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INVESTIGATION OF POTENTIAL FOR OCCURRENCE OF MOLTEN SOIL DISPLACEMENT EVENTS DURING IN SITU VITRIFICATION OF COMBUSTIBLE WASTES

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ABSTRACT

Computer simulations are used to investigate the application of in situ vitrification (ISV) for processing contaminated soil containing high loadings of solid, compressible waste material, typical of landfills and solid waste trenches. Specifically, these simulations predict whether significant displacement of molten soil, due to large, 1 to 2 m diameter, gas bubbles rising up through the ISV melt, are likely to occur during processing of combustible waste-loaded sites. These bubbles are believed to originate from high-pressure regions below the melt caused by vaporization of water and gases generated by the combustion, volatilization, or pyrolyzation of combustible materials in the waste.

The displacement of molten soil is dangerous to both personnel and equipment and can lead to pressurization of the hood, creating the potential for contaminants to escape to the atmosphere. For these reasons, significant displacement of molten soil must be avoided, and any site being considered for processing by ISV should be evaluated for possible situations where a molten soil displacement event may occur.

To investigate this situation, simulations were run using the TOUGH2 computer code to predict pressures underneath the ISV melt. TOUGH2 is an unsaturated groundwater modeling code capable of treating non-isothermal problems. These simulations include moving melt front and simple pyrolysis models and investigate how the gas pressure in the soil below the melt is affected by melt progression rate, soil permeability, combustible and impermeable material loading. The following conclusions have been drawn based on the TOUGH2 simulations:

- A simulation of the ISV of a timber crib predicted that significant displacement of molten soil is not likely to occur during processing; this agreed with empirical evidence from the timber crib ISV demonstration.

- Loading of impermeable wastes in regions to be vitrified can dramatically increase local pressures to the point of creating the potential for a significant displacement of molten soil.

- Soil permeability and melt rate strongly affect the buildup of pressure beneath the melt when combustibles are present.

INTRODUCTION

An effort is currently under way to clean up the 100 Area of the Hanford reservation. This large-scale remediation consists of treating the waste or moving it to the 200 Area to be more permanently stored. The waste relocated to the 200 Area would be stabilized and covered with a protective surface barrier to prevent leaching of contaminants by the groundwater. This barrier is

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an elaborate layering of low permeability soils to prevent water infiltration. If the ground under the barrier subsides due to the decomposition or compression of the waste, it is possible that the barrier may crack and no longer function.

One method of stabilizing the compressible waste is by in situ vitrification (ISV) after the waste is disposed in the 200 Area. In situ vitrification is an innovative technology that treats contaminated soils in situ by melting the soil to form an indelible glass and crystalline form when solidified. The ISV process immobilizes inorganic materials such as plutonium, lead, and cadmium. Vitrification would eliminate the danger of damage to the surface barrier from the soil settling caused by decomposition of combustible material and settling of the compressible waste.

Soil melting in the ISV process is accomplished by passing electrical current through contaminated soils via electrodes inserted into the soil. Because dry soil is not very electrically conductive, a conductive mixture of graphite and glass frit is placed between each electrode to serve as a starter path. An electrical potential is applied to the electrodes to establish an electrical current in the starter path. The flow of current heats the starter path and surrounding soil to well above the initial soil-melting temperatures of 1100°C to 1400°C. Once the soil becomes molten, it becomes more electrically conductive, and the molten region grows outward and downward. Fig. 1 illustrates the ISV process. Power is applied until the melt encompasses the contaminated region.

[place Figure 1 here]

Figure 1. In Situ Vitrification Process[1].

Although ISV would solve the soil settling problem, the waste in the 100 Area includes several components which could influence the feasibility of ISV. Metals are present in small pieces (perforated spacers for nuclear reactor rods) and large sections (aluminum ladders, piping, and steel flooring). These pieces could make regions in the soil impermeable affecting the movement of gas and liquid. The combustible components are also of concern because they are potential gas-generation sources during the ISV process. This work will consider only the potential gas source and confinement problems related to this waste. Potential issues related to the electrical system are not considered.

SAFETY CONCERN OF POTENTIAL "MOLTEN SOIL DISPLACEMENT EVENT"

During the ISV process, the water present in the pores of the soil near the melt is heated to boiling, and combustibles are combusted or pyrolyzed (depending on the availability of oxygen). Both of these processes produce significant quantities of gas. If the permeability of the soil is low due to the tight structure or the presence of solid regions (e.g., metal drum, concrete wall, etc), the gas generated can cause a significant increase in pressure below the melt. When this pressure becomes greater than the static head of the melt, there is the possibility it can rupture the sintered soil layer surrounding the melt and send a bubble of gas into the melt. As the gas bubble rises through the melt, its volume increases due to decreasing pressure until it reaches the surface. This large bubble volume (two or more meters in diameter) displaces an equal volume of melt, causing the molten soil to overflow its boundaries (termed a "molten soil displacement event") and causing a temporary pressurization of the containment hood. When the bubble reaches the melt surface, it bursts, and may result in the expulsion of molten soil onto the off-gas hood.

