 kW) calculation is shown in Figure 15. It should be noted that this approximation only removes heat. Latent heat is not returned during cooling.

With the TRUMP program, the phase change temperature and latent heat may be input directly or, alternatively, the heat capacity may be tabulated as a function of temperature with a suitable increase over a temperature range for the phase change. Three calculations were made to investigate these options. In the first, a temperature of 96.7°C and a heat of vaporization of 8.23×10^4 J/kg were specified. In the other two calculations, the heat capacity variation method was used with a vaporization temperature range of 5°C and 10°C both centered at 96.7°C. All other properties were the "average" properties.

These three calculations are shown along with the original (no vaporization) TWIGS calculation in Figure 16. The TRUMP calculations are practically indistinguishable, indicating that the vaporization range used is unimportant. The only interesting feature is the "flat spots". These are from the first calculation where vaporization takes place at a fixed temperature and are an artifact of the finite mesh size. When a node reaches that temperature it must stay there until it receives enough heat to complete its phase change. Also noted on the cooling side of the curves, is that the phase change is reversible. What goes out comes back in. This may not be physically true. The steam (at least some of it) may escape.

A comparison of Figures 15 and 16 shows the expected result: the TWIGS approximation shows too great a temperature reduction at the wall, but much better agreement with TRUMP at lower temperature locations.

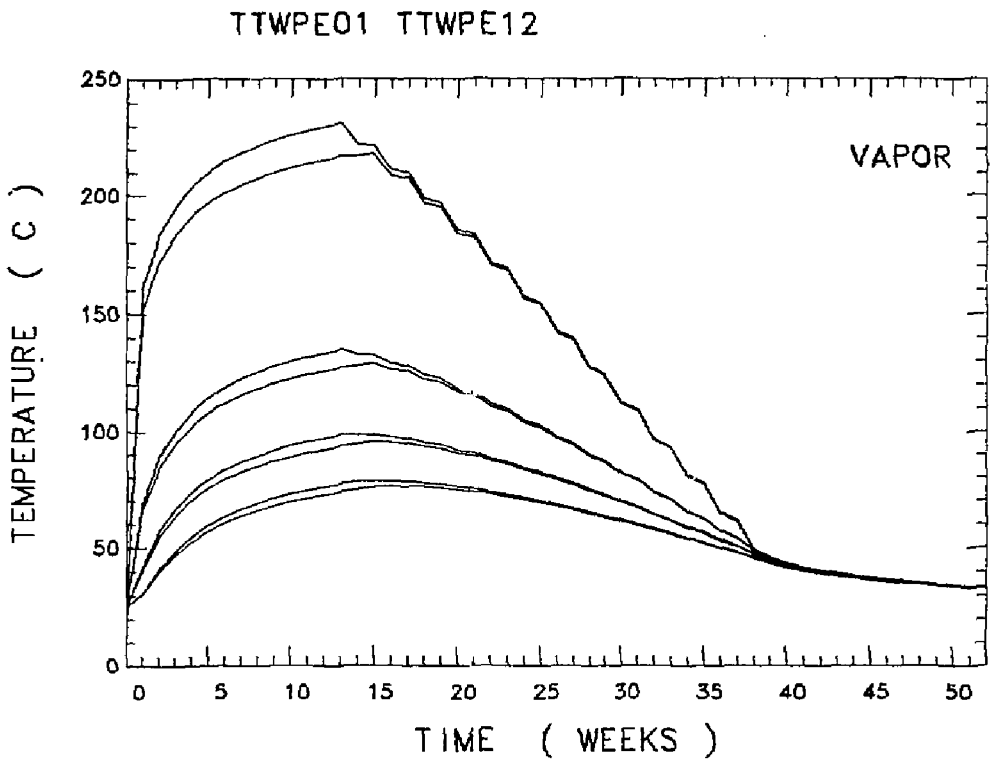

Figure 15. The effect of vaporization of water by a 6 m heater as approximated with TWIGS.

