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CFD Model for the WSRC Am/Cm Melter

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CFD MODEL FOR THE WSRC AM/CM GLASS MELTER (U)

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ABSTRACT

Decades of nuclear material production at the Westinghouse Savannah River Company (WSRC) have resulted in the generation of kilogram quantities of Am and Cm isotopes. The isotopes, which have great commercial value, are stored as a nitric acid solution and are intensely radioactive. In order to stabilize the material, the Am/Cm isotopes will be vitrified by depositing a liquid feed stream containing the isotopes in solution together with a stream of glass frit onto the top of a molten glass pool. Isotope vitrification is to be a batch process with separate feeding, idling and pouring phases.

The melter has the form of a tall rectangular box and is composed of an 80 wt% platinum, 20 wt% rhodium alloy, which is resistively heated. A resistively heated plenum is used to apply thermal radiation to the surface of the glass pool. During the feeding phase, a packed bed of frit and evaporating liquid (referred to as a cold cap) is formed at the surface of the glass pool. Evaporation, along with the heating of the frit and non-volatile feed components in the cold cap, accounts for the majority of the power supplied during the feeding phase. After feeding is complete, the melter is idled and the glass pool is allowed to homogenize. During the idling phase, the power demand at the top of the melter decreases. To accommodate the increased demand for power at the top of the melter during the feeding phase and the requirement for a more uniform power distribution during the idling phase, a unique split power supply was developed.

Natural convection within the glass plays a major role in heat transfer to the cold cap and in the uniform distribution of isotopes in the glass. Variations in the power distribution and heat loss through the walls of the melter result in temperature differences that drive convection. However, the strong dependence of the glass viscosity on temperature significantly affects flow patterns, especially in the neighborhood of the cold cap. In order to gain insight into the complex flow and thermal processes occurring in the melter and to assess design modifications, a computational fluid dynamics model was developed with the AEA CFX-F3D® and CFX-RADIATION® software. The temperature dependent properties for the glass were utilized and the coupled effects of conduction, convection and thermal radiation were included in the model. Because the glass is opaque to thermal radiation, radiation heat transfer calculations were only required in the vapor space of the plenum. Conjugate heat transfer from the glass and the vapor to the surrounding

refractory material was treated in the calculations. External boundary conditions, based on the ambient environment, were applied at the outside of the refractory. Power densities in the platinum alloy, consistent with boundary conditions for the applied electric current, were calculated with the ABAQUS® finite element software and input to CFX-F3D®. The heat sink resulting from evaporation in the cold cap was also included. In the plenum, flow resulting from evaporation at the surface of the cold cap was modeled by defining a mass source. The model predicted flow patterns in the glass pool and the vapor space of the plenum, as well as, temperatures in the melter and refractory material. Heat fluxes and temperature dependent material properties and were also calculated. The model predictions were compared with data from tests on an experimental melter and good agreement was observed.

INTRODUCTION AND BACKGROUND

Nuclear material production campaigns at the Savannah River Site (SRS) have resulted in the generation of kilogram quantities of Am and Cm isotopes. The isotopes possess great commercial value but are in the form of an intensely radioactive nitric acid solution. The isotopes must be transported from SRS to the Oak Ridge National Laboratory (ORNL) for processing, which will take place over several decades. In order to stabilize the isotopes, it has been proposed that they be vitrified.

Vitrification will be a batch process with separate feed, idling and discharge phases. The melter is to be a resistively heated Pt/Rh alloy vessel, see Figure 1.

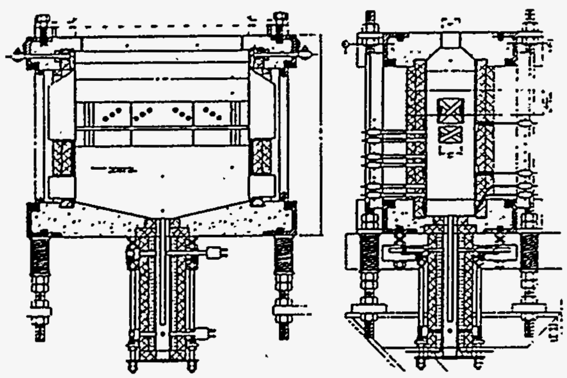

Figure 1 Front and side schematic of melter and drain tube assembly.