This scenario is dangerous to personnel and equipment and can lead to the potential for uncontrolled release of contaminants into the atmosphere as the off-gas hood is pressurized. For these reasons, it is important to avoid pressure buildups beneath the melt. A practical way of addressing this concern, however, is to predict potential pressure buildup problems using computer modeling of the region beneath the melt, including the combustion process.

MODELING APPROACH

Two sets of simulations were run using the TOUGH2 modeling code, one modeling a timber crib (116-B-6A) and the other modeling a trench containing combustible and impermeable waste. The timber crib simulation was selected because data exist on an ISV melt, which successfully consumed a timber crib, that can be compared to the model results. The trench model represents the preliminary investigation of ISV treatment of wastes to be stored in the 200 Area. For this simulation, two melt progression rates and two soil permeabilities were investigated to aid future design of staging of the waste.

The two sets of simulations contained common geometries for the advancing ISV melt front and common soil properties. In addition, the combustible material used for both simulations was cellulose (wood), and approximations for the pyrolysis process were the same.

TOUGH2 Description

TOUGH2 is an unsaturated groundwater modeling code, capable of treating non-isothermal problems, which was developed by Karsten Pruess at Lawrence Berkeley Laboratory[2,3]. TOUGH2 treats unsaturated groundwater and gas flow in response to pressure, temperature, and liquid saturation gradients. It computes the changes in phase between liquid and gas and includes models for relative permeability and capillary pressure. TOUGH2 was used to model the transient hydrothermal phenomena occurring below ISV melts in these simulations.

It should be noted that combustion is not treated in the TOUGH2 code, although it does allow injection of gas, liquid, and heat into any number of locations. This feature was used to approximate the introduction of combustion energy and by-products into the modeled domain.

General Model Features

The crib and trench sites were modeled incorporating as much realism as possible. The models included representations of the melt (with moving melt front), combustibles, off-gas hood at the soil surface, and the thermal-hydraulic phenomena occurring in the soil. Both models used an approximately spherical melt shape to take advantage of symmetry in order to reduce the computational requirements of the model. The phenomena occurring in the soil surrounding the melt typically mimic the shape of the melt, and there is little variation around the perimeter of the melt. For this reason a two-dimensional wedge from a spherical coordinate system was used to model these processes.

Hanford soil typical of the ISV site in the 300 Area of the Hanford reservation was used for these models. Hydraulic properties, measured experimentally by Rockhold, et al.[4], and approximations for the thermal properties based on Hillel[5] are entered in Table I. Both models used initial gas saturations in the soil of 0.82 at 25 °C and 101350 Pa (approximately atmospheric conditions), except near the melt where an exponential temperature profile was used.

Table I: ISV Site Soil Properties

Absolute Permeability	1.01e-11 m^2
Grain Density	2720 kg/m^3
Porosity	0.398
Thermal Conductivity	1.305 W/m °C
Specific Heat	800 J/kg °C
Capillary Pressure and	$\alpha = 5.375$ 1/Pa

Relative Permeability (VanGenuchten functions[6])	$n = 2.6889$ $S_r = .214$ $S_s = 1.0$ $P_{max} = 1.0e+5$ Pa

The advancing ISV melt and off-gas hood parameters were modeled similarly in both sites. The melt front was considered to be an impermeable boundary to gas and liquid flow that maintained at 1300 °C. The melt front was assumed to move at a constant rate and was approximated by a step-wise process. Simulations were run with the melt at a given radius. When a sufficient amount of time was simulated for the melt to move to the next radial node, the melt position was reassigned to this position.

The off-gas hood above the melt directs contaminants originating from the melt and the soil surrounding the melt into the off-gas treatment system. In these models, a region at the soil surface was used to approximate the effects of the hood. This region had a 20-foot radius, partial vacuum of 1.25 in. water (101,039 Pa), and a temperature of 300°C. These numbers are based on typical large-scale, ISV hood operating conditions.

Destruction of the combustible material in both models was assumed to occur at 500 °C. At this temperature, the mass of the combustible material was converted entirely to gas. This is a worst-case assumption. It allows for more gas generation than is likely in reality (it is more realistic to assume that pyrolysis occurs and only half of the mass is converted to gas). The volatiles given off by the pyrolyzation process were assumed to be equal parts of CO and H_2. A gas mass flow rate and enthalpy was given to each node containing combustible material as its temperature rose above 500 °C. The enthalpy of the released gas was taken to be the average of the assumed product gases at 500°C (h_H= 1.7e+7 J/kg and h_{CO} = 3.93e+6 J/kg from the JANAF Thermochemical Tables[7]). The duration of combustion was assumed to be the time for the melt to move through the node.