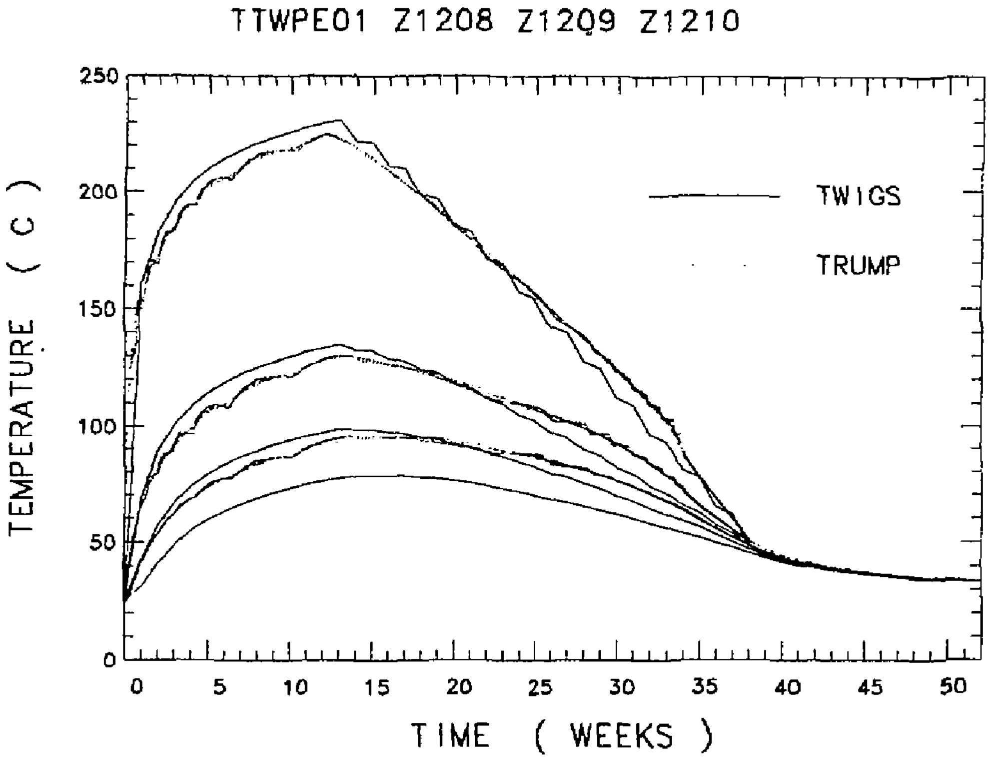

Figure 16. Vaporization and condensation as calculated by TRUMP.
Phase change occurring over a range of 0, 5 or 10°c.

6.0 FINAL CALCULATIONS

Three final TRUMP calculations were made. The first two, one each for the 6 m and 4.5 m heaters, used the complete set of "recommended" properties with one minor modification; the 25°C vaporization range started at 97°C (the appropriate boiling point for the planned experimental area) rather than the 100°C given by Nimick et al. These calculations are shown in Figures 17 and 18 along with the corresponding initial TWIGS calculations using "average" properties and no vaporization. The similarity of the results of the two quite different techniques gives considerable credence to the idea of using simple methods (like the PLUS Family) for some of the design calculations for situations similar to these.

The last calculation (for the 6 m heater) was the same as the one just discussed with the exception that the vaporization range was reduced to 5°C, but still starting at 97°C. These two calculations, shown in Figure 19, show only minor differences.

