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Three-Dimensional Model of Heat Transport During In Situ Vitrification with Melting and Cool Down[1]

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ABSTRACT

A potential technology for permanent remediation of buried wastes is the In Situ Vitrification (ISV) process. This process uses electrical resistance heating to melt waste and contaminated soil in place to produce a durable, glasslike material that encapsulates and immobilizes buried wastes. The magnitude of the resulting electrical resistance heating is sufficient to cause soil melting. As the molten region grows, surface heat losses cause the soil near the surface to re solidify. This paper presents numerical results obtained by considering heat transport and melting when solving the conservation of mass and energy equations using finite element methods. A local heat source is calculated by solving the electric field equation and calculating a Joule Heat source term. The model considered is a three-dimensional model of the electrodes and surrounding soil. Also included in the model is subsidence; where the surface of the melted soil subsides due to the change in density when the soil melts. A power vs. time profile is implemented for typical ISV experiments. The model agrees well with experimental data for melt volume and melt shape.

SUMMARY

This paper presents a thermal analysis performed in support of the Idaho National Engineering Laboratory (INEL) In Situ Vitrification (ISV) treat ability study. The main purpose of this analysis is to determine if ISV equipment[a] with 1.0 meter electrode spacing and power supply of 400 kW is capable of vitrifying soil to a depth of 3.05 m (soil depth), below which is basalt. The analysis was performed using PATRAN[b] and VULCAN[c] computer codes. PATRAN was used to generate the finite element meshes, and VULCAN was used to solve the coupled electric field and heat transport equations. This report also presents a cool down analysis of the ISV process, where the cool down process is simulated for a time of one year. This analysis shows that it would take approximately 8.3 days to melt to a depth of 3.05 m. The cool down analysis shows that the 100°C isotherm reaches a maximum depth of 5.5 m at approximately 115 days. The 100°C isotherm is important to track since it is the temperature where water vapor is generated. The water vapor is capable of transporting melt products through the porous soil.

PROBLEM DESCRIPTION

The region of soil, showing initial and boundary conditions, considered in this analysis is illustrated in Figure 1. The calculation is performed in cartesian coordinate system (x,y,z). One-quarter of a four electrode ISV model[d] is used since symmetry can be assumed for the temperature and electric fields. The electrodes have a 1.07 m spacing and are 0.13 m square. The 0.13 m square electrodes are chosen to have the same cross sectional area as the typical ISV electrodes with a 1.0 m spacing. The assumption is made that there is initially a small square region between the electrodes in which the soil is at its melting temperature. This is done to simulate a graphite starter path that melts very quickly with the electrical current applied. The heated graphite quickly heats soil to its melting point. After the soil is melted, the electrical conductivity is high enough to generate heat in the soil (Eq 3), and maintain electrical connectivity. The initial melt zone extending between the electrodes, is 5-cm thick, and is covered with 5-cm of soil. The remainder of the soil is initially at ambient temperature. Heat energy is lost at the ground surface to the air by radiation. The other five surfaces of the region are assumed to be adiabatic since the external surfaces are far from the heat source and the interior surfaces have no net heat flux by symmetry.

The two electric field equations, the heat transport equation, and the mass conservation equation (used to calculate subsidence) are solved during the heatup. During the cool down, the mesh is fixed and only the heat conduction equation is solved, with the radiant sink temperature (hood temperature) reduced from 500K to 283K. The hood is used to vacuum gases

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produced in the melted soil and then process the gases by filtering hazardous particles out. To start the simulation, an initial voltage of 220 V is applied to the top of the electrode. Two electric fields need to be solved. For the first electric field, a positive voltage is applied to electrodes one and two (electrode number one is shown in Figure 1) and a negative voltage is applied to electrodes three and four. For the second electric field, a positive voltage is applied to electrodes two and three and a negative voltage is applied to electrodes one and four. The electrodes in the preceding example are numbered in a clockwise fashion. For the first electric field a voltage boundary condition of zero is applied on one of the interior faces of the model, while the other five surfaces are zero electric field ($\partial\phi_1/\partial n=0$). The same boundary conditions are applied for the second electric field except the zero voltage boundary condition is applied to the other interior face. The finite element meshes used for the heatup and cool down are shown in Figure 2 with fine grading around the electrode.