Timber Crib Specific Model Features

The timber crib (116-B-6A site) required modeling of the waste crib, which was composed of wooden timbers. This was done by overlaying the crib geometry on the spherical grid and mapping nodes to be specified as wood or soil. The wood nodes were considered impermeable to gas and liquid flow before combustion. After they reached 500°C these nodes were given the same permeability as the soil. Because of the spherical coordinate system used in this problem, it was not possible to model the anisotropic character of permeability between the timbers. In the actual crib, flow is only restricted in one horizontal direction. The horizontal plane is not aligned with any of the spherical coordinates so the restricted flow could not be modeled exactly. Instead, the layers with interspaced wood and soil were assigned an isotropic permeability half that of soil. This simulation assumed a melt rate of 2.54 cm/hr (1 in./hr).

200 Area Trench Specific Model Features

To model the 200 Area trench assumptions were made about the amounts of various constituents present. The constituents modeled were representative of metal (14% by volume), combustible materials (54%), and soil (32%). The cells of the model falling within the trench region were randomly assigned one of these material types, preserving these volume fractions. The nodes assigned with the metal material type were assumed to be impermeable to fluid flow and to have thermal properties midway between aluminum and steel.

For this simulation, it was necessary to make the combustible nodes partially permeable to fluid flow. On average, the scale of these nodes is much larger than the scale of the trench waste pieces.

The assumption that metal and combustible nodes were both impermeable to flow would result in unrealistic restriction and pressure buildup in areas of the model. A permeability half the magnitude of soil was used for the combustible nodes.

Simulations were made that explored the effect of melt progression rate and soil permeability on the buildup of pressure in the soil beneath the melt. The melt rates simulated were 2.54 cm/hr and 5.08 cm/hr (1 in./hr and 2 in./hr). A soil two orders of magnitude less permeable than listed in Table I was also simulated.

RESULTS & DISCUSSION

The results of the crib and trench simulations are discussed in the following section.

Timber Crib Simulation (116-B-6A Site)

The ISV treatment of the timber crib was run for 6.25 simulated days of processing. A trace of the maximum pressure occurring in the soil beneath the melt and the static head of the melt (calculated assuming 70% subsidence) are shown in Fig. 2. The gas pressure beneath the melt is always less than the static head of the melt. This implies that it is unlikely that gas could break through the bottom of the melt and cause a molten soil displacement event. This figure also clearly shows the impact of the burning timbers. Two distinct pressures appear on the graph, one approximately atmospheric (101,350 Pa) and the other approximately 120,000 Pa (2.7 psig). The low pressure regions represent times when the low permeability combustible materials are not burning or affecting the flow patterns. The high pressure region between 42 and 132 hours represents the duration of the timber processing. The high pressure location was consistently located directly below the melt centerline. Pressures steadily decreased along the melt edge toward the soil surface.

[Place Fig. 2 here]

Figure 2. Modeled Pressure History Beneath the Timber Crib ISV Melt

Contour plots in Fig. 3 show the air pressure, temperature, and gas saturation in the soil. These plots represent the conditions 72 hours into the test. The plots represent a vertical plane through the melt, with the melt represented by the black quarter circle in the upper left corner. The region of combustibles (the crib) is outlined in white, with the melt partially penetrating it. The soil surface is along the top of the graphs. Fig. 3 does not show the entire modeled domain, the regions showing interesting phenomena are enlarged to show detail. The entire soil surface shown is covered by the containment hood.

The pressure contour plot shows the pressure buildup in the region of the pyrolyzing crib. Outside the crib, the pressure quickly returns to approximately atmospheric. The gas saturation map shows a dry band surrounding the melt. Beyond this region is the relatively uniform saturation assigned as initial conditions. The effect of the high temperature inside the hood can be seen in the upper right corner of this graph where the region directly below the hood is drying out. The temperature contour plot shows a steep gradient just outside the melt. Temperatures fall from 1300°C at melt surface to 25°C in ~1 meter. The effect of the hood is not as apparent in this plot. The scale required to cover the entire temperature range does not show these more subtle differences.

[Place Fig. 3 here]

Figure 3. Timber Crib Melt after 72 Hours

The calculated flowrates from the soil to the containment hood were approximately 1 m^3/min. This value varied slightly during the test, increasing when combustibles were giving off gas, decreasing when they were not. The off-gas flowrate capacity for the large-scale ISV unit is approximately 10 m^3/min. The difference between the calculated flowrates into the off-gas hood and the capacity of the off-gas treatment system indicate that the off-gas hood would be maintained at a negative pressure.