During the feed phase, a liquid feed stream containing the isotopes in solution, together with a stream of glass frit, will be deposited onto the surface of the molten glass pool. The feed and frit streams form a porous bed, within which the liquid component boils. The majority of heat supplied to the melter is required to evaporate the liquid component of the feed. Due to the boiling process the temperature in the upper part of the bed is near 373 K, which is much lower than the surrounding glass pool. Hence, the bed is referred to as a cold cap. As the bed is incorporated in to the pool, the isotopes chemically combine with the glass to produce durable (low leachability in water) glass. After the melter has been filled, it will be idled to allow the glass to homogenize by convective mixing. Following the idling period, the glass is to be discharged from the melter through a freeze valve located at the bottom of the melter. The glass discharged from the melter is collected in a cylindrical stainless steel canister which is then sealed, cleaned and stored.

During the feeding process, evaporation from the cold cap requires that more power be delivered to the upper portion of the melter than to the bottom. After the feed phase when evaporation from the cold cap has stopped and the material has been incorporated into the glass, the required power distribution between the top and bottom of the melter will become more uniform. During the idling phase, the power distribution may be need to be changed to enhance convective mixing. A split power supply attached to the upper and lower pairs of electrodes on the melter, see Figure 1, will be used to shift the power distribution as needed during the different phases of melter operation.

The isotopes generate a significant amount of heat and radiation. Therefore, it is necessary to homogeneously distribute the isotopes in the product glass to avoid high local concentrations. Further, lanthanides in the liquid feed stream are required to reduce the glass viscosity to values assumed for melter design. Hence, adequate mixing is necessary to distribute the lanthanides throughout the glass. The diffusion rate in the glass is very slow, hence, for practical purposes mixing is driven by natural convection. In the glass pool, natural convection is not only a function of glass density but also of glass viscosity, which is strongly dependent on temperature. Because hot glass from the bottom of the melter is carried to the top, convection also plays a significant role in heat transfer to the cold cap. In order to better understand the convection processes in the melter, a computational fluid dynamics model was developed. The model was compared to experimental data and was capable of predicting quantities, such as glass flow patterns that could not be measured directly. The model was used to guide system design and to evaluate the overall practicality of the system. By using the model to estimate the significance of physical changes to the system, the number of necessary experimental tests was reduced.

SYSTEM DESCRIPTION

The geometry of the platinum alloy vessel is shown in Figure 2. The vessel has the form of a rectangular box whose bottom is in the shape of a truncated V. The drain tube is centered at the bottom of the melter. Inside the melter, there are two pairs of heater screens which span the width of the vessel. The screens act as shunts for the current and provide heated surfaces with large areas for heat dissipation within the melter. The air space above the glass pool, enclosed by the Pt/Rh shell, is referred to as the plenum. The exit from the plenum to the offgas system, located at the top of the vessel, is shown as a slot with semi-circular ends in Figure 2.

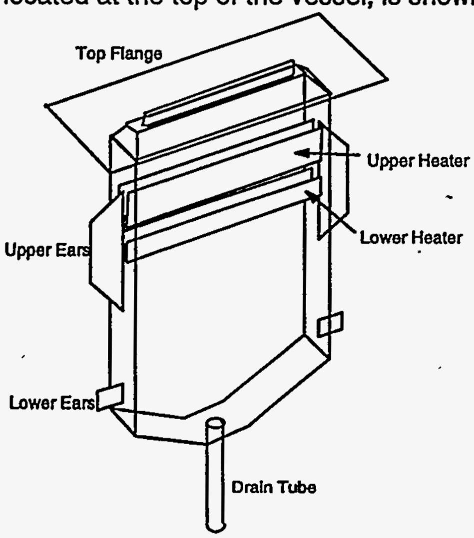

Figure 2 Schematic of Pt/Rh alloy vessel.

