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NUMERICAL STUDIES OF HEAT TRANSFER AND GAS MIGRATION PROCESSES IN RELATION TO IN SITU VITRIFICATION

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ABSTRACT

This document presents numerical studies conducted in support of the In Situ Vitrification (ISV) treatability study. These results will be used for support of hardware design and performance assessments of ISV processes. Four models are presented and analyzed using finite element techniques: (1) heat transport and melting during the ISV process, (2) heat transfer calculations on the Intermediate Field Test (IFT) off-gas confinement hood, (3) gas migration in permeable soil surrounding the vitrified zone, and (4) melt rate calculations. Heat transport in the ISV process describes the temperature field and melt growth in the soil. Thermal radiation heat transfer calculations for the IFT hood demonstrate the sensitivity of the hood temperatures to melt temperature, melt radius, and exterior hood emissivity. The study of gas migration in permeable soil resulting from a buried source predicts that gas may migrate to the soil surface. The one-dimensional melt rate calculations conservatively predict a melt rate of 6 cm/hr.

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NOMENCLATURE

<u>Symbol</u>	<u>Description of Symbol</u>
A_e	finite element area
c_p	heat capacity at constant pressure
d	drum thickness
F	radiation view factor
h	heat transfer coefficient
i	current density
k	thermal conductivity
k_e	electrical conductivity
K	gas permeability
L	latent heat of fusion
n	normal vector
P	pressure
Pr	Prandtl number
Q	source generation rate
r	radius
R	gas constant
Re	Reynolds number
t	time
T	temperature
V	velocity of melting surface
x	cartesian coordinate direction
y	cartesian coordinate direction
z	cartesian or axisymmetric coordinate direction

Greek

α	coefficient of thermal expansion
β	isothermal compressibility
δ	characteristic length scale
ϵ	emissivity
μ	dynamic viscosity
π	porosity

ρ	density
σ	Stefan-Boltzman constant
Σ	summation
Ω	electrical resistance

Subscripts

a	air, atmosphere
c	convection
e	element
i	inside of hood
l	liquid
m	melt
o	outside of hood
oil	oil from drum
r	radiation
s	solid
	parallel to melt surface
$\perp$	perpendicular to melt surface

NUMERICAL STUDIES OF HEAT TRANSFER AND GAS MIGRATION PROCESSES IN RELATION TO IN SITU VITRIFICATION

1. INTRODUCTION

This report presents numerical studies performed in support of the Idaho National Engineering Laboratory (INEL) In Situ Vitrification (ISV) treatability study^{1,2}. These studies include: (1) heat transport and melting during the ISV process, (2) heat transfer calculations on the Intermediate Field Test (IFT) hood, (3) gas migration in permeable soil, and (4) melt rate calculations which support off-gas release rate estimates. Results of these studies have provided preliminary data for melt growth and off-gas release rate estimates and confinement hood temperature predictions.

The studies presented here were performed with PATRAN³ and ABAQUS⁴ computer codes. The finite element mesh generator PATRAN was used to create the finite element models. The finite element code ABAQUS was used to solve the steady state and transient diffusion equations contained in the models. These codes are described in Section 2. A preliminary numerical study of heat transport during ISV is presented in Section 3. Section 4 presents heat transfer calculations for the Intermediate Field Test (IFT) off-gas confinement hood. The transport of carbon monoxide (CO) gas through the soil surrounding a vitrified zone is examined in Section 5. One-dimensional melt rate calculations in support of the off-gas release rates are presented in Section 6.

2. COMPUTATIONAL SOFTWARE

The computer codes PATRAN and ABAQUS are described in the following sections. The codes are discussed in order of their general use.

2.1 PATRAN

PATRAN is a general purpose, three-dimensional computer aided engineering software system. It includes capabilities for generating finite element meshes in cartesian, cylindrical, or spherical coordinate systems, using automated command sequences. Element material properties, volumetric heat generation rates for elements, surface heat flux values and convection heat transfer coefficients for element faces may be specified. PATRAN was used to generate finite element meshes for all the models described in this report. The PATRAN generated meshes were verified by inspecting the nodalization and boundary conditions prior to each use. PATRAN was also used as a pre and post processor for ABAQUS.

2.2 ABAQUS

ABAQUS is a production oriented, general purpose finite element code used to solve a variety of structural, heat transfer, and dynamic problems. It is simple to use for a wide range of nonlinear applications, one of which is the solution of three-dimensional, transient heat conduction, or thermal diffusion problems. Steady-state solutions are obtained by direct integration of the spatial partial differential equation. Transient solutions are obtained by integrating the temporal/spatial equation with the backward difference operator (modified Crank-Nicholson method).

ABAQUS was used to analyze transient heat conduction and heat generation for: (1) a preliminary numerical study of heat transport during ISV, (2) steady state heat conduction in the intermediate field test hood, (3) gas diffusion in soil, and (4) melt rates of soil. ABAQUS uses an adaptive time stepping algorithm to automatically choose the time step. A user supplied tolerance on the maximum temperature change allowed in a time increment is used to adjust the time step. This approach was taken to conserve on computation time while allowing ABAQUS to adapt to rapid changes in the solution.