The governing equation to solve the electric potentials (ϕ_1 and ϕ_2) is given by

$$\frac{\partial}{\partial x}\left(k_\phi(T)\frac{\partial\phi_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_\phi(T)\frac{\partial\phi_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_\phi(T)\frac{\partial\phi_i}{\partial z}\right)=0,\quad i=1,2 \tag{1}$$

where $\phi_1(x,y,z)$ is the first electric potential, $\phi_2(x,y,z)$ is the second electric potential, k_ϕ is the electrical conductivity and T is the temperature. The governing equation of heat conduction is given by

$$\rho c_p\frac{\partial T}{\partial t}-\frac{\partial}{\partial x}\left(k(T)\frac{\partial T}{\partial x}\right)-\frac{\partial}{\partial y}\left(k(T)\frac{\partial T}{\partial y}\right)-\frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right)=Q(T) \tag{2}$$

where T(x,y,z,t) is the temperature, t is the time, ρ is the density, c_p is the specific heat, k is the thermal conductivity and Q is the electrical heat source given by

$$Q(T)=\frac{k_\phi(T)}{2}\left\{\left[\left(\frac{\partial\phi_1}{\partial x}\right)^2+\left(\frac{\partial\phi_1}{\partial y}\right)^2+\left(\frac{\partial\phi_1}{\partial z}\right)^2\right]+\left[\left(\frac{\partial\phi_2}{\partial x}\right)^2+\left(\frac{\partial\phi_2}{\partial y}\right)^2+\left(\frac{\partial\phi_2}{\partial z}\right)^2\right]\right\} \tag{3}$$

Mass is conserved in each column of nodes by calculating the change in volume of each element due to the change in density. Latent heat of fusion is included in the model by simply requiring additional heat to be added at the melt temperature in order to melt the soil. The model did not allow for the soil to vaporize.

The simulation starts with an initial power of 10 kW and follows a ramp up to 100 kW at a time of 28,800 seconds (0.33 days) as is shown in Figure 3. Only 100 kW is used since we are using a 1/4 model and the normal operating power is 400 kW. Also shown in Figure 3 is the power computed by VULCAN. In order to control the power input, a varying voltage boundary condition at the top of the electrode was implemented and maintained by

$$\phi_{(1,2)_i}=\phi_{(1,2)_{i-1}}\sqrt{\frac{P_d}{P_{i-1}}} \tag{4}$$

where i is the current time step, Pd is the desired power, and P_{i-1} is the power at the previous time step given by

$$P_{i-1}=\frac{\sum_{j=1}^{nelm}Q_{j,i-1}(T)Vol_j}{\sum_{j=1}^{nelm}Vol_j} \tag{5}$$

where "nelm" is the total number of elements, j is the element number, and Vol is the jth element volume.

This model also includes the subsidence of the soil due to the loss of porosity during melting. A density vs. temperature curve[e] is used to calculate the change in density with temperature. The model takes a column of nodes in the vertical direction and adjusts the position of the nodes in order to conserve mass.

Also included in this model are moving electrodes. The material properties of the electrodes are adjusted so that they have the properties of electrodes above the melting point of soil, and possesses the properties of soil below the melting point of soil. This abrupt change in conductivity made the code take smaller time steps but ended up being more realistic. The analysis required the following soil properties [e][f]: thermal conductivity, specific heat, density, electrical conductivity, and latent heat of fusion.