The vessel is composed of an 80 wt% Pt-20 wt% Rh alloy. The interior height was approximately 30 cm., the internal width from ear to ear was approximately 25 cm., and internal depth from front to back was approximately 7 cm. The walls of the vessel were 1.52 mm thick. The top flange, shown in Figure 2, was not included in the CFX model.

Because the glass is non-conducting, electrical current only flows in the Pt alloy shell of the melter. Therefore, the heat source for the melter and plenum models is the electrical power dissipation in the platinum alloy vessel. The power distribution in the vessel is governed by the current split applied to the upper and lower electrodes of the melter. The electrodes, also referred to as "ears", are the tabs seen on the narrow side of the melter in Figure 2. The clamps connecting the ears to the power supply are water cooled.

The vertical sides of the melter are insulated with Kaowool® 15C board manufactured by the Thermal Ceramics of Augusta, GA. To allow for thermal expansion, a layer of Fiber-frax® paper, approximately 3 mm thick, was placed between the Kaowool and the platinum alloy vessel. The bottom and top of the melter are insulated with KAST-O-LITE 30® castable refractory material manufactured by A. P. Green Industries, Inc., Mexico, MO. The outer surfaces of the refractories are exposed to air at approximately 30°C. A drain tube assembly (a freeze valve) is located at the bottom of the melter.

When the melter is full, the glass pool is to be at approximately 1.27 cm above the top heater plate. The plenum volume above the glass pool will contain a mixture primarily consisting of air and water vapor, which are respectively introduced through an air purge and from evaporation of the liquid component of the feed.

MODEL DESCRIPTION

Flow and thermal and modeling for the Am/Cm melter was performed with the AEA CFX-F3D® general purpose computational fluid dynamics software. CFX-F3D is a finite volume code which solves the coupled mass, momentum and energy conservation equations in three dimensions. CFX-F3D was used to perform conjugate heat transfer calculations, and with the module CFX-RADIATION®, was used for thermal radiation calculations. CFX-RADIATION performs thermal radiation calculations based on the user's choice of Monte-Carlo or Shah's method (the method of rays). Shah's method was used for all calculations in this paper. Combined CFX-F3D and CFX-RADIATION calculations will be referred to as CFX calculations.

The melter was modeled as a quasi-steady process in which the glass level was constant and the cold cap experienced a steady rate of evaporation set equal to the feed rate of volatile liquid. The approximation of a fixed glass level was justified by the low feed rate, approximately 2.5 L/hr. Material properties which vary with temperature, as well as complex boundary conditions were incorporated in the user FORTRAN subroutines of CFX-F3D. The glass and the air-steam mixture in the melter were thermally coupled to ambient conditions by conjugate heat transfer and conduction calculations through the vessel and refractory walls. Although the glass is opaque to thermal radiation, it is the dominant mode of heat transfer in the plenum which is filled with a mixture of water vapor and air.

To reduce the number of cells to a manageable level, the melter was modeled in quarter symmetry. Based on the prescribed mode of operation, geometry and power distribution, the melter system possessed reflective symmetry about the normal vertical planes passing through the centers of the wide and narrow sides of the melter. The symmetric model tacitly assumed that the melter would retain its symmetric shape throughout operation. Some asymmetries were introduced via modifications to the offgas and cover designs but it was felt that these effects would not be excessive relative to other assumptions made in the model.

CFX4 is only capable of performing thermal radiation calculations for a single phase fluid system. Therefore, the system was divided into two separate models, one for the melter below the surface of glass pool and one for the melter plenum above the glass pool. The model assumed steady feeding with the top of the glass pool located at 1.27 cm above the top heater screen. In this paper, the part of the system (including refractory material, platinum alloy vessels and contents) below the glass pool will be referred to as the melter model and the part of the system above the glass pool will be referred to as the plenum model. The combined melter and plenum model will be referred to as the melter system model. The two models were linked by supplying calculated temperatures at the top of the melter model as boundary conditions to the bottom of the plenum model, while heat fluxes calculated at the bottom of the plenum model were supplied as boundary conditions to the top of the melter model. UNIX script was used to run the two models for a fixed number of iterations and to launch programs that estimated the iterative error in the interfacial boundary conditions of temperature and heat flux.

