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Heat Transfer Model of the February 1991 Saltstone Pilot Pour Test (U)

Task Number: 93-016-0

by

M. A. Shadday Jr.

June 1993

Patent Status

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Introduction and Summary

A byproduct of the DWPF high-level waste vitrification process will be 25 million gallons of low-level salt solution. This salt solution will be mixed with cement and a flyash/slag mixture and solidified in surface vaults in the Z-area Saltstone Facility. The curing process of saltstone involves exothermic reactions, and there is a maximum temperature limit of 90^0 C for the saltstone. If this temperature limit is exceeded, the physical properties of the saltstone can be degraded. NES was requested to develop a heat transfer model of the saltstone pouring process, and as part of this task NES was also requested to analyze thermocouple data from a test pour of saltstone in a cylindrical hole. The data has been analyzed and a transient heat transfer model of the test was developed. The agreement between the model results and the test data is excellent. The analysis of the test pour is the first part of this task, and it is the subject of this document. This is the first of two reports that will document the work on this task. When the investigation is completed, a second report will document the model of the saltstone pouring process and results of the study conducted with the model.

The internal heat generation rate, as a function of elapsed time after pouring, of the curing saltstone was determined by direct analysis of the thermocouple data. The response of the thermocouples on the hole centerline was assumed to be due to an adiabatic heatup. This allowed the heat generation rate due exothermic curing reactions to be determined for the first 20 hours after pouring. Most of the energy was released during this period. Heat generation due to secondary reactions can persist for months. The heat generation rate was therefore used to tune the numerical model to the test results, and the excellent agreement between model and experiment is not unexpected. The model is sensitive to the heat generation due to the secondary reactions, and therefore this tuning process is a good way of determining the functional form of the heat generation rate for the saltstone.

Test Description

On February 19, 1991, saltstone was poured into a hole, six feet in diameter and five feet deep, with ten thermocouples distributed axially and radially. Figure 1 is a schematic of the hole and the tree that supported the thermocouples. For the next twenty-six days, the thermocouple temperatures were recorded on a half-hourly basis, as the saltstone cured. The test data is presented in (Aurah, 1991). The initial temperature of the saltstone, measured in the Saltstone Hold Tank, was 25^0 C.

The saltstone vaults consist of cells that are 100 ft. square and 25 ft. deep, and they are covered with a metal roof. The hole was dug in previously poured saltstone in vault #1 cell #2 approximately six to nine months prior to the pilot pour test. The saltstone was poured into cell #2 by the normal process, covering the entire top surface of the cured saltstone, and allowed to run over the lip of the hole and fill it. Since the hole was a low spot in the cured saltstone surface it filled quickly, at least within thirty minutes. Thermocouple temperatures were recorded every thirty minutes, and the hole was filled in the period between two consecutive readings.

Ten thermocouples in the hole were installed on a cross shaped tree made of #4 rebar. Eight of the thermocouples were type J (iron constantan) and two were type K (chromel alumel). The data acquisition system did not correctly compensate for the output of the two type K thermocouples, and they therefore gave false readings. These two thermocouples, (# 7 & 8), are not shown in figure 1. Most of the thermocouples occasionally exhibited unexplained nonphysical behavior. This generally occurred during periods of rapid internal heat generation. Figure 2 shows the temperature data from thermocouples #1 through #6 for the first twenty-five hours following the pour. With the exception of thermocouple #2, all show discontinuous behavior during the period from two to nine hours after the pour. This was the period when there was a large spike in the internal heat generation rate. Though not shown, thermocouples #9 and #10 displayed similar nonphysical behavior.

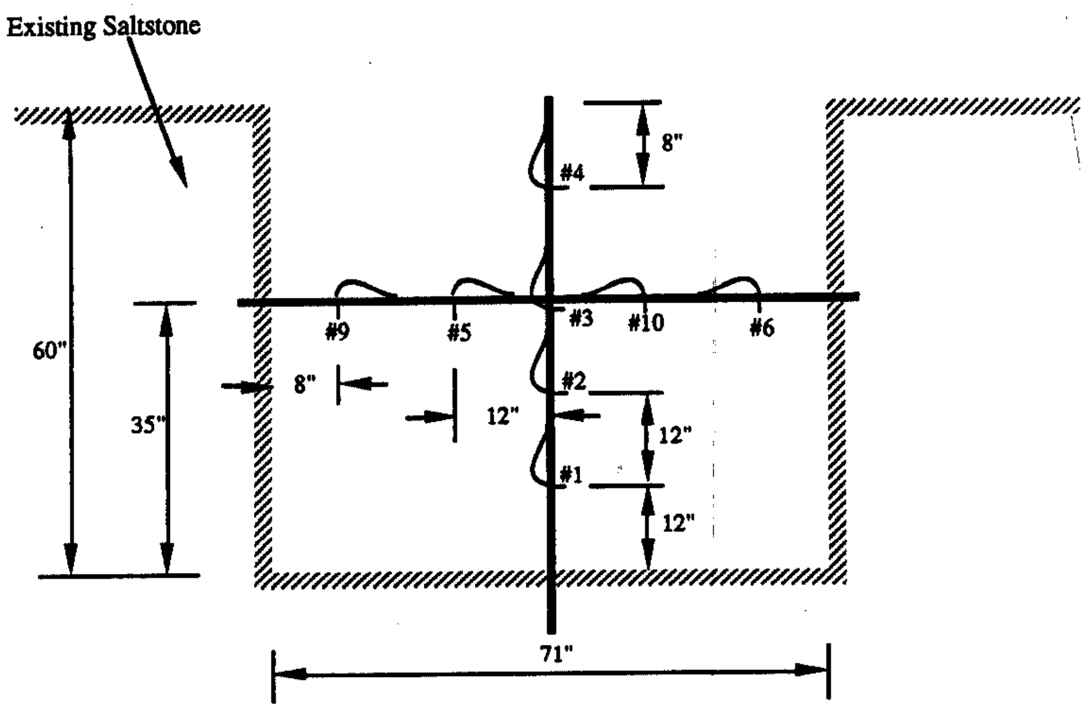

Figure 1: Schematic of the pilot pour hole and thermocouples

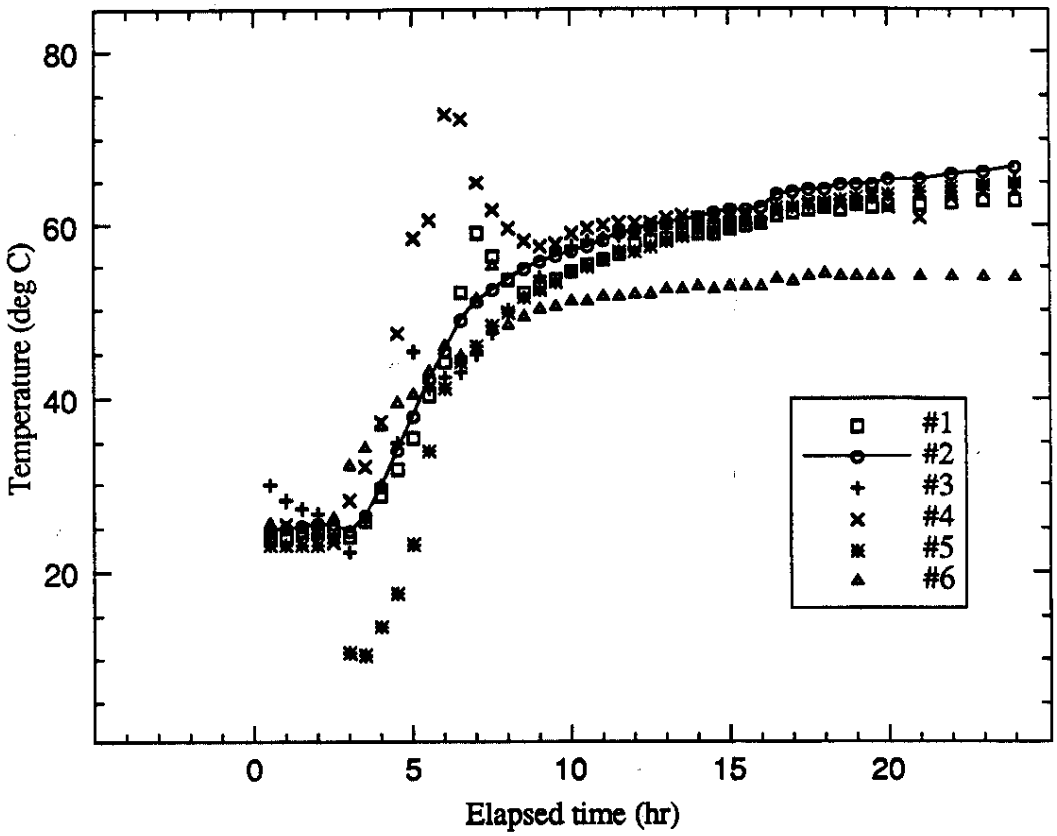

Figure 2: Response of thermocouples #1 through #6 for the first 25 hours

Internal Heat Generation

The time dependence of the internal heat generation, due to curing of the saltstone, was determined directly from the test data. Thermocouple #2 was the one thermocouple that did not exhibit erratic behavior during the first fifty hours after the saltstone was poured into the test hole. Fortunately this thermocouple is on the hole centerline and close to the horizontal midplane. Since the initial temperature distribution in the saltstone is uniform and the internal heat generation due to curing is essentially uniform, the the thermal conduction losses of the saltstone in the vicinity of thermocouple #2 are negligible until the influence of conduction losses at the hole boundaries reach the thermocouple. In the interim, the heat up is adiabatic, and can be used to calculate the internal heat generation rate. One-dimensional transient thermal conduction in cylinders and plates are straightforward problems with well known analytical solutions. The solutions are presented graphically in many Heat Transfer texts, (Chapman, 1974). It takes approximately sixty hours for losses through the bottom of the hole to be sensed at a position two feet above the bottom.