3. A PRELIMINARY NUMERICAL STUDY OF HEAT TRANSPORT

A preliminary numerical study of soil melting⁵ is described in this section. The aim is to use a simplified mathematical model to simulate the soil temperature, heat generation, and melting rate. Based on experimental data⁶, the soil temperature reaches a maximum of about 2000 °C and the melting rate is about 2-3 cm per hour. A representative vitrification process is considered and numerical results are obtained that agree well with experimental data.

3.1 Problem Description

A region of soil is considered whose cross-sectional geometry is illustrated in Figure 3.1. The calculation is performed in a cylindrical coordinate system (r, θ, z) and a two-dimensional problem is obtained by assuming an axisymmetric temperature field. The assumption is made that there is initially a small square region, having an area of $1/9 \text{ m}^2$, in which the soil is at its melting temperature. The rest of the soil is initially at ambient temperature.

As a result of electrical resistance heating, the soil temperature increases above the melting point. Heat energy is lost to the air by radiation and convection. At the other three surfaces of the region, in which two are far from the heat source and one is an axis of symmetry, it is assumed that there is no heat flux.

The governing equation of heat conduction⁷ is given by

$$\rho c_p \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k(T) \frac{\partial T}{\partial r} \right) - \frac{\partial}{\partial z} \left(k(T) \frac{\partial T}{\partial z} \right) = Q(T) \quad (3.1)$$

where $T(r, z, t)$ 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. Equation (3.1) is assumed to hold in a square region having sides of length $L=20 \text{ m}$.

Boundary conditions for Equation (3.1) are

$$\frac{\partial T}{\partial r}(0, z, t) = \frac{\partial T}{\partial r}(L, z, t) = \frac{\partial T}{\partial z}(r, L, t) = 0 \quad (3.2)$$

and

$$-k \frac{\partial T}{\partial z}(r,0,t) = h [T(r,0,t) - T_a(r,t)] \quad (3.3)$$

where T_a is the ambient air temperature and h is the total heat transfer coefficient given by

$$h = h_c + h_r \quad (3.4)$$

where h_c and h_r are the convective and radiative heat transfer coefficients. Boundary conditions at the liquid-solid interface are given by

$$T(r_m, z_m, t) = T_m \quad (3.5)$$

$$k(T_m) \frac{\partial T}{\partial n_s}(r_m, z_m, t) + k(T_m) \frac{\partial T}{\partial n_l}(r_m, z_m, t) = \rho L V_s \quad (3.6)$$

where r_m , z_m are the coordinates of the liquid-solid interface, T_m is the melting temperature, L is the heat of fusion, n_l and n_s are unit vectors normal to the interface that point into the liquid and solid, and V_s is the melting rate.

3.2 Electrical Resistance Heating

The electrical resistance heating, Q is given by

$$Q(T) = \frac{i^2}{k_e(T)} \quad (3.7)$$

where i is the current density and k_e is the electrical conductivity.

The current density may be obtained from the solution of the electrostatic potential equation. For this preliminary numerical study, a simplified mathematical representation of the electrical heat source has been chosen. In particular, the current density is assumed to have a constant value which is determined from a measured average electrical power. Although this is an unsophisticated approximation, it provides a heat source model with which to use to investigate solutions of Equation (3.1). This model is not capable of precisely simulating an ISV process, and

is limited to numerical studies in which the dominant physical phenomena are examined and the performance of numerical methods is assessed.

An average electrical power density of $1.3 \times 10^5 \text{ W/m}^3$ has been measured⁶. At the melting temperature of soil, this power is associated with a current density of $0.36 \times 10^3 \text{ A/m}^2$. This average current density is used in Equation (3.7) to obtain the heat source Q . The temperature and position dependence of the heat source is shown in Figures 3.2-3.3. The position dependence accounts for the presence of a region of soil that is initially liquid.

3.3 Surface Heat Transfer Coefficient Correlations

The convective heat transfer coefficient from a heated surface to air is given by⁷

$$h_c = \frac{k}{\delta} 0.332 \text{Pr}^{\frac{1}{3}} \text{Re}^{\frac{1}{2}} \quad (3.8)$$

in which the properties are those of air. The Prandtl number Pr is given by

$$\text{Pr} = \frac{\mu c_p}{k} \quad (3.9)$$

and the Reynolds number Re is given by

$$\text{Re} = \frac{\rho V \delta}{\mu} \quad (3.10)$$

where V is the air velocity and δ is a characteristic length scale. The properties of air are evaluated at the temperature which is the average of the soil surface and ambient air temperatures. For a soil temperature of 1200°C , an air temperature of 200°C and an air pressure of 20 atm, with V equal to 10 m/s and δ equal to 4 m (electrode separation), h_c is $13 \text{ W/m}^2\text{-}^\circ\text{C}$.

The radiation heat transfer coefficient h_r is given by

$$h_r = \sigma \epsilon (T^2 + T_a^2) (T + T_a) \quad (3.11)$$

where σ is the Stefan-Boltzmann constant and ϵ is the emissivity of soil. For a representative temperature difference $T - T_a$ equal to 1000°C , h_r is $250 \text{ W/m}^2\text{-}^\circ\text{C}$. Thus radiative heat loss will dominate convective heat loss.