The mesh for the melter model was generated with CFX-MESHBUILD and contained 155,548 cells. The overall grid was based on a 4 cell thickness across all components of the Pt/Rh shell. The remainder of the grid was built by smoothly transitioning cell sizes as the mesh moves outward from the platinum alloy shell. To keep the number of cells to a reasonable value, two geometric approximations were made to the geometry of the melter model. First, the castable refractory was assumed to follow the bottom of the platinum alloy vessel. The approximation was made because the triangular topology formed by the castable refractory and the sloped bottom of the platinum alloy shell is difficult to represent as hexahedral blocks and cells, as required by

CFX-4. The second approximation was the representation of the circular holes in the melter screen as rectangles.

The mesh for the plenum model was generated with CFX-MESHBUILD and contained 118,239 cells. The fluid in the plenum was modeled as air with water vapor which was introduced at a rate equal to rate of evaporation of the liquid component of the feed. Evaporation was represented by locating a volumetric mass source at the cold cap and introducing water vapor at the saturation temperature. The plenum outlet was assumed to extend over the entire slot at the top of the plenum and is represented with a pressure boundary patch. The plenum outlet was assumed to be a black absorber for thermal radiation.

Heat Source

The heat source for the melter system is the dissipation of electrical energy in the platinum shell. For a given power split, the local power densities in the shell were calculated with the ABAQUS® finite element code [Gong and Hardy, 1997]. ABAQUS solves the microscopic form of Ohm's Law and utilizes the electrical currents applied to the top and bottom ears as boundary conditions. It was found that for a given power split, the local power density is directly proportional to the total power. For all calculations presented in this paper the total melter power was 13.5 kW with 100% of the power delivered to the upper ears.

Because the electrical current flows in the Pt/Rh shell of the plenum, the heat source must be applied there, as for the melter model. The power distribution in the plenum shell results in thermal radiation heat transfer to the surface of the glass pool, which is applied to the glass pool of the melter model through the interface with the plenum model.

Boundary Conditions

Correlations for natural convection and thermal radiation boundary conditions were applied to the exterior refractory surfaces. The plenum exit was assumed to be 500°C and to be a black absorber of thermal radiation. At the outer edge of the ears, the temperatures were maintained at 60°C due to water cooling of the power supply clamps attached there.

Interfacial Conditions

The interface between the melter and plenum serves as a boundary for each of the individual models. At the interface, plenum and melter model temperatures must be equal and energy must be conserved. The physics of the melter system dictate that the interface be divided into three regions: 1) the cold cap, 2) the glass pool and 3) the Pt/Rh shell and refractory. At the cold cap, the interfacial temperature was fixed. Plenum calculations accounted for thermal radiation heat transfer to the glass pool and cold cap. At the interface of the refractory, vessel and the surface of the glass pool outside the cold cap the temperature and heat fluxes were equated.

As the frit and liquid feed are deposited onto the glass surface they form the cold cap, which is a porous bed. The liquid component of the feed undergoes packed bed boiling within the cold cap and the frit and non-volatile materials from the feed become heated. Because heat transfer and flow within the cold cap is extremely complex, it was not explicitly modeled in this study. In the model, the cold cap was assumed to be of infinitesimal thickness and of fixed area. Further, it was assumed that the liquid component of the feed had the same properties as pure water. Therefore, for both the plenum and melter models it was assumed that the temperature of the area subtended by the cold cap was the saturation temperature for water at atmospheric pressure, namely, 100°C (373.15 K). The feed rate of the volatile liquid (assumed to be water) was 2.5 l/hr and the feed rate of glass frit was 0.4 kg/hr.

In reality, the cold cap area will vary depending on the amount of heating and the feed rate. Fixing the cold cap area and temperature will be exactly correct only if the total heat flux to the cold cap equals the energy required to evaporate the liquid and heat the frit and dissolved solids to the local glass pool temperature at the feed rate. However, specifying the cold cap area and temperature, while letting the heat flux vary, prevents over specification of the problem. From the steady state energy balance and the frit to solution feed ratio, the required feed rate to obtain an energy balance was calculated. The calculated feed rates were then compared to the actual feed rates to determine whether the assumed cold cap area was approximately correct. In this way, fixing the cold cap temperature and area leads to reasonable estimates for the glass temperature profile away from the cold cap without introducing excessive complexity to the model.