The internal heat generation rate per unit mass is directly proportional to the rate at which the temperature changes in an adiabatic process:

$$q^* = C_p \frac{dT}{dt} \qquad (1)$$

Figure 3 shows the temperature data from thermocouple #2 for the first fifty hours of the test. Also shown is the rate of change of the temperature as a function of time. There is a large spike in the internal heat generation rate between approximately three and nine hours of elapsed time. There is a smaller secondary spike in the internal heat generation rate at approximately sixteen hours. After about twenty-five hours, the internal heat generation rate is lost in the noise of the thermocouple data.

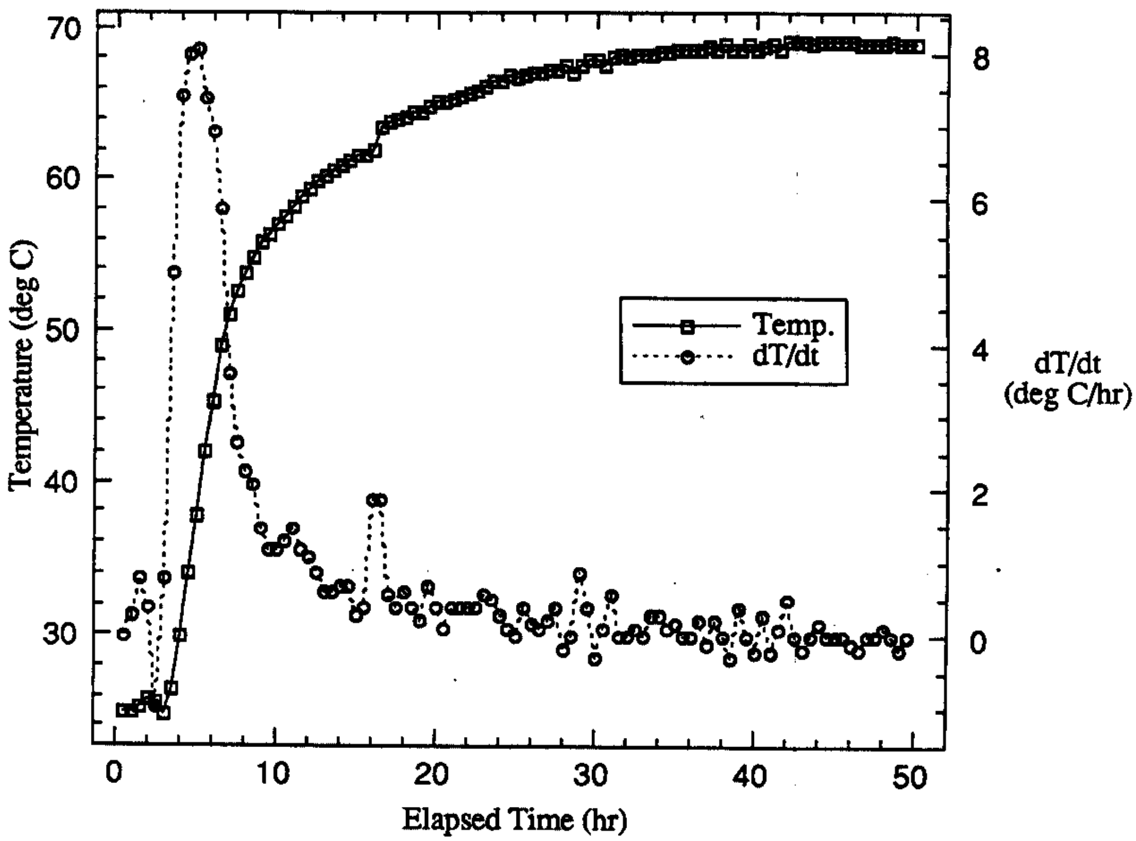

Figure 3: Temperatures and time derivatives of the temperature for thermocouple #2

The two spikes in the heat generation rate are modelled as sine functions, and between the two spikes the heat generation rate is assumed to change linearly with time. Equations (2) through (4) are the expressions for the time rate of change of temperature for thermocouple #2 for the first 17.0 hours. These expressions are shown in figure 4 along with the data from thermocouple #2.

$$\frac{dT}{dt} = 0.0 \rightarrow t \leq 2.5hr. \qquad (2)$$

$$\frac{dT}{dt} = 8.2 * \sin\left(1 - \frac{t-2.5}{5.5}\pi\right) \rightarrow 2.5 \le t \le 7.5hr. \tag{3}$$

$$\frac{dT}{dt} = 2.31 - .23875 * (t - 7.5) \rightarrow 7.5 \le t \le 15.5hr. \tag{4}$$

$$\frac{dT}{dt} = .4 + 1.7 * \sin\left(1 - \frac{t-15.5}{1.5}\pi\right) \rightarrow 15.5 \le t \le 17.0hr. \tag{5}$$

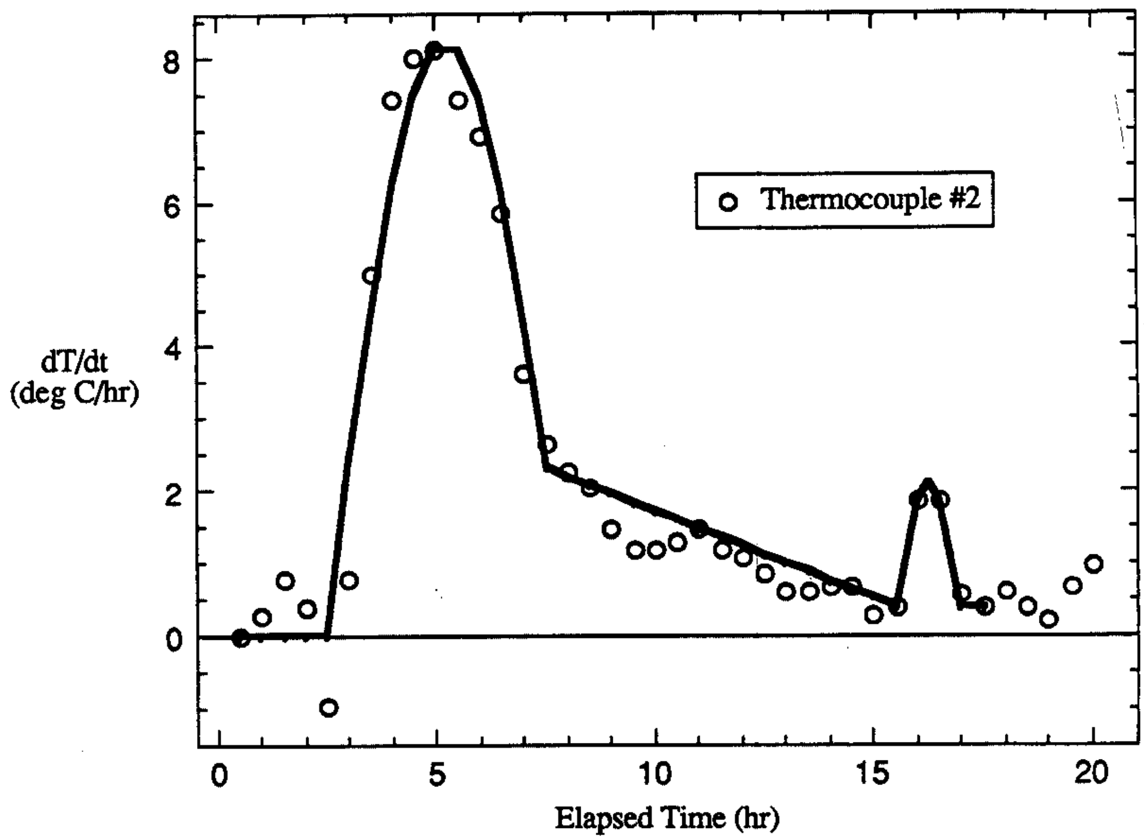

Figure 4: Model of the adiabatic heat up rate and thermocouple #2 data

Equations (2) through (4) were determined directly from data analysis. The time rate of change of temperature data in figure 3 suggests that the internal heat generation drops to zero when 38.0 hours have elapsed, but (Hay, 1991) indicates that secondary exothermic reactions can persist for months. When the model was run with the internal heat generation shown above, the model systematically underperdicted the thermocouple temperatures in the latter stages of the test. The internal heat generation was used as a free parameter to bring the model results and data into agreement. Equations (6) through (10) are the expressions for the time rate of change of temperature for elapsed times after 17.0 hours. Figure 5 is a plot of these expressions. Figure 6 shows the predicted transient temperatures for thermocouple #2 with and without the modified internal heat generation. Also shown is the thermocouple data. While the internal heat generation rate after 45.0 hours is less than 1.5% of the peak rate, it significantly influences the rate at which the saltstone cools down.