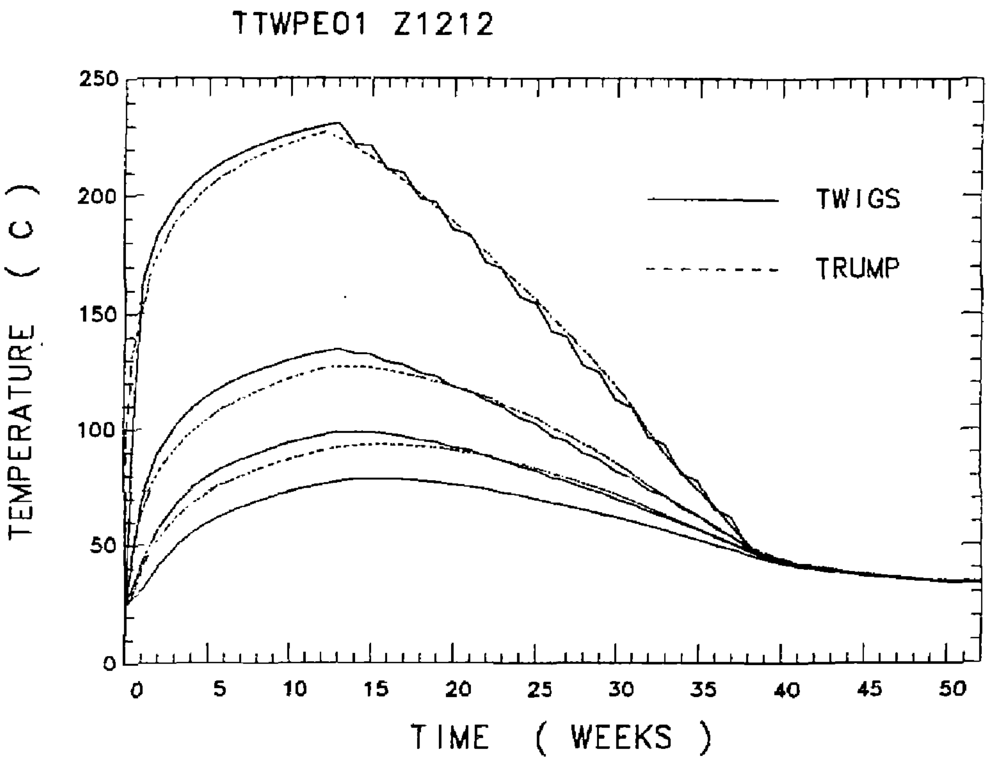

Figure 17. The 6 m heater using "average" properties (TWIGS) and "recommended" properties (TRUMP).