Material Properties for Glass

Glass Viscosity

If T > 1703 K then

$$\mu_{glass} = 1.024\ \mathrm{Pa-s}\ .$$

If T ≤ 1703 K then

$$\mu_{glass} = 48440.-83.760\times T + 4.826\times 10^{-3}\times T^2 - 9.266\times 10^{-6}\times T^3\ .$$

Where: m_{glass} = glass viscosity in Pa - s
T = glass temperature in K.

Glass Thermal Conductivity

If T > 1423.15 K then

$$k_{glass} = 6.07\ \frac{W}{m\ K}\ .$$

If 1221.15 K ≤ T ≤ 1423.15 K then

$$k_{glass} = -28.060 + 0.024\times T\ .$$

If T< 1221.15 K then

$$k_{glass} = 1.32\ \frac{W}{m\ K}\ .$$

Where: k_{glass} = glass thermal conductivity in $\frac{W}{m K}$
T = glass temperature in K.

Glass Density

If T ≥ 1221.15 K then

$$\rho_{glass} = 2811.364 - 0.111\times T - 1.050\times 10^{-4}\times T^2\ .$$

If T< 1221.15 K then

$$\rho_{glass} = 2419.88\frac{kg}{m^3}\ .$$

Where: ρ_{glass} = glass density in $\frac{kg}{m^3}$
T = glass temperature in K.

Glass Specific Heat

Over the range of temperatures for the Am/Cm melter model, the specific heat is given by

$$C_{P_{glass}} = 803.366 + 0.565\times T - 1.400\times 10^{-4}\times T^2\ .$$

Where: $C_{P_{glass}}$ = glass specific heat in $\frac{J}{kg K}$
T = glass temperature in K.

Platinum Alloy and Refractory Data

Constitutive property data for the Pt alloy of the melter vessel and the refractory materials are given in Table 1.

Table 1
Pt/Rh Alloy and Refractory Data

Material	k (W/m °C)	ρ (kg/m³)	C_p (J/kg °C)
90/10 Pt/Rh Alloy	79.	18720.	133.98
Castable Refr.	0.63	1450.0	1250.
Kaowool 15c	0.25	192.	1130.

RESULTS

The steady state melter and plenum calculations showed the temperature distributions and flows occurring during the feed phase with a total power of 13.5 kW and 100% of the power applied to the upper ears. The most important result of the CFX4 calculations was the three-dimensional visualization of flow patterns and temperature profiles that could not be measured. External temperatures predicted by the model were in reasonable agreement with those measured during operation of an experimental melter. From the temperature profiles in Figures 3 and 4, it can be seen that the lowest temperatures in the melter occur at the side to which the electrodes (ears) are attached. Although the current, and thus the power density, is greatest in the ears, the cooling of the power supply clamps removes sufficient heat to offset the higher heat generation rate. This situation emphasizes the need to include all components of the energy balance for the melter, rather than focusing only on the rate of electrical energy dissipation. The cold cap, fixed at 100°C (373.13 K), can clearly be seen in Figures 3 and 4. Figure 3 shows the extent to which the cold cap affects the temperature of the glass pool.