$$\frac{dT}{dt} = .3 * e^{-.036484*(t-17.0)} \rightarrow 17.0 \le t \le 45.0hr. \quad (6)$$

$$\frac{dT}{dt} = .10801 - .0006*(t-45.0) \rightarrow 45.0 \le t \le 175.0hr. \quad (7)$$

$$\frac{dT}{dt} = .03 + .012*\sin\left(\frac{t-175.0}{100.0}\pi\right) \rightarrow 175.0 \le t \le 275.0hr. \quad (8)$$

$$\frac{dT}{dt} = .02 + .01*e^{-.065788*(t-275.0)} \rightarrow 275.0 \le t \le 450.0hr. \quad (9)$$

$$\frac{dT}{dt} = .015 + .005*e^{-.065788*(t-450.0)} \rightarrow 450.0hr. \le t \quad (10)$$

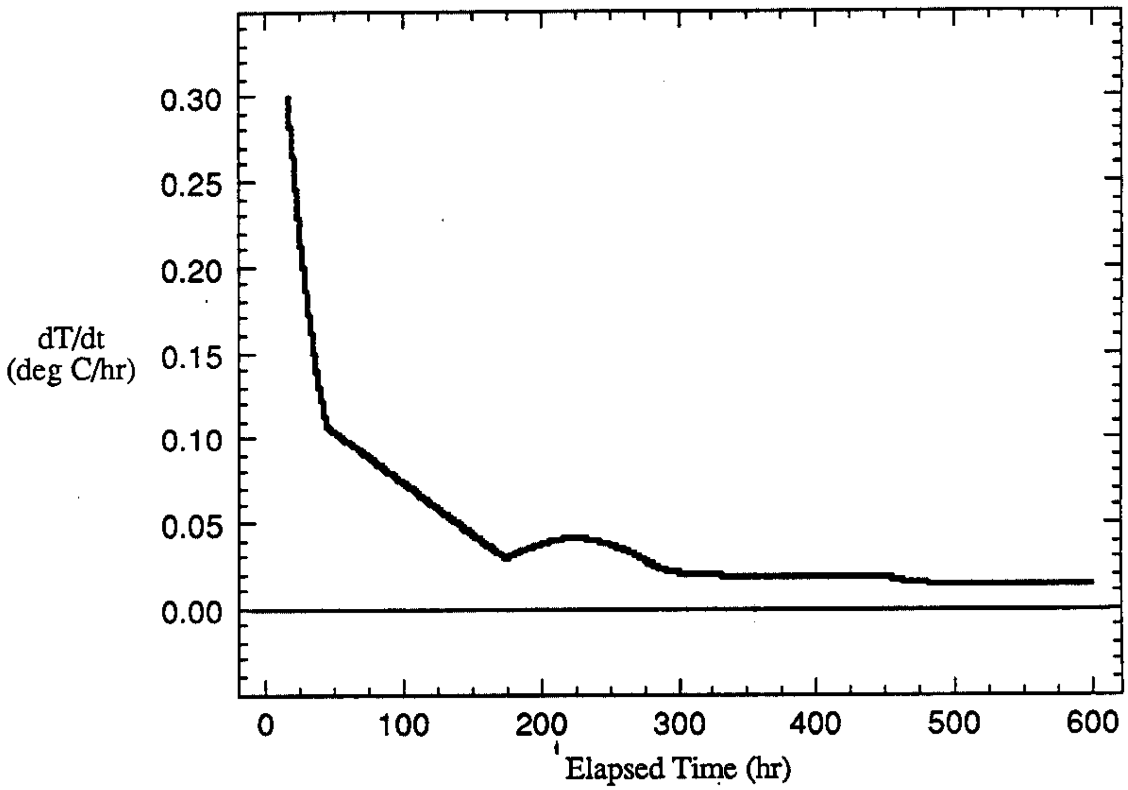

Figure 5: Time rate of change of temperature, after 17.0 hours, for an adiabatic heat up of the saltstone

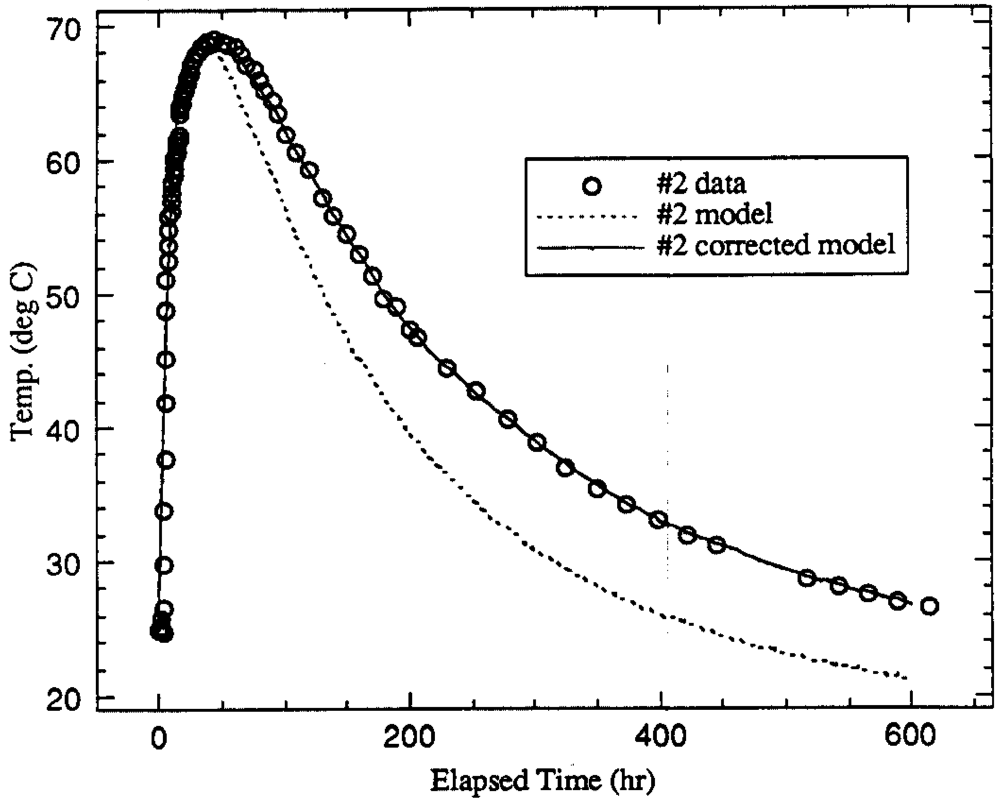

Figure 6: Thermocouple #2 predicted temperatures with and without corrected internal heat generation after 17.0 hours.

Model Description

A two-dimensional cylindrical coordinates transient conduction numerical model of the curing saltstone in the hole was developed. There are no apparent azimuthal variations in the hole geometry or the boundary conditions, so a two-dimensional model, with the hole centerline as an axis of symmetry, is sufficient for this problem. The hole is assumed to be in cured saltstone with infinite extent in the radial and downward directions. The surrounding cured saltstone is modelled as a large cylindrical volume with adiabatic outer and bottom boundaries. The distances from the hole boundaries to the adiabatic boundaries are sufficiently large enough for the boundary temperatures to be negligibly affected by the heat transfer from the curing saltstone in the hole. The adiabatic boundary is 11.4 ft. radially outward from the vertical side of the hole and 14.3 ft. axially downward from the bottom of the hole. Figure 7 is a schematic of the computational domain.