Soil Properties

density (ρ) = 2000 kg/m^3
melting temperature = 1473 K
latent heat of fusion = 4.4e+05 J/kg

Temperature (K)	c_p (J/kg-K)	k (W/m-K)	k_ϕ (1/Ohm-m)
0.0	1125.	0.20e-0	0.10e-2
673.	915.	0.23e+0	0.10e-2
1073.	2699.	0.45e+0	0.16e-1
1428.	1370.	0.85e+1	0.84e+0
1773.	1337.	0.18e+2	0.46e+1
2173.	1337.	0.50e+2	0.16e+2
2573.	1337.	0.80e+2	0.38e+2
5000.	1337.	0.80e+2	0.72e+2

Electrode Properties

density (ρ) = 7000 kg/m^3

Temperature (K)	c_p (J/kg-K)	k (W/m-K)	k_ϕ (1/Ohm-m)
0.0	1125.	0.20e-0	0.10e-2
673.	915.	0.23e+0	0.10e-2
1073.	2699.	0.45e+0	0.16e-1
1473.	1370.	0.85e+1	0.84e+0
1500.	400.	0.70e+2	0.10e+6
2173.	400.	0.70e+2	0.10e+6
2573.	400.	0.70e+2	0.10e+6
5000.	400.	0.70e+2	0.10e+6

RESULTS

The results of the thermal analysis are shown in Figures 4 through 13. Figure 4 shows the temperature contour plot at 722,000 seconds (8.3 days). The power was turned off at this time since the soil had melted all the way to the basalt layer, which is at a depth of 3.05 m. The melting temperature of the soil is taken at 1473K. The bottom three elements in the model are basalt and are slightly larger. The ground surface is slightly hotter than the starting temperature of 283K because of the insulating effect of the off-gas hood, which is assumed to be at 500K. Reference [a] reports that the average temperature in the hood is 573K, thus the 500K radiant sink temperature permits more heat loss. Figure 4 also shows the subsidence of the soil in the melted region. The surface is not exactly smooth since the nodes are adjusted in height only due to the conservation of mass in each node column in the vertical direction. The maximum temperature is at 1982 K at the center of the melt.

Figure 5 shows the maximum temperature in the melt vs. time. The maximum temperature levels off by about 1950K and rises to 1980K between 100,000 seconds and when the power is turned off at 722,000 seconds (8.3 days). The maximum temperature at the end of one year is 350K. The "knee" in the cooling curve between 10^6 and 10^7 seconds is due to the larger specific heat value around 1000K. Figure 6 shows a phase 1 voltage contour plot with a cutaway view of the electrode at 722,000 seconds (8.3 days). The phase 2 voltage would be exactly the same except the gray face would be on the left front face instead of the right front face. The large voltage drop between the electrode and the face with zero potential is the cause of the heat generation, Q, as given by Eq 3. Figure 7 shows the voltage boundary condition applied at the top of the electrode vs. time. The voltage starts out at 220V and ramps up quickly to meet the necessary power requirements shown in Figure 3. As the melt increases the total resistance decreases, which makes the voltage drop for a given power as is shown in Figure 7.

Volume of melted soil for 1/4 of the melt is plotted vs. time in Figure 8. This is the total volume of soil above the melting temperature of soil. The melt volume reaches a maximum of 5.2 m^3 (20.8 m^3 for the entire melt). The melt volume continued to grow for 20,000 seconds (0.23 days) after the power was shut off. This is due to the thermal energy stored in the hot soil, which conducted downward and outward, melting more soil before enough heat was lost to stop the melt from growing. Molten soil was present for about 200,000 seconds (2.3 days) after the power was turned off. Figure 9 shows the melt depth in the center of the melt vs. time. The melt reached a depth of 3.1 m which is 0.05 m into the basalt. When comparing results with the experiment in report [a] at a time of 70 hours, 7.7e+10 J were put into the soil for the experiment and melted 17,430 kg, whereas this simulation put in 10.0e+10 J and melted 14,140 kg. The difference is because the density used in this analysis was 2,000 kg/m^3, and in reality it is about 1600 kg/m^3. This was done since a higher density would take longer to vitrify the soil. Higher density was conservative since we wanted to make sure the currently available equipment could vitrify the described soil and geometry.