The ambient air temperature T_a is modeled as

$$\begin{aligned} T_a(r,t) &= \frac{1}{6} T(r,0,t) \quad \text{for } r \leq 2\text{m} \\ T_a(r,t) &= 0^\circ\text{C} \quad \text{for } r > 2\text{m} \end{aligned} \quad (3.12)$$

This model is chosen to account for the presence of a confinement hood at $r = 0$ to $r = 2 \text{ m}$, in which the maximum temperature is assumed to be 200°C .

3.4 Soil Properties

The material properties of soil used in this analysis are given by⁶

$$\begin{aligned} \rho &= 2200 \text{ kg/m}^3 \\ c_p &= 1000 \text{ J/kg-}^\circ\text{C} \\ T_m &= 1200^\circ\text{C} \\ L &= 240,000 \text{ J/kg} \\ \epsilon &= 0.94 \end{aligned}$$

The temperature dependence of the thermal conductivity k and electrical conductivity k_e are shown in Figures 3.4-3.5.

3.5 Results

The finite element mesh used for the calculation is shown in Figure 3.6. The grid size is small in the region that is initially liquid, in order to calculate accurately the sharp transition from melting to ambient temperature.

Heat transport and melting have been simulated to a time of 60 hours. Figure 3.7 shows the temperature contours at the final time. The melted soil region has grown to a depth of about 2 m, and growth is more rapid in the vertical direction than the horizontal direction. This preferential growth occurs because there is a large heat loss by radiation to the air. Also because of heat loss,

the soil near the ground surface has solidified, producing a solid cap above the liquid melt. The region of high temperature moves downward as the soil melts, and there is a sharp transition from high to low temperature that occurs near the liquid-solid interface. The solid soil, about a half meter away from the interface, is at ambient temperature.

The analysis shows that the melt rate averages about 2.5 cm per hour and a maximum temperature of about 2000°C is attained, and these values agree well with experimental measurements⁶. The ability to simulate heat transport and melting is essential for modeling in situ vitrification, because many phenomena that occur during vitrification are sensitive to temperature changes. This simulation capability will be used in Section 6 to predict the melt rate in the case where a layer of waste is buried in the soil.

Figure 3.1 Geometry for an axisymmetric simulation of the in situ vitrification process.

Figure 3.2 Power vs temperature (initial liquid region).

Figure 3.3 Power vs temperature (initial solid region).

Figure 3.4 Thermal conductivity vs temperature.

Figure 3.5 Electrical conductivity vs temperature.

Figure 3.6 Finite element mesh; the cross-sectional area is 20 x 20 m.

Figure 3.7 Soil temperature at a time of 60 hours.

4. HOOD HEAT TRANSFER CALCULATIONS

Heat transfer calculations of the ISV Intermediate Field Test (IFT) hood are presented in this section. The aim is to conservatively bound the maximum hood temperature, and the maximum thermal gradient within the hood. A steady state heat transfer calculation is performed for a base case and seven other cases, with parameters changed from the base case. The model description is presented in Section 4.1, followed by the results in Section 4.2.

4.1 Problem Description

The model used to analyze the hood is presented in Figure 4.1. The calculation is performed with a cylindrical coordinate system (r, θ, z) , and a two-dimensional problem is obtained by assuming that the temperature is independent of the θ coordinate. The molten soil and interior hood surface radiate heat to each other by means of gray body radiation. The heat is conducted from the interior hood to the exterior surfaces and then radiated to the sky by means of black body radiation. Convection was not included in this model in order to conservatively bound the problem. Steady state calculations were performed for this analysis.

The governing equation of steady state heat conduction⁷ is given by

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r k(T) \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k(T) \frac{\partial T}{\partial z} \right) = 0 \quad (4.1)$$

where $T(r, z)$ is the temperature, and k is the thermal conductivity. Equation (4.1) is assumed to hold only in the hood.

The boundary condition at the inside of the hood is

$$-k(T) \frac{\partial T}{\partial n_i}(r, z) = h_r [T(r_i, z_i) - T_m] \quad (4.2)$$

where h_r for gray body radiation⁷ is described as

$$h_r = \frac{\sigma [T_m^2 + T^2(r_i, z_i)] [T_m + T(r_i, z_i)]}{A_e \left(\frac{1 - \epsilon_m}{\epsilon_m A_m} + \frac{1}{F_{im} A_e} + \frac{1 - \epsilon_i}{\epsilon_i A_e} \right)} \quad (4.3)$$

where σ is the Stefan-Boltzman constant, T_m is the melt temperature, $T(r_i, z_i)$ is the temperature on the inside of the hood, ϵ_m is the emissivity of the melt, A_m is the melt area, F_{im} is the shape factor⁸ from the inside of the hood to the melt, A_e is the element area, and ϵ_i is the emissivity on the inside of the hood.

The shape factor F_{im} for the top of the hood parallel to the melt is described as

$$(F_{im})_{\parallel} = \frac{1}{2} \left(1 - \frac{1 + H^2 - R^2}{\sqrt{Z^2 - 4R^2}} \right)$$

where

$$H = \frac{z}{r}$$

$$R = \frac{r_m}{r}$$

$$Z = 1 + H^2 + R^2 \quad (4.4)$$

where r_m is the radius of the melt.