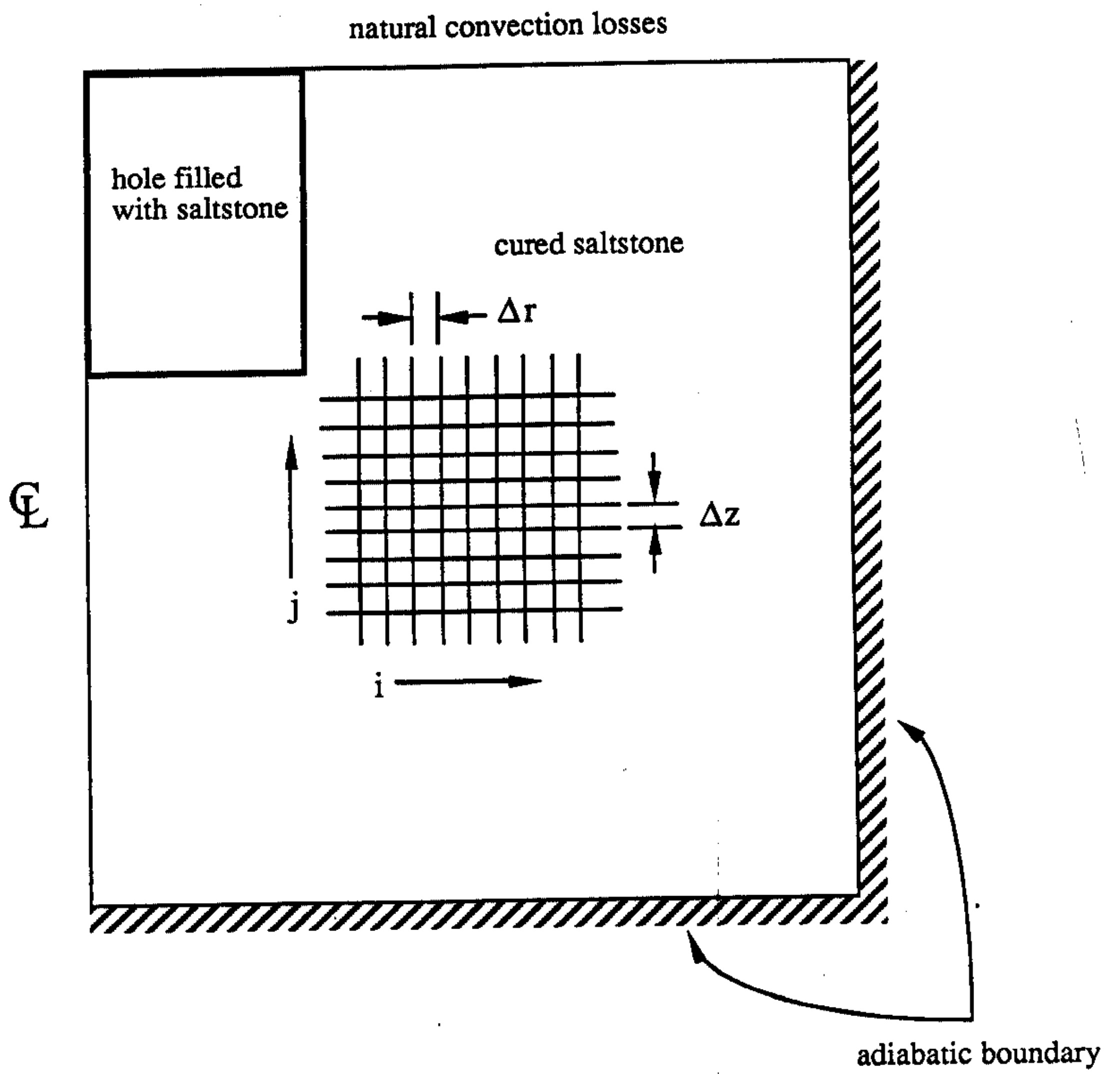

Figure 7: Pilot pour model computational domain

The numerical model is an explicit finite-difference model with a uniform mesh. The finite-difference equations were derived by application of the integral form of the energy equation to nodal control volumes. This insures that the interior and boundary equations are consistent. The computational domain has 32 nodes in the radial direction and 41 in the axial direction. The poured saltstone in the hole is modelled with 77 nodes, 7 radial and 11 axial. A timestep of 15 minutes was used. This allowed the internal heat generation rate, as a function of elapsed time, to be adequately resolved, and it met the stability criterion for the explicit equations. The increased complication of an implicit scheme was therefore not justified.

The cured saltstone served as the primary heat sink for the curing saltstone, and therefore it was important to correctly model the initial temperature distribution in the cured saltstone. Since the hole and the surrounding cured saltstone had been undisturbed for a long time, in excess of six months, I assumed that the temperature distribution was a function of the annual variation of the environmental temperature, and this initial temperature distribution was determined with a numerical model of the cured saltstone. The surfaces exposed to air were assumed to be heated or cooled by natural convection. The mean daily temperatures were assumed to vary sinusoidally between a low on January 15, with a mean temperature of 45^0 F, and a high on July 15, with a mean temperature of 85^0 F. The diurnal variation in air temperature was neglected in this analysis. The model was run for over one year to insure that a periodic solution for the cured saltstone temperature distribution on February 19 was obtained. Figure 8 is a plot of the initial temperature distribution in the cured saltstone.

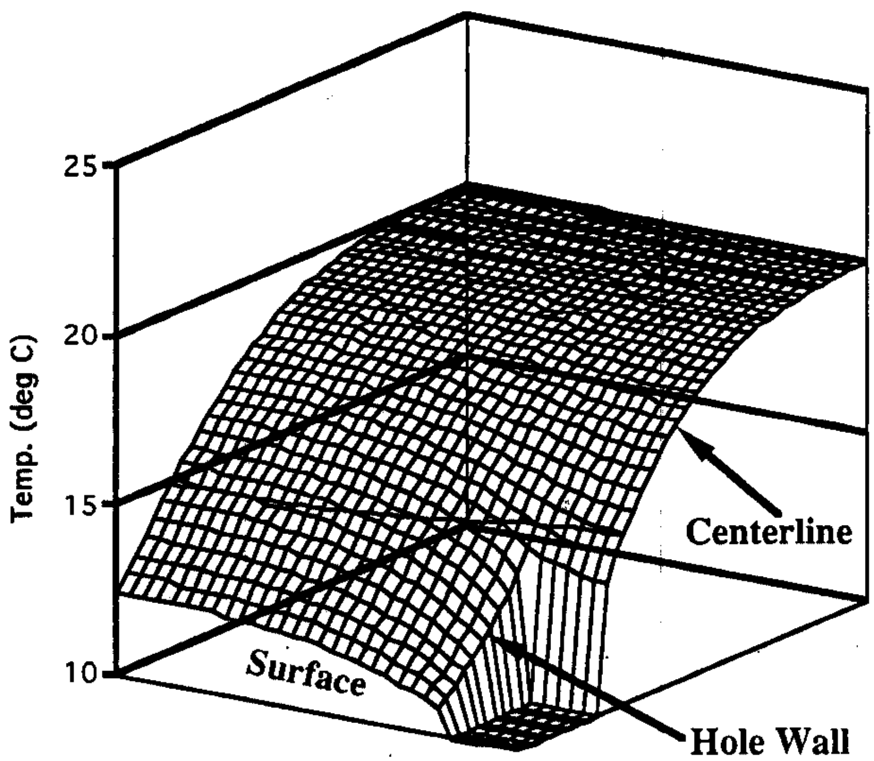

Figure 8: Initial temperature distribution in the cured saltstone

The surface of the poured saltstone and the surrounding cured saltstone was cooled by natural convection of the air in the vault cell. The cell is covered by a metal roof, so the air temperature in the cell is not necessarily the same as the outside air temperature. Figure 9 is a plot of the average daily outside air temperatures for a period commencing five days before the pour and extending beyond the conclusion of data collection for the test. This air temperature data was obtained from the SRTC Environmental Technology Section. The mean temperature for this period is 12.55^0 C. On the day that the saltstone was poured, the mean outside air temperature was 19.7^0 C. The thermocouples in the hole were reading approximately 11.6^0 C for nine hours before the saltstone was poured. The variations in the air temperature in the vault cell apparantly lag behind the outside air temperature variations, and are probably significantly attenuated relative to the outside temperature variations. Over an extended period, the outside air and the cell air should have essentially the same mean temperature. In the model, the air temperature was assumed to be the mean outside air temperature, 12.55^0 C. The natural convection heat transfer coefficient was assumed to have a constant value of 1.0 W/m^2K. This mean value for the heat transfer coefficient was determined by a trial and error procedure. Thermocouple #4 is the thermocouple closest to the surface of the poured saltstone, and therefore it is most influenced by the heat losses from the surface. Values of the heat transfer coefficient between 0.6 and 1.5 W/m^2K were tried, and the predicted transient temperatures for thermocouples #1 and #4 were compared with the data. The predicted results for thermocouple #1 were insensitive to the value of the heat transfer coefficient. With a heat transfer coefficient of 0.6 W/m^2K, the predicted temperatures for thermocouple #4 were systematically higher than the data, and with a heat transfer coefficient of 1.5 W/m^2K, the temperatures were systematically underpredicted. A value of 1.0 W/m^2K was optimum. This is right in the middle of the range of expected values for natural convection from a horizontal surface. The use of mean values for the air temperature and the heat transfer coefficient is justified because convection losses were of secondary importance in this test due to the small surface area of the deep hole, and the environmental conditions are not known well enough to justify a more rigorous treatment.