Figure 10 shows the horizontal melt position measured from the center of the melt; the maximum horizontal melt position was at a depth of 1.94 m. Figure 10 shows that it takes about 340,000 seconds (3.9 days) to reach a depth of 1.94 m and then grows outward to a melt position of 1.8 m when the power is turned off. Figure 11 shows the 100°C isotherm depth position at the center of the melt as it varies with time. The 100°C isotherm reaches a maximum depth of 5.5 m between 5 and 10 million seconds (57-115 days) after the process started. Figure 12 shows the 100°C isotherm horizontal position at a depth of 1.94 m. The 100°C isotherm reaches a maximum position of 3.75 m measured from the center of the melt at an earlier time of about 5.0e+06 seconds (57 days). Finally, Figure 13 shows an isotherm plot of the temperatures with the cool down mesh when the 100°C isotherm is at its maximum position at a time of 6.6e+06 seconds. The cool down mesh is 14.5 x 14.5 14.5 m.

The model contained 1694 nodes and 1300 (8 noded) hexagonal elements while heating up. The cool down model used 4864 nodes and 4050 elements. CPU timed involved to solve the problem was 3.5 CPU hours for the heatup portion, and 3.0 CPU hours for the cool down model. The cool down model was shorter since only the energy equation was solved. A DECstation 5000 was used during the simulation. Time stepping was controlled by adjusting the time step so as not to allow any node to change more than 100K during any time step. Higher values were tried, but the value of 100 was time step converged.

CONCLUSIONS

Heat transport and melting have been simulated to a time of 722,000 seconds (8.3 days) using the VULCAN computer code with typical ISV equipment. The ISV process was simulated by calculating two electric fields and using a 1/4 model due to symmetry. This process continued until the melted soil reached a depth of 3.05 m, then a cool down was simulated after the power was turned off for a period of 31.5e+06 seconds (one year). Subsidence was also included in the model. Melt volume, electrode voltage, and maximum melt temperature were tracked during the simulation. Melt depth and width, along with 100°C isotherm depth and width were also followed during this analysis. The final conclusions are that the ISV equipment with a 1.0 m electrode spacing and power supply of 400 kW can melt 3.05 m of soil after 722,000 seconds (8.3 days), and that the 100°C isotherm reaches a maximum depth of 5.5 m after 10.0e+06 seconds (115 days).

REFERENCES

a. R. A. Callow et al., "In Situ Vitrification Application to Buried Waste: Final Report of Intermediate Field Tests at Idaho National Engineering Laboratory", EG&G Informal Report EGG-WTD-9807, August 1991

b. PDA Engineering, "PATRAN Plus User Manual", version 2.3, PDA Engineering, Costa Mesa California, July 1988

c. P. E. Murray, and M. O. Fryer, "Simulation of Heat Conduction and Electric Fields During In Situ Vitrification of Soil: Method Design and Verification", EG&G Informal Report EGG-WM-9045, 1990, Idaho National Engineering Laboratory

d. M. O. Fryer, G. L. Hawkes, P. E. Murray, "Parametric Melting Studies for In Situ Vitrification", EG&G Informal Report EGG-WM-9872, February 1991

e. J. L. Buelt et al., "In Situ Vitrification of Transuranic Waste: An Updated Systems Evaluation and Applications Assessment", PNL-4800 Supplement 1, March 1987
f. J. B. Henderson, H. Groot, "Thermophysical Properties of Soils and Basalt Rock, A Report to EG&G Idaho, Inc.", TPRL 1144, Thermophysical Properties Research Laboratory, School of Mechanical Engineering, Purdue University, April 1992