200 Area Trench Simulations

The model of the region below the ISV melt for the processing of the 200 Area trench was run for 6.25 days for the 2.54 cm/hr melt-rate case, and 3.125 days for the 5.08 cm/hr melt-rate case. This amount of time would be required for processing the waste (the trench modeled was approximately 4.57 m [15 ft] deep).

Fig. 4 shows the predicted gas pressure beneath the melt for the 2.54 cm/hr melt progression rate case. Also shown in this figure is the static head of the melt through the duration of the simulation. The predicted gas pressure is consistently below the melt static head, implying that a breakthrough induced melt displacement event is unlikely. The gas pressures shown in Fig. 4 are the highest pressures observed anywhere around the melt perimeter. These locations were not consistently at the melt centerline. Typically, these were locations with one or more of the neighboring nodes impermeable (metal).

The results shown in Fig. 4 were computed assuming that the combustible nodes were semi-permeable (half the permeability of the soil). An earlier simulation with combustible nodes impermeable showed extreme pressure buildups, far exceeding the static head of the melt. In this simulation, some areas of soil were completely confined, with no means of escape for accumulating gas. This shows the sensitivity of the results from these models to the assumptions made.

[Place Fig 4 here]

Figure 4. Modeled Pressure History Beneath the 200 Area Trench ISV Melt

Figure 5 shows the pressure history for the 5.08 cm/hr (2 in./hr) melt rate. The gas pressure shows the same peaks as the 2.54 cm/hr melt rate simulation, but their magnitude is greater. At 0.6 days, the gas pressure beneath the melt actually exceeds the static head of the melt. This implies that a molten soil displacement event could potentially occur.

[Place Fig. 5 here]

Figure 5. Modeled Pressure History Beneath the 200 Area Trench ISV Melt, 5.08 cm/hr Melt Rate

Figure 6 shows the pressure history of the lower permeability soil simulation (2.54 cm/hr melt progression rate). Again, the same pressure peaks appear in the figure, but the magnitude is much greater. The maximum pressure seen during this simulation occurred at 4 days, at 245,000 Pa (21.8 psig). This figure shows the potential danger of vitrifying combustible wastes in low permeability soil.

[Place Fig. 6 here]

Figure 6. Modeled Pressure History Beneath the 200 Area Trench ISV Melt, Low Permeability Soil

Pressure, temperature, and gas saturation contour plots of the 200 Area trench (2.54 cm/hr and baseline soil permeability) 99 hours into the simulation are shown in Fig. 7. Small areas of locally high pressure (up to 140,000 Pa - 5.6 psig) can be seen in the area beneath the melt. These areas have elevated pressures due to impermeable metal regions near them. Liquid in the nodes boils or combustion gases are released and are unable to dissipate into the surrounding soil. The temperature contour plot is very similar to that of the timber crib simulation. The steep temperature gradient near the melt and the slight warming at the soil surface due to the presence of the off-gas hood are the only remarkable features. The gas saturation plot shows local areas of high saturation within the trench. These areas are partly an artifact of the modeling method. Metal nodes were assigned gas saturations of ~1. These areas, as well as the dry soil nodes, appear red in this plot. The soil surface is much drier than in the simulation for the timber crib because these plots are made later in the test (99 hours versus 72 hours, respectively).

[Place Fig.7 here]

Figure 7. Trench ISV Melt after 99 Hours

Contour plots were not included for the faster melt rate and lower soil permeability simulations because they closely resemble those presented in Fig. 7.

The flowrate into the off-gas hood is approximately the same as predicted in the 116-B-6A simulation, ~1 m^3/min. As was the case for the timber crib simulation, this implies that the off-gas hood could be maintained at a negative pressure. This does not consider the added flowrate that could be released if a significant displacement of molten soil event occurs. Such an event could cause a sudden increase in gas flowrate to the hood.

CONCLUSIONS AND RECOMMENDATIONS

The following conclusions have been drawn based on the TOUGH2 simulations of the timber crib and 200 Area trench with compressible material:

- The timber crib ISV melt simulation predictions agreed with observed evidence that large-scale "glass displacement events" did not occur.

- Given the assumptions in loading (32% soil, 54% combustibles, and 14% metal by volume), random distribution, and combustion by-products, a "glass displacement event" is unlikely to occur while vitrifying the wastes typical of the 200 Area trench.

- Loading of impermeable wastes in regions to be vitrified can dramatically increase local pressures to the point of creating a "glass displacement event".

- Soil permeability and melt rate strongly affect the buildup of pressure beneath the melt when combustibles are present.

Based on these findings, the following recommendations for future work are given:

- To ensure that the particular random loading used in this work represents reality, a statistical sampling of ISV with other random loadings should be modeled.

- The loading of metals was only considered for the effect on soil permeability in this work. It is important to also consider the effect of metals on electrical driving and uniform melt progression.

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