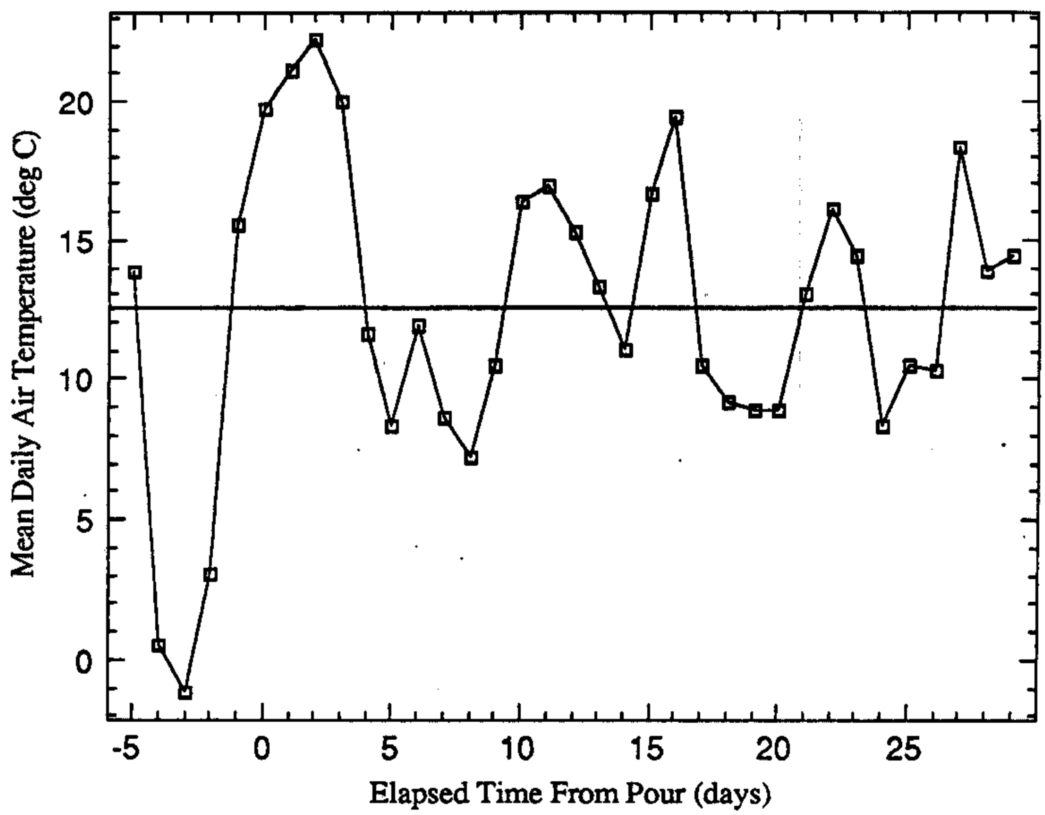

Figure 9: Mean daily air temperatures for the test pour

In this model, the saltstone is assumed to have constant thermodynamic properties. (Langton, 1986) and (Yu, 1990) are the references for the properties. The values for the density, thermal conductivity, and specific heat for the saltstone, that were used in the model, are listed below:

Density (ρ) 1797.63 kg/m^3

Thermal Conductivity (k)	.744 W/m K
Specific Heat (C_p)	1302.06 J/kg K

The development of this code is documented in detail in (Shadday, 1993). The derivation of the finite-difference equations, stability considerations, a code listing, and model results are included in this laboratory notebook. The global conservation of energy by the model was verified, and the coding of the computational section of the code was checked line by line. The confidence level that the code was working as planned is high.

Discussion and Results

The model simulated the transient heat transfer in the poured saltstone and the surrounding cured saltstone for a period of twenty-five days after the saltstone was poured into the hole. The initial temperature of the saltstone was assumed to be 25^0 C. Figures 10 through 12 are surface plots that show the temperature distributions in the poured saltstone and the surroundings. Figure 10 shows the initial temperature distribution. Figure 11 shows the temperature distribution after 50.0 hours have elapsed, and figure 12 shows the temperature distribution at the end of the computation, after 600.0 hours have elapsed.

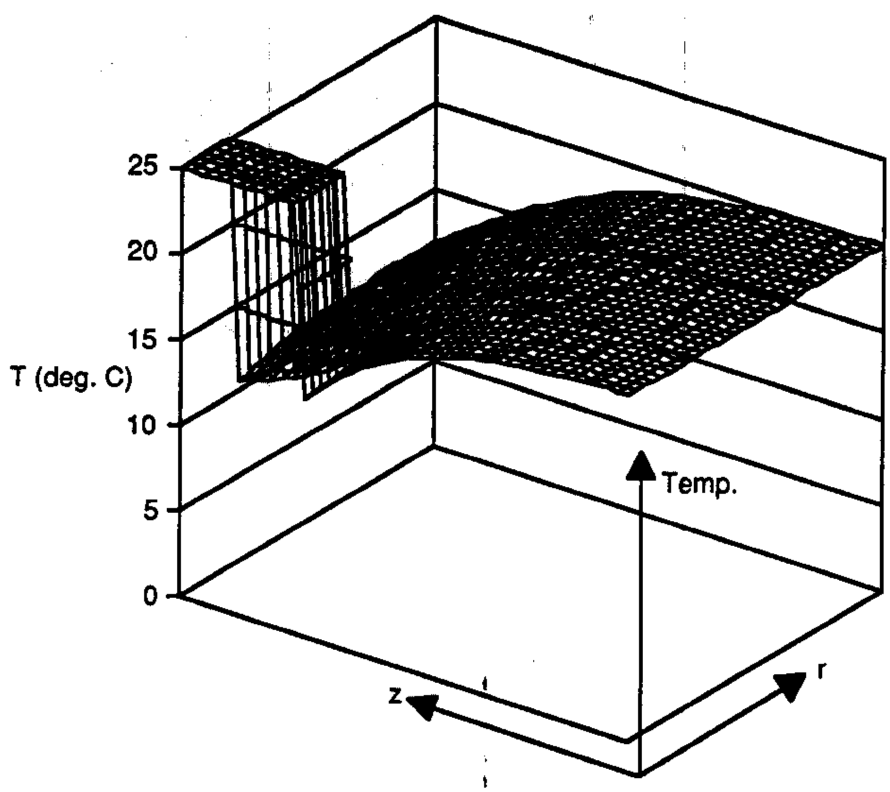

Figure 10: Initial temperature distribution

Figure 11 shows the temperature distribution at the approximate time that the peak temperature occurred. The calculated peak temperature occurred at an elapsed time of 45.0 hours, and it occurred at the intersection of the hole horizontal midplane and the centerline. The peak calculated temperature was 70.1^{0} C. Figure 13 is a plot of the transient peak temperature in the poured saltstone. Note the excellent agreement with the thermocouple #2 data that is shown in figure 3. Thermocouple #2 is approximately 7.5 inches below the point where the peak calculated temperature was predicted to occur.