Glass flow patterns in the melter are displayed in the vector profile of Figure 5 and the streamlines of Figure 6. Figure 6 shows the large scale pattern for convective flow predicted by the model. For the glass properties and melter powers used in this analysis, the predicted glass velocities were very low. Overall, the model predicts that the convective flow within the glass pool goes upward along the large side of the melter, flows over the upper screen and then downward through the center of the melter between the opposing screens. By using the CFX4 post processor to apply animated markers which move in the direction of the glass flow, it was seen that the glass followed along a spiral path about the upper and lower screens from the narrow vertical midplane of the melter toward the wall at which the ears are attached. The narrow side wall is at a low temperature due to the water cooled clamps on the ears. Hence, near the wall the glass cools, increases in density, and falls to the bottom of the melter, moving downward along the tapered bottom. As the glass moves along the bottom of the melter it becomes heated, less dense, and begins to rise near the narrow vertical midplane of the melter, adjacent to the large face, to repeat the flow pattern. At the narrow midplane beneath the center of the cold cap, the glass is cooled and flows downward to the bottom of the melter. Flow is observed to pass through the perforations in the screens, as well as between the upper and lower screen. Consistent with the flow pattern of Figures 5 and 6, the temperature profile of the glass surface in Figure 4 shows an upwelling of hot glass in the corner of the pool. Glass upwelling at the corners of the pool have been visually observed during melter experiments. The streamlines shown in Figure 6 and the velocity vectors shown in Figure 5 indicates that glass flows around the region of cold, high viscosity glass below the cold cap. In the neighborhood of the cold cap, the glass is of sufficiently high velocity to be nearly rigid.

Volatilized material and small particles entrained in the plenum vapor can result in deposition and fouling of the offgas system. In the past offgas system design has relied on rough approximations and limited empirical data. Therefore, the ability to predict plenum flows and temperatures, as shown in Figures 7 and 8, is particularly important. In future models, particles having size and density characteristic of those ejected from the glass surface will be inserted into the flow. The calculated particle trajectories will determine the potential for carryover in to the offgas system and will be used to identify necessary system modifications.

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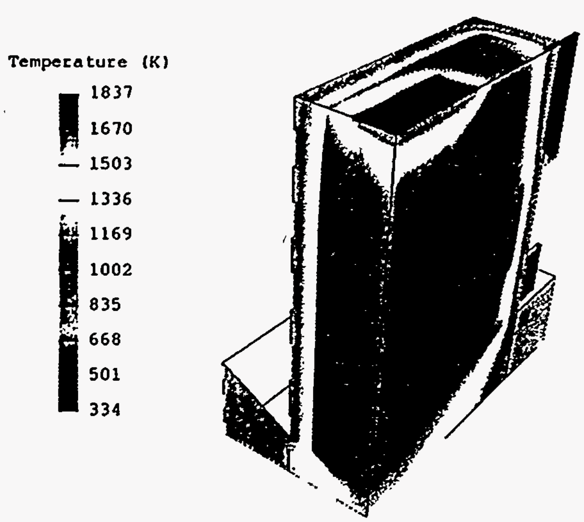

Figure 3 Temperature profile in glass pool.

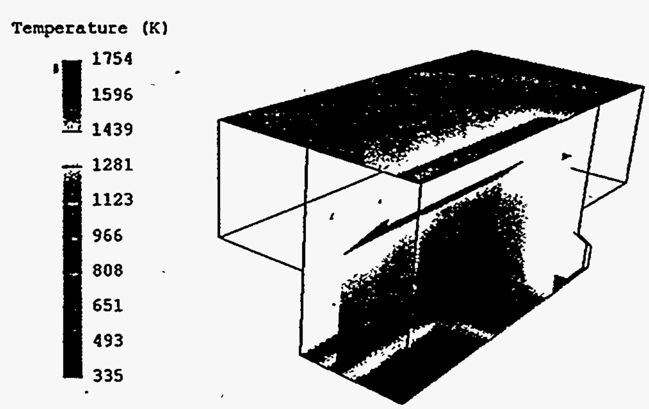

Figure 4 Plenum temperature profile.

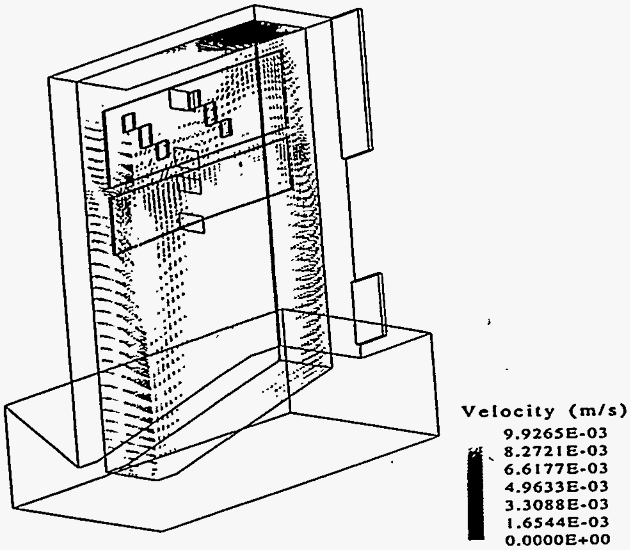

Figure 5 Velocity vectors in glass pool.