The shape factor for the side of the hood is the maximum of a plane parallel to the melt $(F_{im})_{\parallel}$, and a plane perpendicular to the melt $(F_{im})_{\perp}$. Where $(F_{im})_{\perp}$ is described as

$$(F_{im})_{\perp} = \frac{H}{2} \left(\frac{Z}{\sqrt{Z^2 - 4R^2}} - 1 \right)$$

where

$$H = \frac{z}{r}$$

$$R = \frac{r_m}{r}$$

$$Z = 1 + H^2 + R^2 \quad (4.5)$$

The boundary condition at the outside of the hood is

$$-k(\vec{r}) \frac{\partial T}{\partial n_o}(\vec{r}, z) = h_r [T(r_o, z_o) - T_a] \quad (4.6)$$

where h_r for black body radiation⁸ is described as

$$h_r = \sigma \epsilon_o [T^2(r_o, z_o) + T_a^2] [T(r_o, z_o) + T_a] \quad (4.7)$$

where ϵ_o is the emissivity on the outside of the hood, $T(r_o, z_o)$ is the outside hood temperature, and T_a is the outside air temperature. The boundary conditions at the centerline and bottom edge of the hood are assumed to be adiabatic.

The finite element model consists of 300 elements with four nodes per element. The mesh is only one element thick to account for the hood thickness. Maximum aspect ratio of the elements is four. The hood is made of stainless steel type 304. The thermal conductivity⁹ of the hood at selected temperatures is given by

k (W/m-°C)	T (°C)
16.3	0.0
19.0	300.0
22.0	600.0
22.0	2000.0

Linear interpolation is used to obtain the conductivity at intermediate temperatures. It is assumed that the hood does not radiate to the unmelted soil. The top and side of the hood were modeled such that they did not radiate to each other. The only radiation is from the melt to the hood and from the hood to the air.

4.2 Results

Heat transfer calculations due to steady state radiation from melted soil have been performed for the IFT hood. The calculations were performed for a base case and seven variations from the base case. Table 4.1 shows the values used for the base case (case 0) along with the maximum and minimum temperatures calculated in the hood. The parameters used in the base case are: $T_m = 1400^\circ\text{C}$, $r_m = 0.688$ m, $\epsilon_m = 0.90$, $\epsilon_i = 0.90$, $\epsilon_o = 0.30$, $T_a = 30^\circ\text{C}$ (a hot summer day).

Figure 4.2 shows the non-dimensional temperature and shape factor for the base case. One can see that the shape factor equations change at the corner of the hood. The transition hump in the shape factor curve is due to the perpendicular equation becoming larger than the parallel equation for the maximum. The maximum of the parallel and perpendicular equations was chosen so that the curve would be continuous. The summation of the shape factors of the elements inside the hood multiplied by each element's area should be equal to the shape factor of the melt (equal to one) times the area of the melt. The sum inside the hood is 1.34 m^2 , and the area of the melt is 1.49 m^2 . The discrepancy is due to the shape factor approximation along the side of the hood. It was felt that the difference was small enough to not warrant a more detailed shape factor in the model. The temperature profile has the same trend as the shape factor. This result shows that the temperature is a strong function of the shape factor.

The IFT uses 500 kW of electrical power. This value of 500 kW is used as a reference for discussion. The heat flux is calculated for each case. The total heat flux radiated to the sky was calculated to be 508 kW for the base case. This means that all of the electrical heat is being radiated to the sky. Table 4.1 shows the changes made in each variable, in cases one through seven, along with the maximum and minimum temperatures in the hood and the total heat radiated to the sky. The temperatures were affected most by changing melt temperature, melt radius, and emissivity on the outside of the hood. In case seven, the temperature was fixed at the bottom of the hood which created the sharpest thermal gradient in the hood.

Case 1 has the highest maximum and minimum temperatures due to the melt temperature being raised to 2000°C . The total heat flux is unreasonably high at 1700 kW. When changing the melt radius to 0.90 m in case 2, the temperatures also increase and the heat flux is too high at 794 kW. The model is not very sensitive to the emissivity of the melt as is shown in case 3, 3a, and 3b where ϵ_m was changed to 0.30, 0.01, and 0.001 respectively. The maximum and minimum temperatures changed very little. When changing the emissivity on the inside of the hood to 0.30 in case 4 it had the effect of lowering the temperatures. This occurred since the absorptivity ($1 - \epsilon_i$) (inversely proportional to heat flux) was increased and so less heat was absorbed and conducted through the hood, which lowered the temperatures as Equation (4.3) shows. Case 5 shows the temperatures are strongly dependent on the emissivity on the outside of the hood. Temperatures decreased significantly since more heat was radiated to the sky. Changing the ambient temperature to 0°C in case 6 had little effect on the temperatures or heat flux. This result is because of the small change in ambient temperature. Case 7 shows the sharpest thermal gradient in the hood, which

resulted from fixing the bottom temperature to 0°C . The maximum hood temperature still remained the same.

Table 4.2 shows the temperature profile along the hood for each of the different cases. For the base case, the temperatures drop about 100°C along the top of the hood, and 600°C along the side. This is indicative of all the cases since the shape factor is so small at the bottom of the hood.