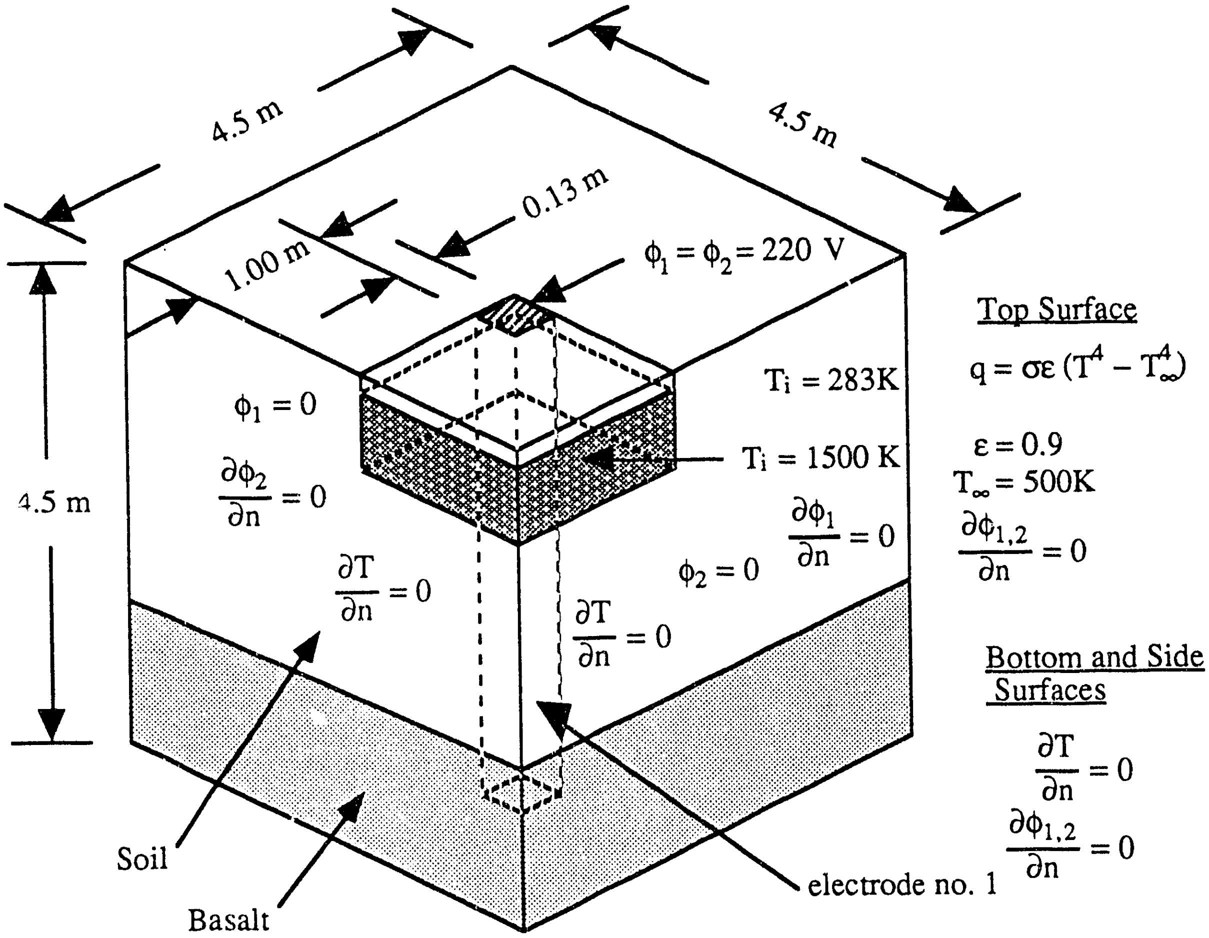

Figure 1. One-quarter ISV model description.