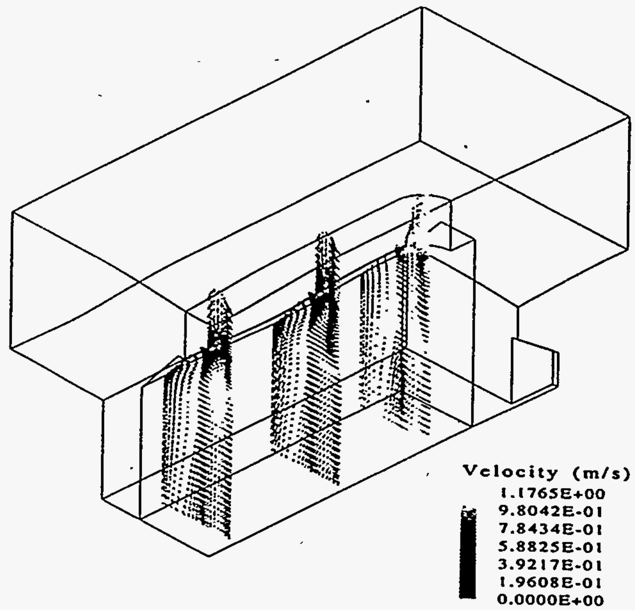

Figure 7 Plenum velocity vectors.

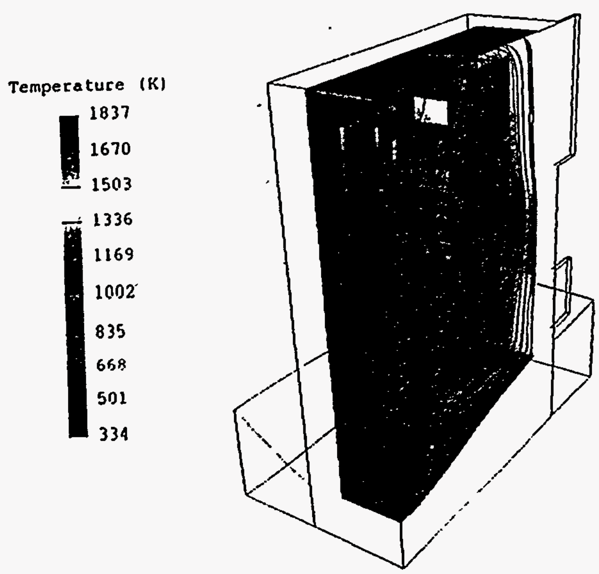

Figure 6 Streamlines and temperatures in glass pool.

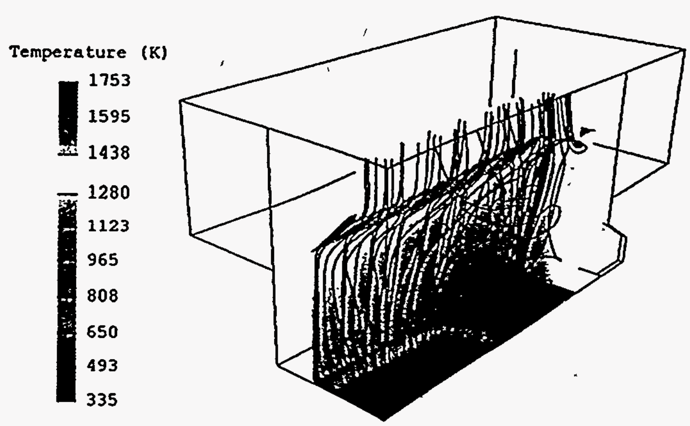

Figure 8 Plenum streamlines and temperatures.