Figure 4.1 Schematic of IFT hood model.

Figure 4.2 Non-dimensional temperature and shape factor vs radius.

Table 4.1 Results from IFT hood sensitivity study

	C0	C1	C2	C3	C3a	C3b	C4	C5	C6	C7
Change		$T_m=2000$	$r_m=0.90$	$\epsilon_m=0.30$	$\epsilon_m=0.01$	$\epsilon_m=0.001$	$\epsilon_i=0.30$	$\epsilon_o=0.90$	$T_a=0.0$	$T_{bot}=0.0$
Tmax (°C)	875.	1290.	979.	875.	874.	862.	837.	638.	875.	875.
Tmin (°C)	175.	274.	219.	175.	174.	165.	174.	87.	168.	0.
Qtot (kW)	508.	1700.	794.	506.	440.	204.	466.	561.	500.	500.
										$T_a=0.0$

Table 4.2 Temperature profiles along IFT hood for various cases

<u>x</u> <u>(m)</u>	<u>y</u> <u>(m)</u>	<u>C 0</u> <u>(°C)</u>	<u>C 1</u> <u>(°C)</u>	<u>C 2</u> <u>(°C)</u>	<u>C 3</u> <u>(°C)</u>	<u>C 3a</u> <u>(°C)</u>	<u>C 3b</u> <u>(°C)</u>	<u>C 4</u> <u>(°C)</u>	<u>C 5</u> <u>(°C)</u>	<u>C 6</u> <u>(°C)</u>	<u>C 7</u> <u>(°C)</u>
0.00	2.25	876.	1290.	980.	876.	874.	863.	837.	638.	875.	875.
0.16	2.25	874.	1288.	978.	874.	866.	809.	835.	636.	873.	873.
0.33	2.25	868.	1279.	973.	867.	853.	754.	830.	631.	867.	867.
0.51	2.25	857.	1265.	964.	857.	837.	709.	821.	621.	857.	857.
0.68	2.25	843.	1245.	951.	842.	818.	670.	809.	608.	842.	842.
0.85	2.25	825.	1220.	935.	824.	796.	636.	794.	592.	824.	824.
1.02	2.25	803.	1191.	916.	803.	772.	605.	775.	573.	803.	803.
1.18	2.19	788.	1169.	902.	787.	750.	566.	762.	559.	788.	788.
1.28	2.02	789.	1170.	905.	788.	748.	555.	762.	560.	789.	789.
1.39	1.85	784.	1163.	902.	783.	741.	543.	758.	556.	784.	784.
1.49	1.68	772.	1146.	893.	770.	728.	530.	747.	545.	771.	771.
1.60	1.52	750.	1116.	875.	749.	708.	516.	728.	526.	749.	749.
1.71	1.35	746.	1112.	860.	745.	702.	507.	725.	523.	746.	746.
1.81	1.18	741.	1104.	859.	740.	696.	498.	720.	519.	741.	741.
1.92	1.01	723.	1080.	845.	722.	679.	486.	704.	504.	722.	722.
2.02	0.84	690.	1035.	815.	689.	651.	471.	674.	477.	690.	690.
2.13	0.67	641.	968.	766.	640.	609.	452.	628.	436.	640.	640.
2.24	0.50	573.	874.	695.	573.	550.	424.	565.	382.	572.	572.
2.34	0.33	481.	748.	594.	481.	467.	382.	476.	311.	480.	480.
2.45	0.16	346.	561.	439.	346.	340.	301.	344.	212.	343.	341.
2.55	0.00	175.	275.	219.	175.	174.	166.	175.	87.	168.	0.

5. GAS DIFFUSION IN SOIL

This section describes calculations performed which simulate gas diffusion in the soil during the ISV process. The aim is to simulate gas diffusion of carbon monoxide (CO) in the soil. The CO results from pyrolyzation of regal oil in a buried drum. During the active vitrification and cooldown phases of the ISV process, heat conducts away from the melt into the surrounding soil and waste. Temperatures in this region range from the soil melt temperature 1200°C at the melt front to ambient temperature at some distance away from the melt front. Wastes present in this region may pyrolyze and volatilize and generate gases. Temperature, concentration, and pressure gradients will force this multiphase multicomponent gas to migrate into the melt zone and through the surrounding soil. To simplify the problem, gases not entering the melt zone are treated as a single-phase single component ideal gas which is forced through the permeable soil and waste regions surrounding the melt by gas pressure gradients. The model description is discussed in Section 5.1, followed by results in Section 5.2.

5.1 Model Description

A region of soil whose cross-sectional geometry is illustrated in Figure 5.1 is considered. Calculations are performed with a cartesian coordinate system (x,y,z), and a two-dimensional problem is obtained by assuming that the gas diffusion is independent of the z coordinate. The pressures in the model are assumed to initially be at zero gage pressure. The melted soil is not included in the mesh since the permeability of the melted soil is assumed to be much smaller than the unmelted soil and that the boundary condition of no mass transfer between the melted soil and unmelted soil is appropriate.