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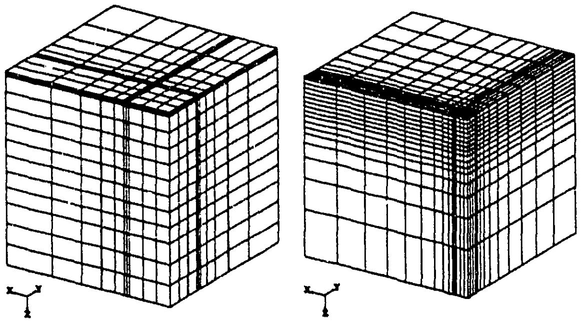

Figure 2. Finite element meshes for heatup and cooldown

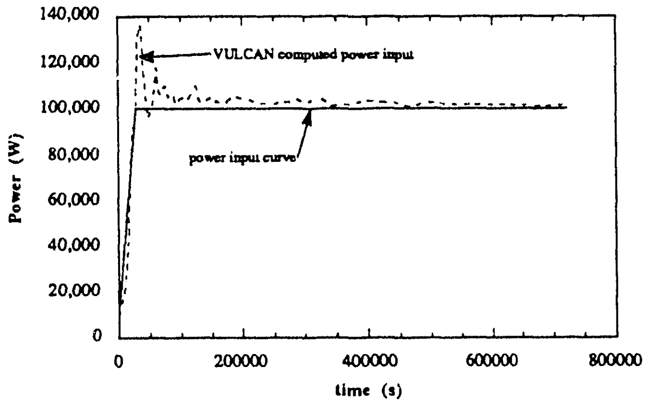

Figure 3. VULCAN computed power vs. power input curve.

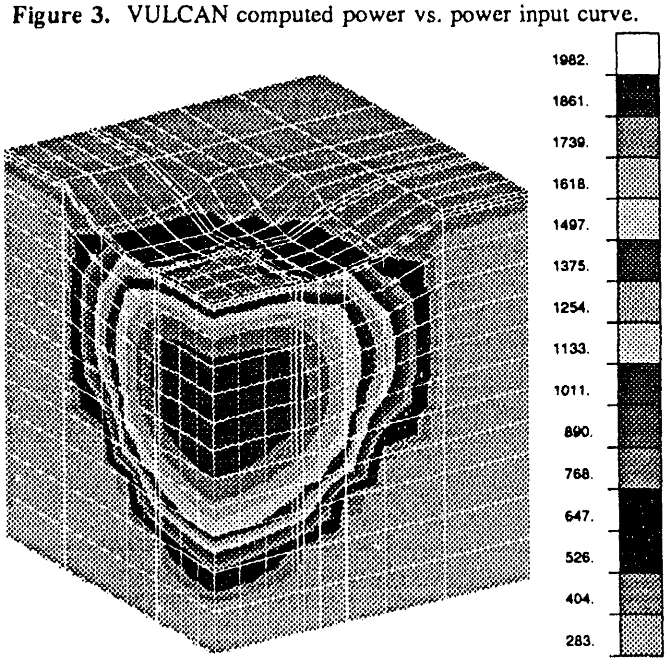

Figure 4. Temperature when power is turned off.

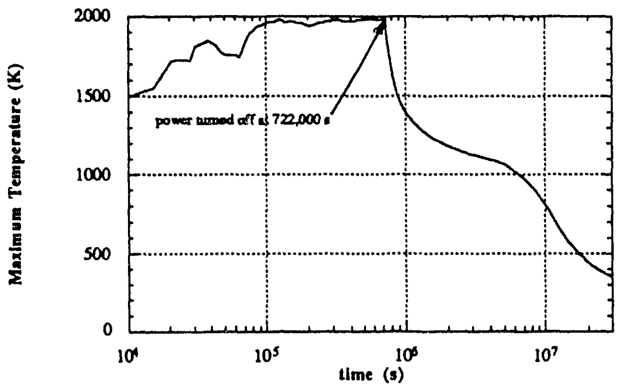

Figure 5. Maximum temperature in melt.