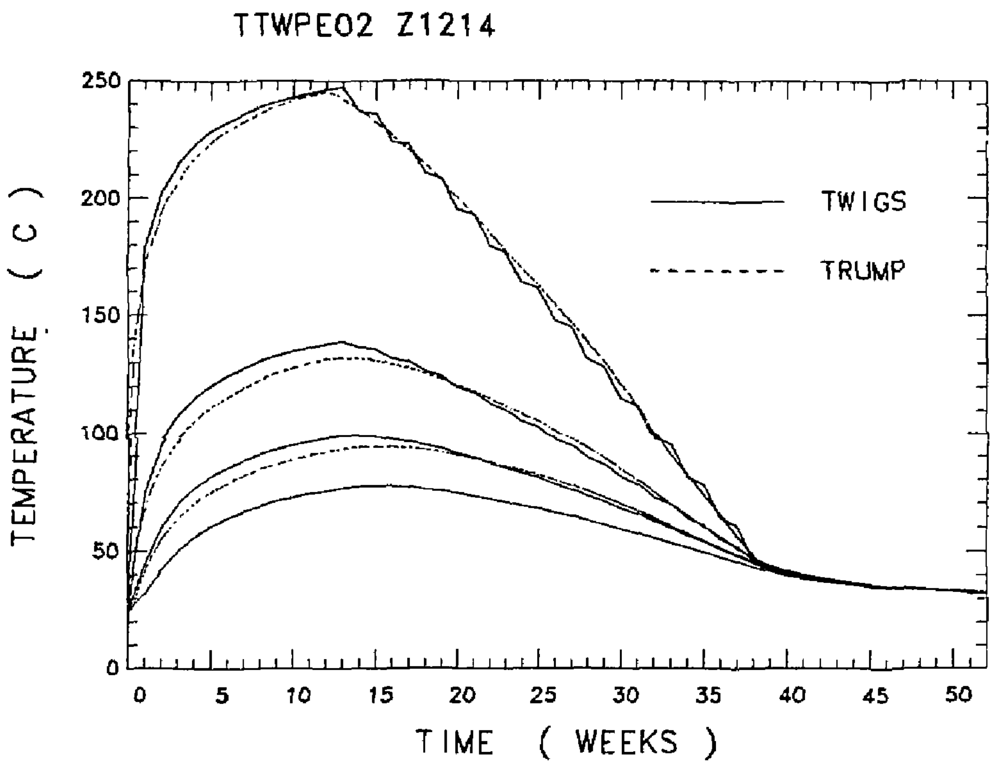

Figure 18. The 4.5 m heater using "average" properties (TWIGS) and "recommended" properties (TRUMP).

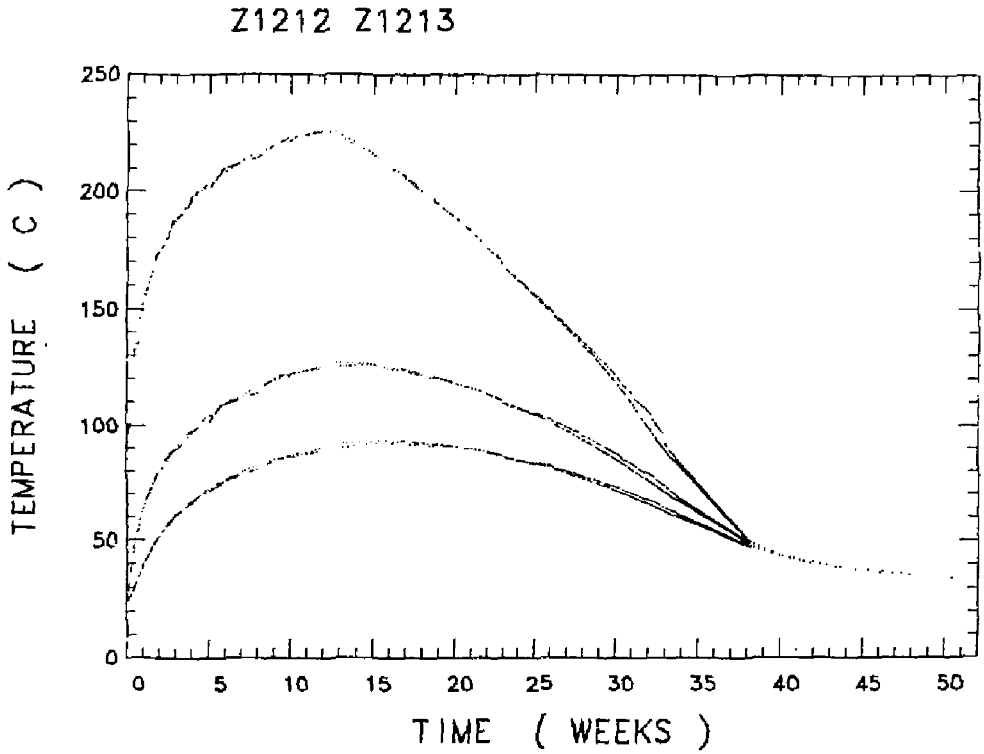

Figure 19. TRUMP calculations for the 6 m heater using "recommended" properties. Phase change range 5 and 25°C starting at 97°C.

7.0 COMMENTS ON THE PROPERTIES USED

We used the "recommended" properties for Unit II-NL at 80% saturation as given in Table 2 of the SNL Keystone Document (Nimick et al. 1984) in our thermal calculations. However we have carefully examined these "recommended" values and also the "intact" values given in Table 1 of the Document. We find some apparent problems and/or inconsistencies that should be borne in mind by anyone using our calculational results.