By assuming Darcy flow, applying the principle of mass conservation, and using the definitions of fluid compressibility and thermal expansivity, the basic equation for single phase gas flow in porous media is

$$\frac{\partial}{\partial x} \left(\frac{\rho K}{\mu} \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\rho K}{\mu} \frac{\partial P}{\partial y} \right) = \rho \pi \left(\beta \frac{\partial P}{\partial t} + \alpha \frac{\partial T}{\partial t} \right) + Q(T) \quad (5.1)$$

where $P(x,y,t)$ is the pressure, t is the time, ρ is the gas density, μ is gas viscosity, K and π are soil/waste permeability and porosity respectively, β is gas compressibility, α is the gas thermal expansion coefficient, T is temperature, and Q is the gas mass source rate per unit volume. The gas compressibility is described as

$$\beta = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial P} \right)_T \quad (5.2)$$

The gas thermal expansion coefficient is

$$\alpha = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P \quad (5.3)$$

The equation of state for an ideal gas is

$$P = \rho R T \quad (5.4)$$

where R is the gas constant. When combining Equation (5.2) with (5.4), the compressibility factor can be described as

$$\beta = \frac{1}{P} \quad (5.5)$$

After combining Equation (5.3) with (5.4), the thermal coefficient of expansion is

$$\alpha = \frac{1}{T} \quad (5.6)$$

When substituting Equations (5.4), (5.5) and (5.6) into (5.1), Equation (5.1) becomes

$$\frac{\partial}{\partial x} \left(\frac{PK}{\mu} \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{PK}{\mu} \frac{\partial P}{\partial y} \right) = \pi \left(\frac{\partial P}{\partial t} + \alpha P \frac{\partial T}{\partial t} \right) + RTQ(T) \quad (5.7)$$

Equation (5.7) holds for the unmelted soil for this analysis. Boundary conditions for Equation (5.7) are shown in Figure 5.1.

A moving temperature wave was assumed for this model. This temperature wave is the $\partial T / \partial t$ term in Equation (5.7). A linear temperature difference of 1400°C over 0.5 m, moving radially outward at 9 cm/hr, was imposed on the mesh. The temperature wave starts at time zero an equidistance of four meters and moves outwardly (in the x and y directions) from the origin. The only term to change in Equation (5.7), before the temperature wave reaches the oil drum is the

$\partial T/\partial t$ term. The pyrolyzation temperature of the oil is set at 500°C. When the temperature is above 500°C in the drum, the source term Q is prescribed as a function of temperature as

$$\begin{aligned} Q &= 0 & \text{for } T < 500^\circ\text{C} \\ Q &= \frac{\rho_{\text{oil}} V}{d} & \text{for } T \geq 500^\circ\text{C} \end{aligned} \quad (5.8)$$

where ρ is the oil density, V is the temperature wave velocity (9 cm/hr), and d is the drum thickness (0.5 m).

Properties used in this analysis are

$$\begin{aligned} K &= 10^{-10} \text{ m}^2 \\ \mu &= 2.7 \times 10^{-5} \text{ kg/m-s} \\ \pi &= 0.25 \\ \rho_{\text{oil}} &= 850 \text{ kg/m}^3 \\ R &= 296 \text{ J/kg-}^\circ\text{C} \end{aligned}$$

5.2 Results

A simulation has been performed of gas migration in soil to a time of 20 hours. Shown in Figure 5.2 is the finite element mesh used in the model and the pressure contours that correspond to 17 hours. The scale in Figure 5.2 is gage pressure (Pascals). The elements are small in the region around the oil drum, in order to accurately calculate the high pressure gradients in the region. The gas source term was turned on at 8 hours when the temperature reached 500°C at the top of the drum and lasted until 17 hours, at which time the temperature at the bottom of the drum reached 1400°C. The last three hours of simulation had no source term and hence the pressures decrease over time. The maximum pressures were obtained at 17 hours. There exists a pressure gradient at the surface of the soil which indicates that gas migrates to the atmosphere. The relatively small pressure rise is due to the large permeability constant of the soil.

Figure 5.3 shows the pressure contours at 17 hours for the soil permeability of 10^{-12} m^2 . The maximum pressure is 1.2 atmospheres. The higher pressures are due to a smaller permeability constant. Figure 5.4 shows the pressure contours at 7 hours. The pressure gradient is due to the soil heating the gas and causing the pressure to rise from the $\partial T/\partial t$ term in Equation (5.7). The gas heated in the soil before the CO has been released has the same properties as CO. The $\partial T/\partial t$

term was treated as a source term, since the temperature field was assumed, and was calculated to be about 0.2% of the Q source term.

Figure 5.5 shows the pressure contours at 14 hours for a soil permeability of 10^{-14} m^2 . An intermediate time is presented to show how the contours progress. The maximum pressure is about 18 atmospheres since the permeability constant is low which allows the pressure to build up and decrease the diffusion through the porous soil. Figure 5.6 shows the pressure contours at 17 hours with the melt region included in the mesh. The permeability of the soil is 10^{-10} m^2 and the permeability of the melted soil was assumed to be 1/1000th of the unmelted soil. Even with the low permeability in the melted region, the gas still migrates up to the surface.

In conclusion, we have successfully been able to model gas migration in the soil resulting from a CO source buried in a drum below the melted region. This model shows that for the permeabilities selected, gas may flow through the permeable soil and migrate to the surface.