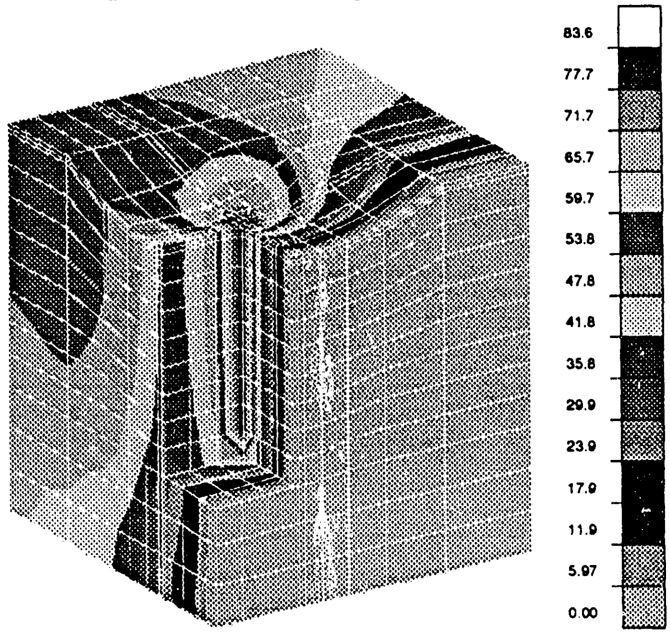

Figure 6. Phase 1 Voltage at 722,000 seconds.

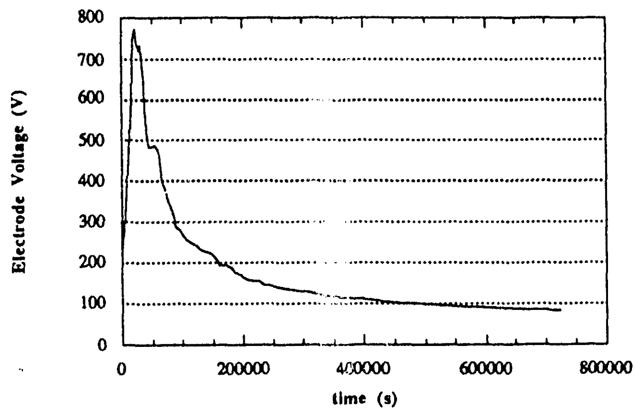

Figure 7. Electrode voltage vs. time.

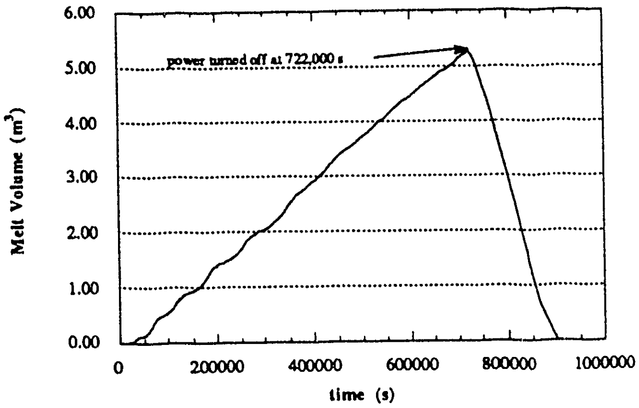

Figure 8. Melt volume vs. time

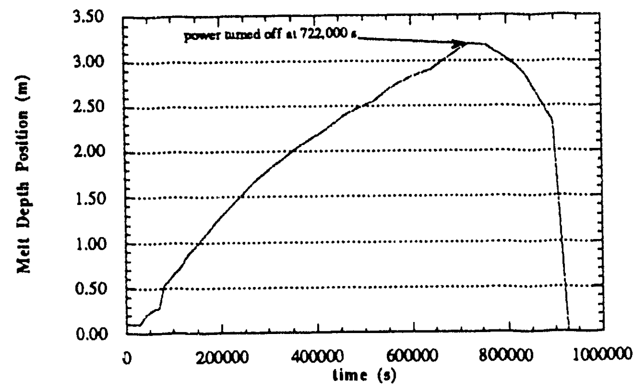

Figure 9. Melt depth position in center of melt vs. time.