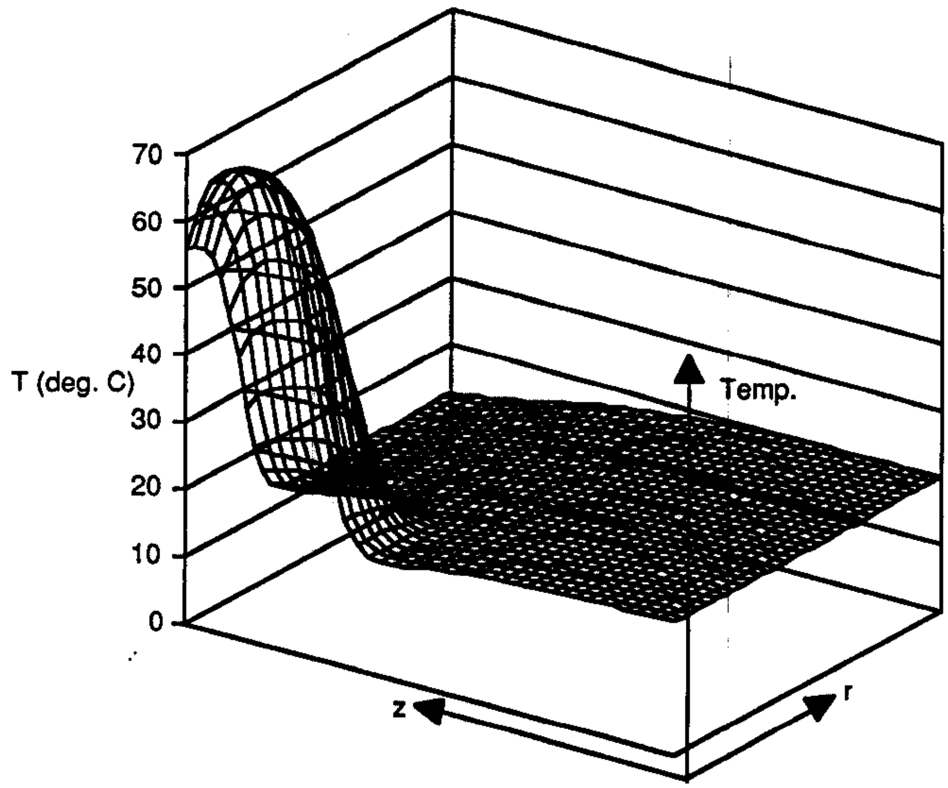

Figure 11: Temperature after 50 hours have elapsed

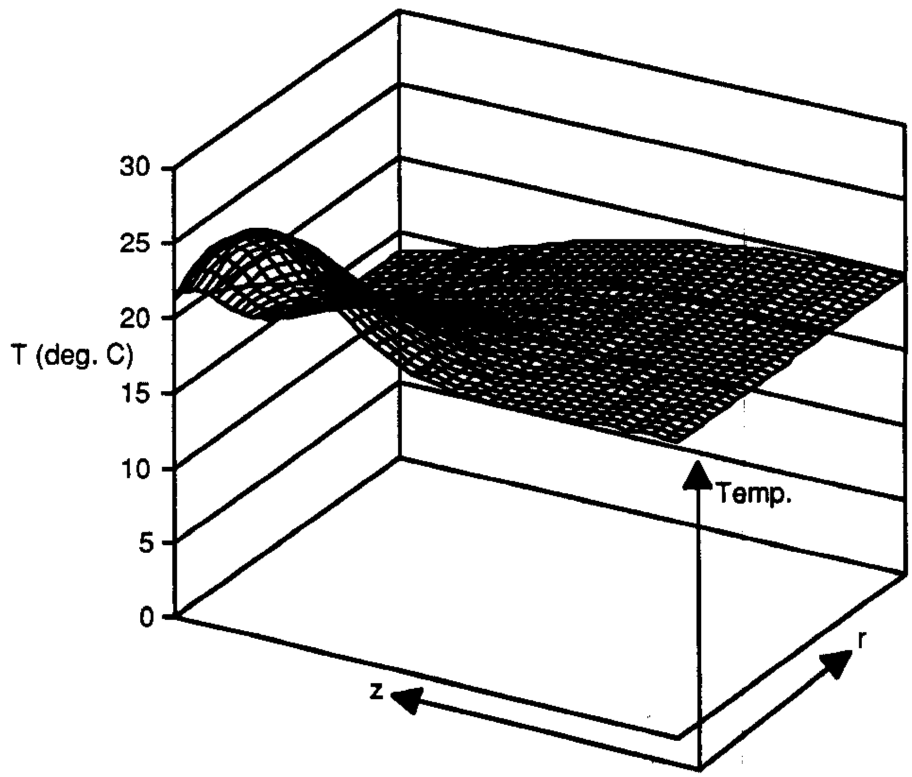

Figure 12: Temperature after 600 hours have elapsed

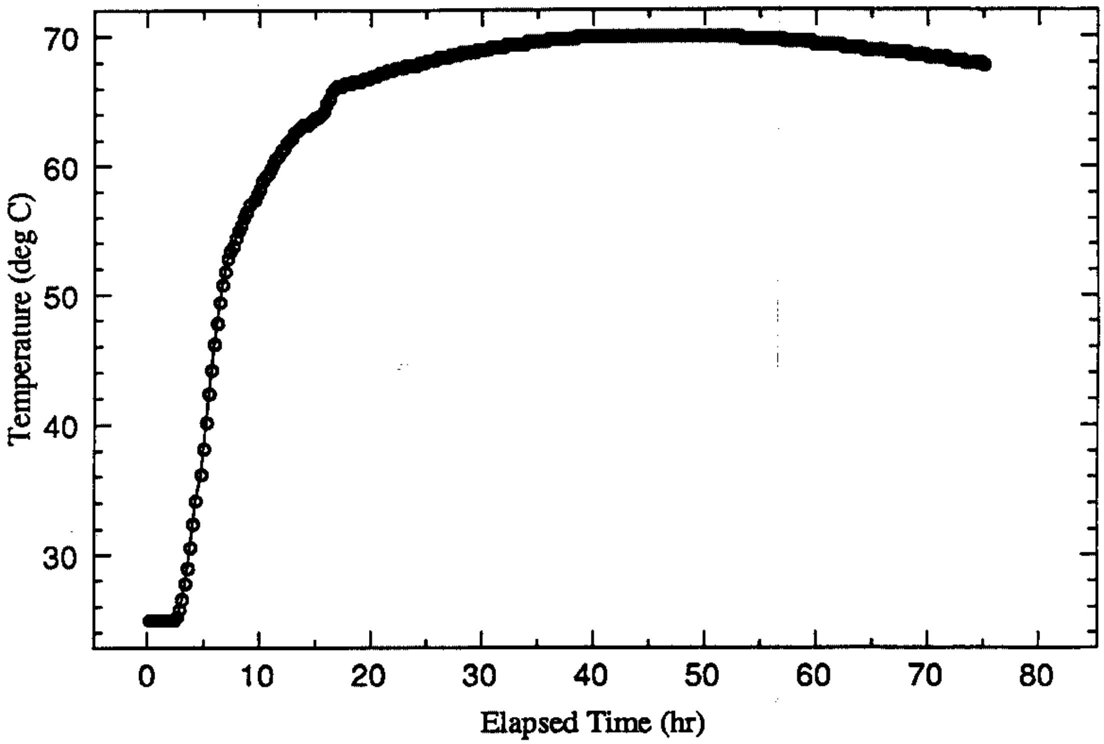

Figure 13: Calculated transient peak temperatures in the saltstone pour

The predicted transient temperatures of thermocouples #1 through #6 are shown in figures 14 through 19. Also shown are the thermocouple data. The agreement between the model and the data is excellent. This excellent agreement is not unexpected, since the data to which the model is being compared was used to develop the functional form of the internal heat generation term. After the initial seventeen hours of the transient, the internal heat generation term was used as a free parameter to fit the model to the thermocouple #2 data.

The predicted behavior, near the time that the temperature peaks, of thermocouples #6 and #9 is not as good as the predicted behaviors of the other thermocouples. Thermocouples #6 and #9 are the two thermocouples closest to the vertical wall of the hole. There is a steep radial temperature gradient in the vicinity of the vertical boundary of the hole, as shown in figure 11, and consequently these two thermocouples were sensitive to errors in radial position. Figure 20 shows the predicted responses of these two thermocouples in the radial position shown in figure 1 and for a radial 2.5 inches closer to the hole wall. Moving the thermocouples further out from the centerline lowers the peak temperature by a little over 2.0^0 C. The discrepancy could also be due to errors in the assumed initial temperature distribution of the surrounding cured saltstone, or a combination of the two.