Figure 5.1 Geometry for a 2-D simulation of gas diffusion from a buried source.

Figure 5.2 Gas diffusion pressure contours at 17 hours, $K = 10^{-10} \text{ m}^2$.

Figure 5.3 Gas diffusion pressure contours at 17 hours, $K = 10^{-12} \text{ m}^2$.

Figure 5.4 Gas diffusion pressure contours at 7 hours, $K = 10^{-14} \text{ m}^2$.

Figure 5.5 Gas diffusion pressure contours at 14 hours, $K = 10^{-14} \text{ m}^2$.

2017. =	A
1878. =	B
1739. =	C
1600. =	D
1461. =	E
1321. =	F
1182. =	G
1043. =	H
904. =	I
765. =	J
626. =	K
487. =	L
348. =	M
209. =	N
69.5 =	O

Figure 5.6 Gas diffusion pressure contours at 17 hours with melt included, $K = 10^{-10} \text{ m}^2$.

6. ONE-DIMENSIONAL MELT RATE CALCULATIONS

One-dimensional melt rate calculations are performed in this section in support of off-gas release rate predictions for the full scale confinement hood¹⁰. This section describes the models used to simulate melting of soil and waste layers in a one-dimensional geometry. The model descriptions and boundary conditions are presented in Section 6.1. The results of the one-dimensional melt rate calculations are presented in Section 6.2.

6.1 Model Description

Three different models are used in the melt rate analysis. The first model assumes that the entire model region is soil. The second model assumes that there is one meter of soil on top of nine meters of waste. The thermal conductivity of the waste is assumed to be constant. The third model is the same as the second except that the thermal conductivity of the waste layer is allowed to vary with temperature. The thermal conductivity of the soil layer varies with temperature for all three models.

A schematic diagram showing the physical setup for models 2 and 3 is given in Figure 6.1. A radiative heat transfer coefficient boundary condition is used for the surface of the melt (with heat flowing out from the melt). This coefficient is dependent on the temperature of the surface but remains near 150 W/(m² °C) for all of the calculations. At the other boundaries, it is assumed that no heat transfer occurs. This is equivalent to using a far-field condition where ambient conditions are undisturbed. Since the melt front progresses only 4 m within the waste layer, the far-field assumption is valid.

The model is one-dimensional in order to simplify the calculations and model the melt rate. The one-dimensional transient heat conduction equation is given by

$$\frac{\partial}{\partial y} \left(k(T) \frac{\partial T}{\partial y} \right) + Q(T) = \rho c_p \frac{\partial T}{\partial t} \quad (6.1)$$

where k is the thermal conductivity, $T(y,t)$ is the temperature, Q is the electrical heat source, ρ is the density, and c_p is the specific heat. Equation (6.1) holds for the entire domain for the three models described above.

The initial configuration of the soil and waste used for each model assumes that the top 0.5 m of soil is molten with the remaining soil at ambient temperature. A heat source (due to

electrical power) of 140 kW is continually input into the 1 m x 1 m x 10 m deep model volume. This heat source is not uniformly distributed with time or position. Rather, it is distributed according to the heat transport model detailed in Section 3 of this report. Since the cross-sectional area is 1 m x 1 m when looking down onto the model, a power per unit area of 140 kW/m² is obtained. This is a representative power density for the full scale test. The latent heats of the soil and waste are neglected, adding to the conservatism of the calculations. (When latent heat is included, it slows the melt rate by 10-20%.)

The following material properties for the soil⁶ are used for all three models. (Linear interpolation is used in all cases to estimate property values in between tabulated values.)

Specific Heat c_p (J / kg- °C) Temperature (°C)

772.0	0.0
772.0	1190.0
1250.0	1210.0
1250.0	5000.0

Thermal Conductivity k (W / m- °C) Temperature (°C)

0.1	0.0
1.0	1000.0
30.0	2000.0
30.0	5000.0

Density ρ (kg / m³) Temperature (°C)

2200.0	All
--------	-----

Electrical Conductivity k_e (Ohm - m)⁻¹ Temperature (°C)

1.0	0.0
1.0	1210.0
20.0	2000.0
20.0	5000.0

In order to be able to obtain values for the thermal properties for the waste layer, the properties of each component are volumetrically averaged. Table 6.1 summarizes the component thermal properties and the volume-averaged calculations. Material properties are obtained from References 6 and 11.

Table 6.1 Thermal conductivity and density-specific heat products for the materials included in the volume-average calculation for the thermo-physical properties for the waste layer.