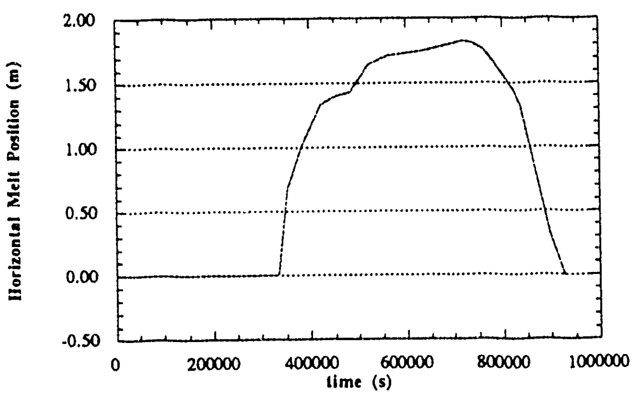

Figure 10. Horizontal melt position at 1.94 m depth vs time.

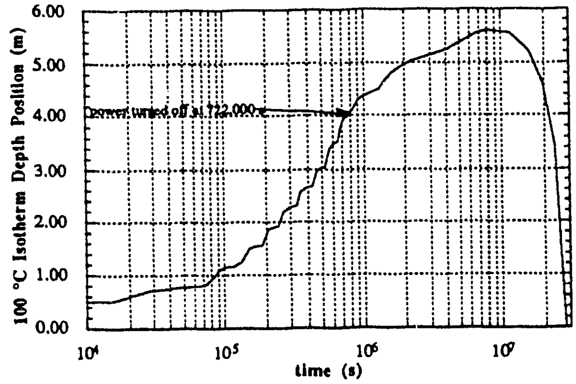

Figure 11. 100°C isotherm depth in center of melt vs. time.

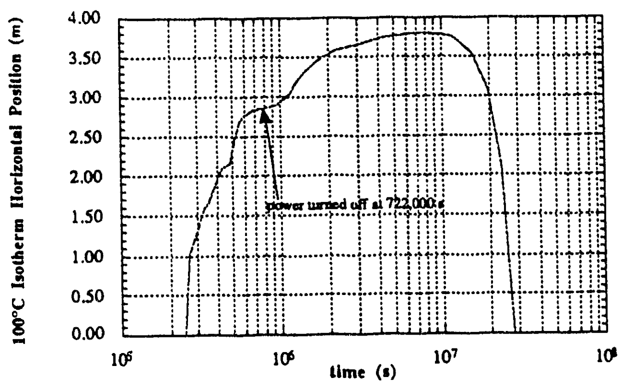

Figure 12. 100°C isotherm horizontal position at 1.94 m depth vs. time.

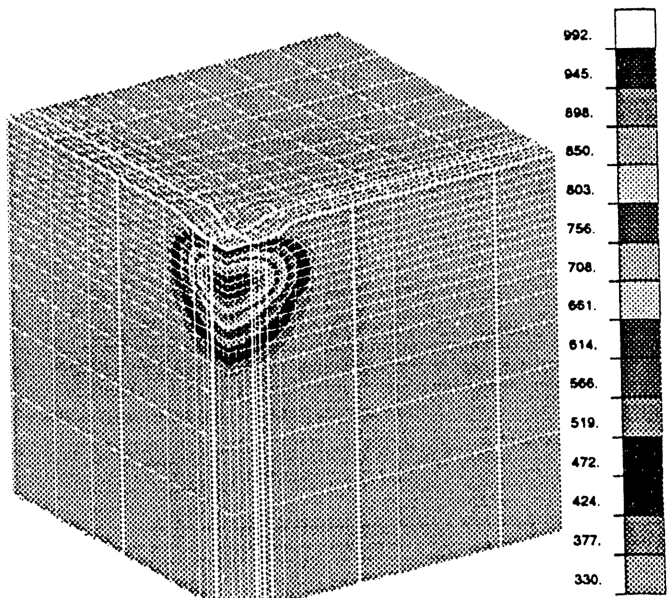

Figure 13. Temperature at maximum 100°C isotherm.

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