In particular, the "recommended" values in Table 2 lump two Units II-NL and III into a single set while Table 1 treats them individually. There are some significant differences. The porosity of the III unit is only 1/3 of that of the II-NL unit, while the thermal conductivity is about 2/3 that of the II-NL unit. The lumped set of "recommended" values for density, heat capacity and thermal conductivity appear to be computed as mix of 84% II-NL and 16% III. The principal effects are on conductivity (~ 5% low) and heat of vaporization (~ 10% low).

If the experimental area is indeed in the II-NL unit our calculated temperature changes might be expected to be ~ 6% high.

Also noted, the dry thermal conductivity given for the III unit is greater than the saturated value. This is not physically reasonable.

8.0 CONCLUSIONS AND RECOMMENDATIONS

A series of thermal calculations have been presented that appear to satisfy the needs for design of the Yucca Mountain Exploratory Shaft Tests. The accuracy of the modeling and calculational techniques employed probably exceeds the accuracy of the thermal properties used. The rather close agreement between simple analytical methods (the PLUS Family) and much more complex methods (TRUMP) suggest that the PLUS Family might be appropriate during final design to model, in a single calculation, the entire test array and sequence.

Before doing further calculations it is recommended that all available thermal property information be critically evaluated to determine "best" values to be used for conductivity and saturation. Another possibility is to design one or more of the test sequences to approximately duplicate the early phase of Heater Test 1 (Montan and Bradkin 1984). In that experiment an unplanned power outage for about two days that occurred a week into the experiment gave extremely useful data from which to determine the conductivity and diffusivity.

In any case we urge that adequate, properly calibrated instrumentation with data output available on a quasi-real time basis be installed. This would allow us to take advantage of significant power changes (planned or not) and also help "steer" the tests to desired temperatures.

Finally, it should be kept in mind that the calculations presented here are strictly thermal. No hydrothermal effects due to liquid and vapor pressures have been considered.

9.0 REFERENCES

Dudley, W. W., Jr., and B. R. Erdal, 1982. "Site Characterization for Evaluation of Potential Nuclear Waste Isolation at Yucca Mountain, Nevada", in Proceedings of the 1982 National Waste Terminal Storage Program Information Meeting, DOE/NWTS-30, pp. 10-12.

Edwards, Arthur L., 1972. "TRUMP: A Computer Program for Transient and Steady-State Temperature Distributions in Multidimensional Systems", Lawrence Livermore National Laboratory, Livermore, Ca, UCRL-14754, Rev. III.

Goodman, R. E., 1980. Introduction to Rock Mechanics, John Wiley & Sons, New York, NY.

Montan, D. N., 1986. "The PLUS Family, A Set of Computer Programs to Evaluate Analytical Solutions of the Diffusion Equation", UCID-20680, Lawrence Livermore National Laboratory, Livermore, CA.

Montan, D. N., and W. E. Bradkin, 1984. "Heater Test 1, Climax Stock Granite, Nevada", UCRL-53496, Lawrence Livermore National Laboratory, Livermore, CA.

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

O'Neal, W. C., D. W. Gregg, J. N. Hockman, E. W. Russell, and W. Stein, 1984. "Preclosure Analysis of Conceptual Waste Package Designs for a Nuclear Waste Repository in Tuff", UCRL-53595, Lawrence Livermore National Laboratory, Livermore, CA.

Vieth, D. L., 1982. "Nevada Nuclear Waste Storage Investigations Project Overview", in Proceedings of the 1982 National Waste Terminal Storage Program Information Meeting, DOE/NWTS-30, pp. 9-10.

Yow, J. L., Jr., 1985. "Concept for Waste Package Environment Tests in the Yucca Mountain Exploratory Shaft", UCID-20450, Lawrence Livermore National Laboratory, Livermore, CA.