Material	Volume (m ³)	k (cal/s-cm-°C)	$\rho \cdot c_p$ (cal/cm ³ -°C)	k * Vol (cal-m ³ / s-cm-°C)	$\rho \cdot c_p \cdot Vol$ (cal-m ³ / cm ³ -°C)
Water	8.70	0.00140	1.00	1.22 x 10 ⁻²	8.7000
NaNO ₃	2.50	0.00500	0.05	1.25 x 10 ⁻²	0.1183
KNO ₃	1.35	0.00500	0.44	6.75 x 10 ⁻³	0.5982
Graphite	1.50	0.40000	0.36	6.00 x 10 ⁻¹	0.5400
Wood / Paper	12.30	0.00082	0.27	1.01 x 10 ⁻²	3.3628
Lead	0.23	0.08200	0.35	1.89 x 10 ⁻²	0.0809
Steel	1.40	0.17000	0.86	2.38 x 10 ⁻¹	1.2104
Hydrate Oxides	3.50	0.04200	0.46	1.47 x 10 ⁻¹	1.6093
CaSiO ₂ + CaO	1.20	0.00050	0.14	6.00 x 10 ⁻⁴	0.1710
Soil	48.00	0.00026	0.53	1.25 x 10 ⁻²	25.3440
Regal Oil *	5.00	0.00034	0.12	1.70 x 10 ⁻³	0.6050
Asbestos	1.408	not incl.	not incl.		
Void Volume	50.0				
Total	137.088			1.06	42.3399
* Regal Oil, EDTA, Misc Oils, Org Oils					
k =	$\Sigma(k \cdot Vol)$ /Total vol.	=	7.73 x 10 ⁻³ (cal/s-cm-°C)	=	3.24 (W/m-°C)
ρc_p =	$\Sigma(\rho c_p \cdot Vol)$ /Total vol.	=	3.09 x 10 ⁻¹ (cal/cm ³ -°C)	=	1.29 x 10 ⁶ (J/m ³ -°C)

The values in Table 6.1 are used for model 2. A summary of all the properties for the waste layer for model 2 is given below.

Model 2 (Soil and Waste. Constant Thermal Conductivity in Waste)

Specific Heat c_p (J / kg- °C) Temperature (°C)

943.5 All

Thermal Conductivity k (W / m- °C) Temperature (°C)

3.26 All

Density ρ (kg / m³) Temperature (°C)

2000.0 All

<u>Electrical Conductivity k_e (Ohm - m)⁻¹</u>	<u>Temperature (°C)</u>
1.0	0.0
1.0	1210.0
20.0	2000.0
20.0	5000.0

For model 3, the thermal conductivity of the waste layer varies with temperature as a function of the soil constituent thermal conductivity. All other constituent conductivities are held constant. A summary of the properties used for model 3 is given below.

Model 3 (Soil and Waste, Variable Thermal Conductivity in Waste)

<u>Specific Heat c_p (J / kg- °C)</u>	<u>Temperature (°C)</u>
943.5	All

<u>Thermal Conductivity k (W / m- °C)</u>	<u>Temperature (°C)</u>
0.326	0.0
6.890	1000.0
14.400	2000.0
14.400	5000.0

<u>Density ρ (kg / m³)</u>	<u>Temperature (°C)</u>
2000.0	All

<u>Electrical Conductivity k_e (Ohm - m)⁻¹</u>	<u>Temperature (°C)</u>
1.0	0.0
1.0	1210.0
20.0	2000.0
20.0	5000.0

6.2 Melt Rate Calculations

The three models are run to a time of 300,000 seconds (83 hours). The heat convected from the top for all three models is calculated to be 36 kW/m². This value compares well with 38 kW/m² from Reference 6. The melting temperature of the soil is taken as 1200°C.

First Model:

The melt reaches a distance of 3.75 m in 83 hr for a melt rate of 4.51 cm/hr. The maximum temperature reached is 2300 °C at a depth of 1.5 m. The temperature vs. position vs. time curve is presented in Figure 6.2. The power vs. time is presented in Figure 6.3. The power remains near 140 kW/m² for the entire transient.

Second Model:

The melt reaches a distance of 2.60 m in 83 hr for a melt rate of 3.13 cm/hr. The maximum temperature reached is 2945 °C at a depth of 1.5 m. The temperature vs. position vs. time curve is presented in Figure 6.4.

Third Model:

The melt reaches a distance of 4.75 m in 83 hr for a melt rate of 5.7 cm/hr. The maximum temperature reached is 2801°C at a depth of 2.0 m. The temperature vs. position vs. time curve is presented in Figure 6.5. The melt rate remains fairly constant during the entire transient. The power remains near 140 kW/m² for the entire transient.

The melt front velocities reported above are time-average values, although the velocities computed are typically very constant over the time of the calculation. Since model 3 yields the highest value for the melt front velocity, it serves as the basis for the rate used in support of the off-gas release rate calculations. In fact, the slightly more conservative value of 6 cm/hr is used.

Figure 6.1 Geometry and boundary conditions for the one-dimensional melt model.

Figure 6.2 Temperature vs time for model one.

Figure 6.3 Power vs time for model one.

Figure 6.4 Temperature vs time for model two.

Figure 6.5 Temperature vs time for model three.

7. CONCLUSIONS

Numerical calculations have been performed for four models in support of ISV calculations. Heat transport in the ISV process shows the temperature field and melt growth for an axisymmetric model that agree well with experimental data. Thermal radiation heat transfer calculations for the IFT hood shows the sensitivity of the hood temperatures to melt temperature, melt radius, and exterior hood emissivity. The maximum hood temperature for the base case study was 875 °C. The study of gas migration in permeable soil resulting from a buried source shows that gas may migrate to the soil surface. The gas migration was found to be a strong function of soil permeability. The one-dimensional melt rate calculations predict a melt rate of 6 cm/hr.

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