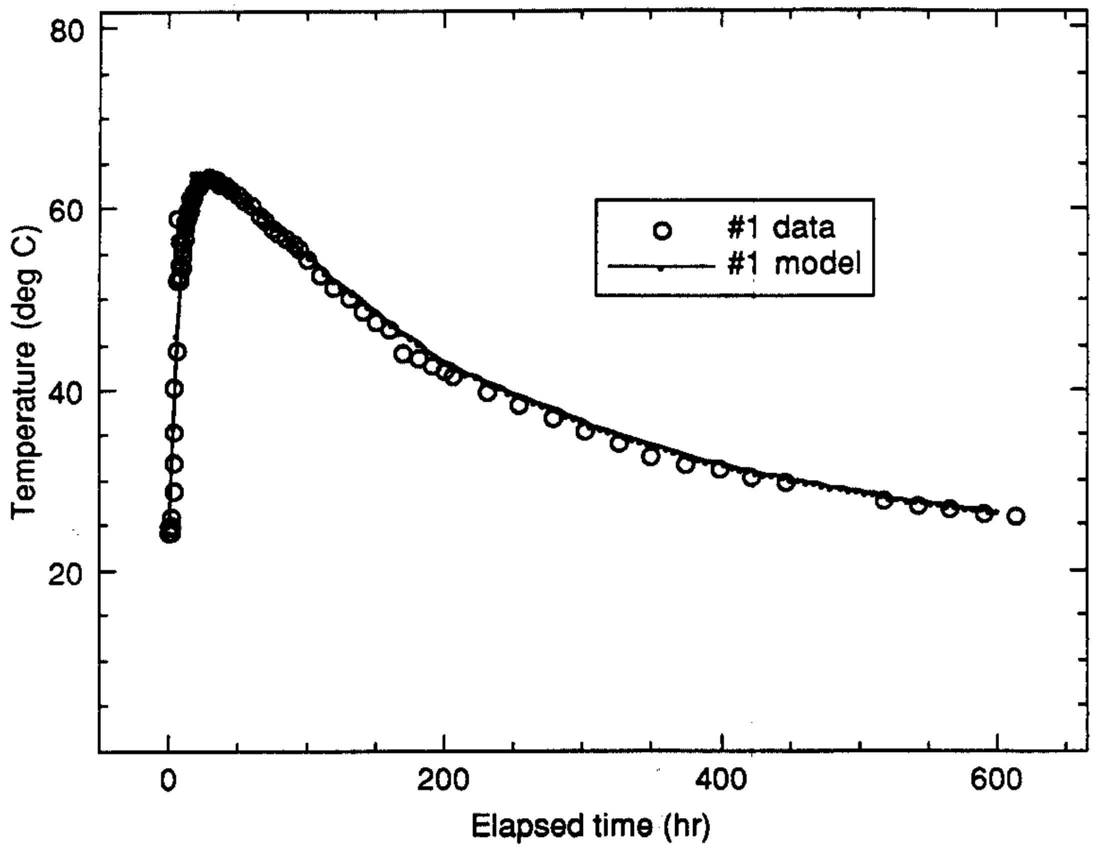

Figure 14: Transient temperature prediction for thermocouple #1 and data

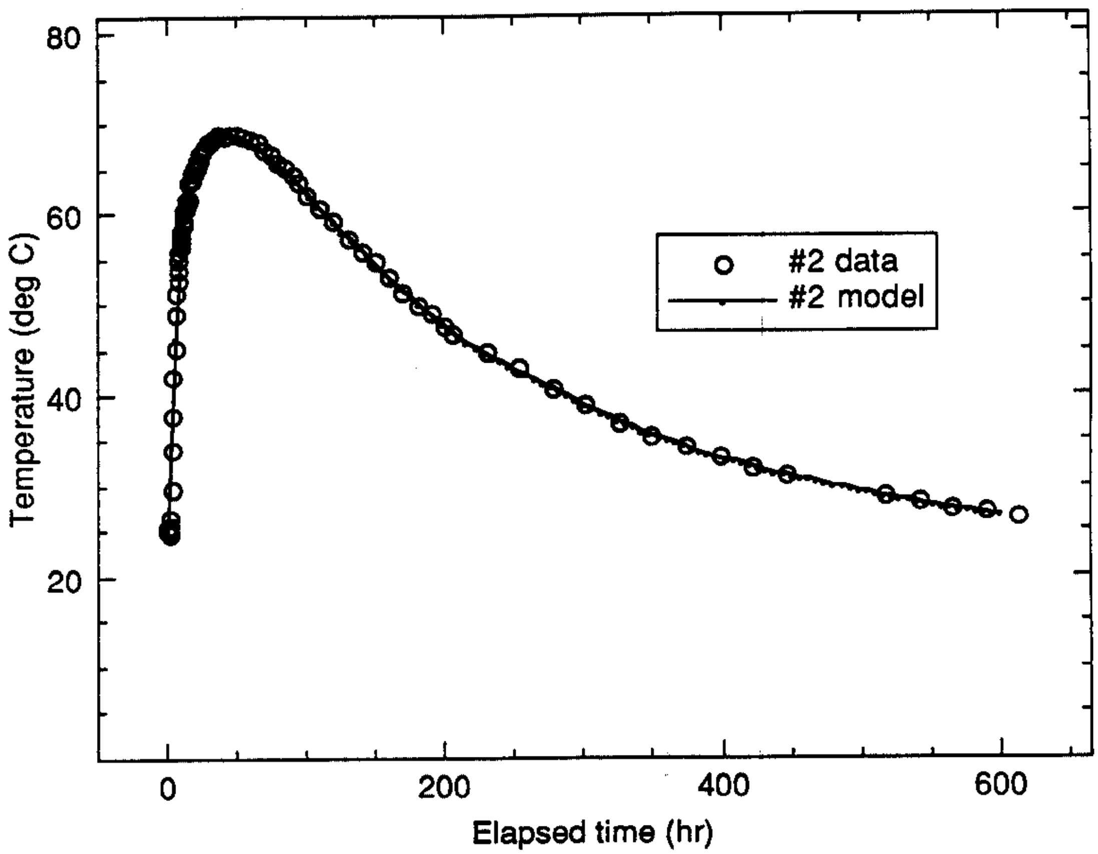

Figure 15: Transient temperature prediction for thermocouple #2 and data

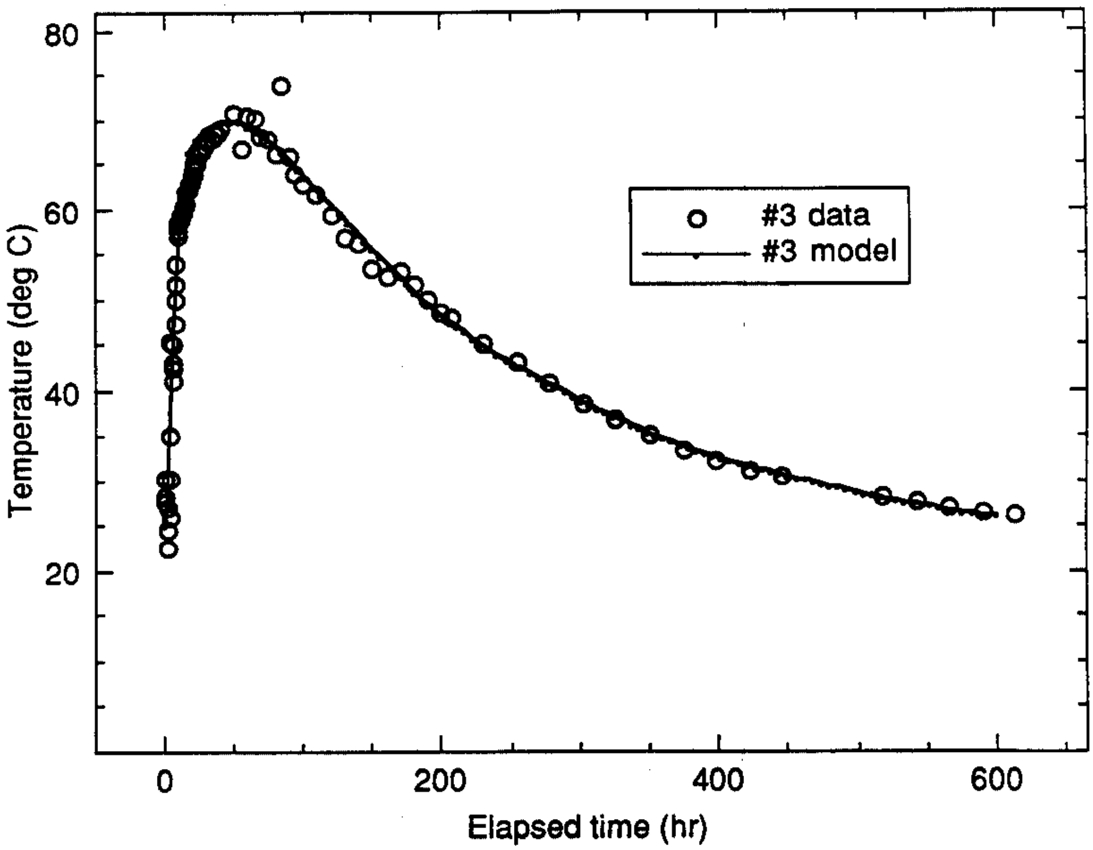

Figure 16: Transient temperature prediction for thermocouple #3 and data

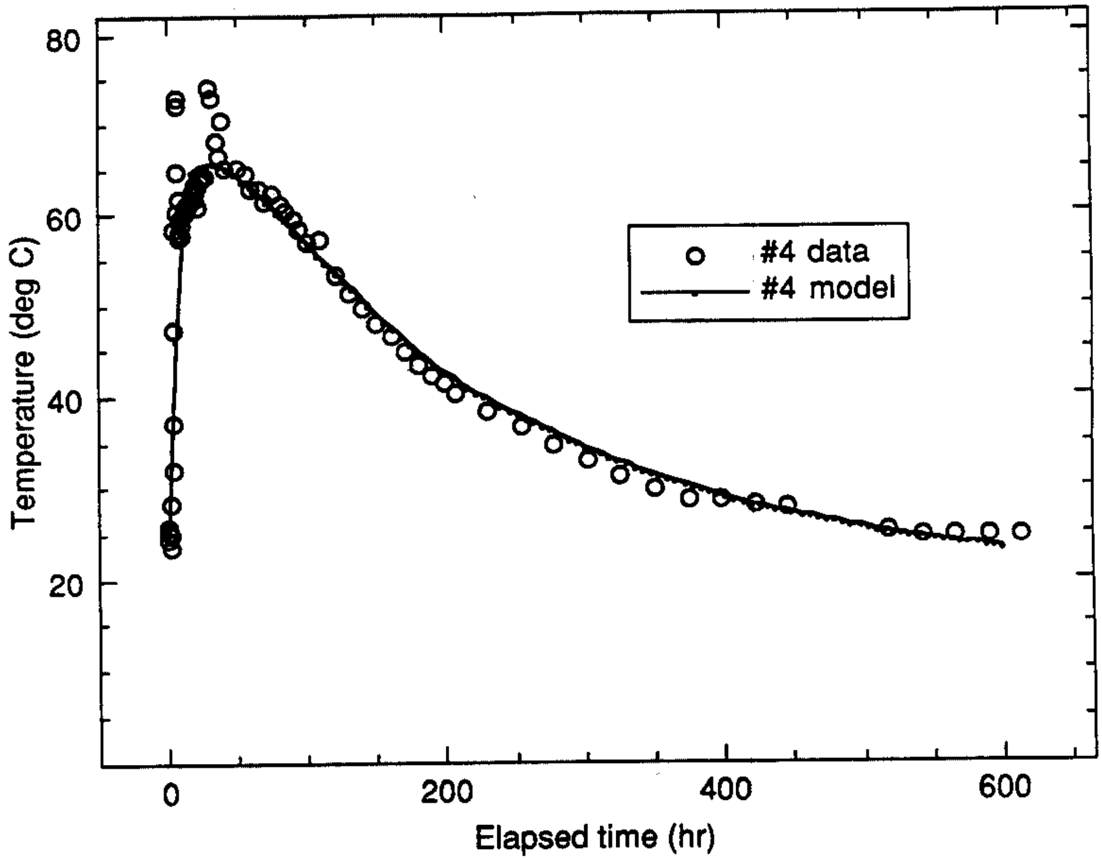

Figure 17: Transient temperature prediction for thermocouple #4 and data

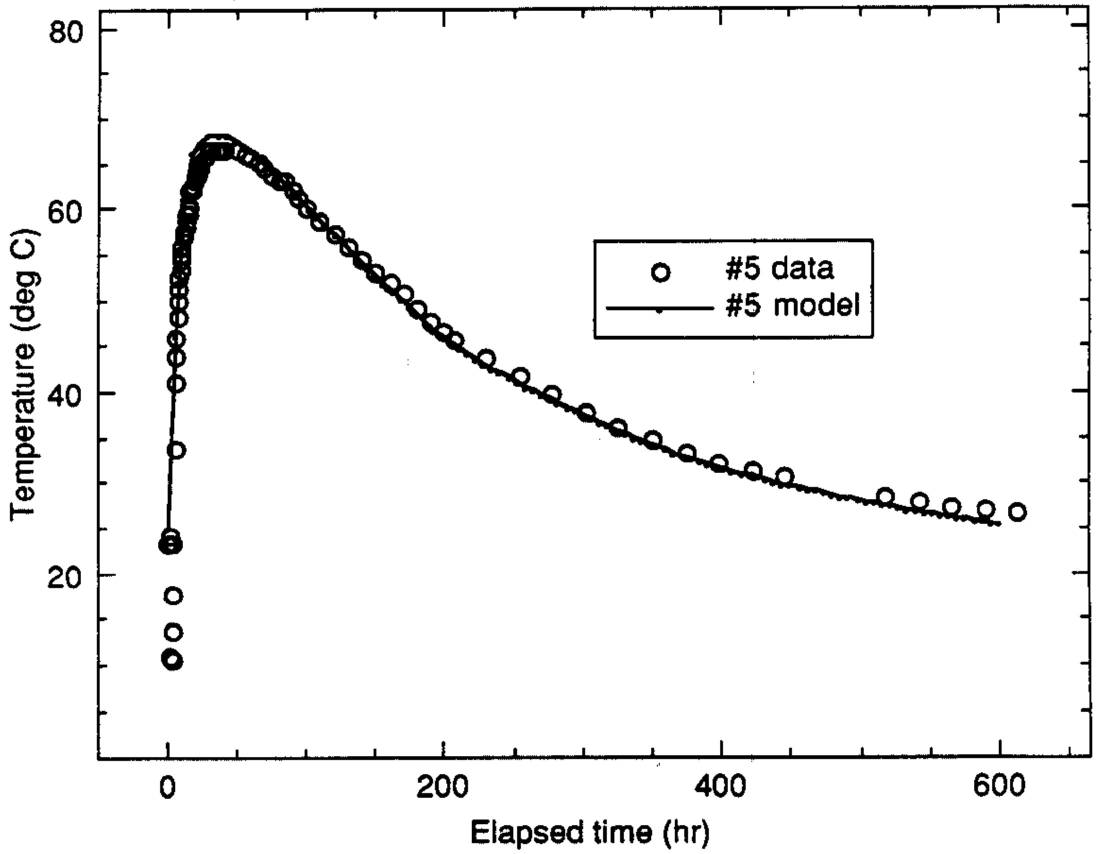

Figure 18: Transient temperature prediction for thermocouple #5 and data

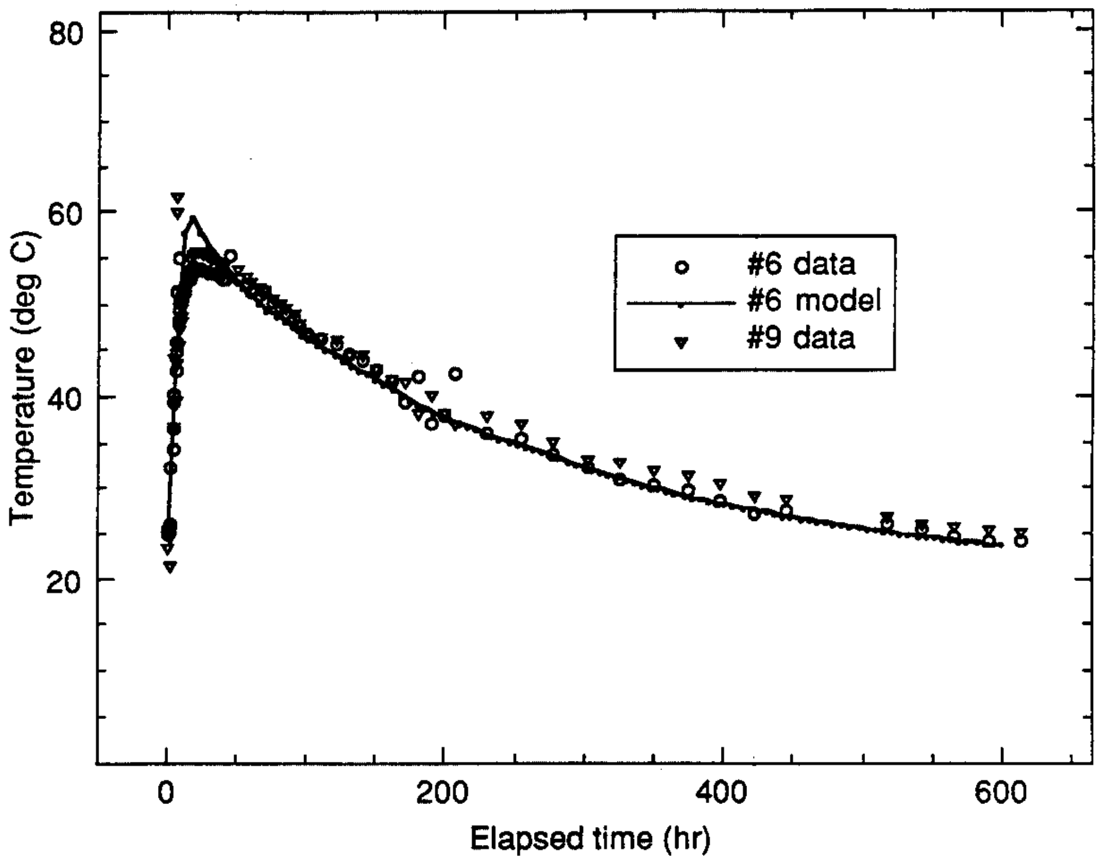

Figure 19: Transient temperature prediction for thermocouple #6 and data

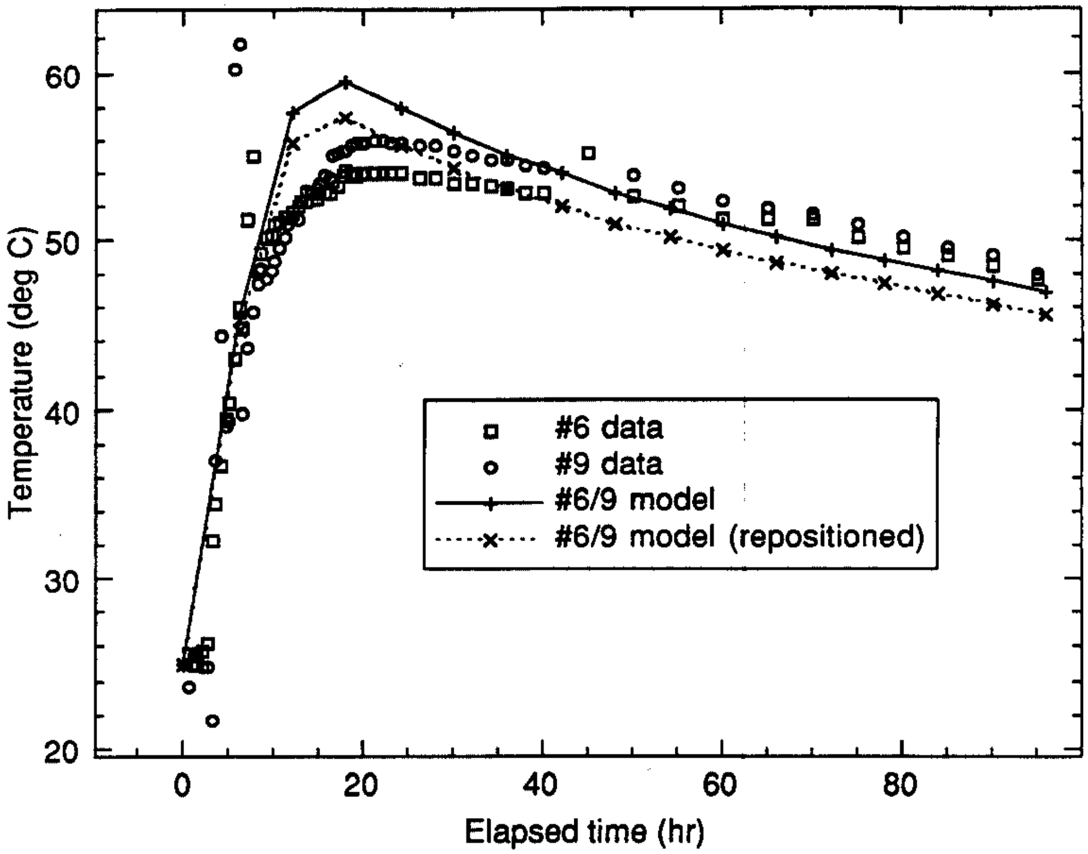

Figure 20: The influence of radial position on the output of thermocouples # 6&9

Conclusions

The most significant contribution of this study is the demonstration that the long term cooling of curing saltstone is strongly influenced by the energy released by secondary exothermic reactions reactions that can persist for months. Though the energy production rate per unit volume, due to secondary reactions, is small, the thermal conductivity of the saltstone is also small. The temperature distribution in cooling and curing saltstone is therefore measurably impacted by small rates of internal heat generation. Since the peak transient temperature of the curing saltstone is expected to be the limiting parameter of the pouring process, secondary exothermic reactions should be important.

The pilot pour test utilized actual low level waste with the same mixture that it is anticipated will be used in the actual storage process. The internal heat generation rate function, equations (2) through (10), was therefore calculated from the best available data, and the function herein presented is the best available. The calorimeter tests conducted at SRTC used a simulated salt solution rather than real liquid waste, (Hay, 1991). Most of the energy released by exothermic reactions occurred during the first twenty hours following the pour, and during this period the assumption of adiabatic heating, near the center of the cylinder of poured saltstone, is very good. The internal heat generation rate function determined in this analysis will be used in a model of the actual pouring process. This model and results will be documented in a second and final technical report that will close out this QA task.

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