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# NUMERICAL MODELS OF WASTE GLASS MELTERS
# PART II - COMPUTATIONAL MODELING OF DWPF

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## ABSTRACT
Computational fluid-dynamics numerical models are developed for joule-heated slurry fed waste glass melters, such as the Defense Waste Processing Facility Melter. An important feature of the analyses is the simulation of the cold cap region with its thermally resistant foamy layer. Using a simplified model which describes the foam void fraction as a function of temperature, based on laboratory sample testing, characteristic features of the cold cap are simulated. Two- and three-dimensional models are presented.

## INTRODUCTION
The performance of radioactive waste glass melters, such as the Defense Waste Processing Facility, would benefit from a detailed thermal-hydraulic analysis using computational methods in order to improve the prediction of glass melt rates and thus glass production rate of the melter. Specific goals of such an analysis would be:

- to predict the melt rate for known thermo-physical properties of various waste batches,
- to optimize melter operating conditions for maximum glass production, and
- to evaluate the effect of melt rate enhancing devices such as bubblers.

By providing predicted temperature distributions within the bulk glass, melter temperature readings can be interpreted properly with respect to operational limits to avoid local glass overheating, or reaching lower glass transition temperatures. Further, knowing potential flow distributions may lead to strategies for increasing convection to the melting cold cap.

The model presented in this paper is a simple one but still incorporates important features of the melt pool and cold cap by which some insights can be made on the melter temperature and flow distributions. This is first illustrated with a two-dimensional model, which is useful for parametric studies. Finally, a three-dimensional model was generated to demonstrate the effect of a full three-dimensional geometry. The computational model complements the Lumped Parameter approach (Ref. 1) by providing the average effect of nonuniform temperature and flow distributions on heat transfer coefficients to the cold cap.

On the other hand, the Lumped Parameter model, based on melter operating data provides known boundary conditions for the computational model.

The DWPF Melter, a joule-heated glass melter, uses a slurry feed of glass frit, water and waste which forms a semi-solid cold cap on top of the glass. The thermal analysis of the melter is complicated by the interplay of three separate heat transfer problems. First, the glass pool is electrically heated by passing direct current through the molten glass. Temperature gradients set up by the introduction of a glass slurry on top of the glass surface produce natural convection currents within the bulk glass. Further, these temperature gradients set up non-uniform electrical heat generation due to the positive temperature coefficient of electrical conductivity of the glass. Second, the cold cap formed by evaporation of the slurry water, is heated from above by radiant heat from the dome heaters and plenum walls and from below by convection from the bulk glass. The cold cap consistency, its radial thickness variability, and foaming characteristics are largely unknown. Third, the radiant heat impinging on the cold cap depends on radiant heat exchange between the cod cap, the dome heaters' surfaces, the walls, and the steam, which participates in the exchange.

ANALYTICAL METHOD

The approach taken here is to analyze the glass and cold cap as a unit and utilize the radiant heat absorbed by the cold cap as a boundary condition. The radiant heat problem in the plenum would be solved separately, where the boundary conditions at the cold cap surface (temperature and heat flux) must match the assumed boundary conditions in the glass/cold cap model.

The computational fluid-dynamics software package, FIDAP, was used to predict the temperature and flow distributions in the electrically-heated glass pool. FIDAP has the advantage that joule heating is already incorporated in the code. The differential equations solved are:

<u>Continuity and Momentum Equations</u>

$$\nabla . u = 0 \qquad [1]$$

$$\rho\, u\, .\nabla u = -\nabla P + \rho\, g\; \beta (T - T_r) + \mu \nabla^2 u \qquad [2]$$

<u>Energy</u>

$$\rho\, c_p\, u \cdot \nabla T \quad = \quad k\, \nabla^2 T \quad + \quad \rho\, \alpha_E\, (\nabla \Phi)^2 \qquad [3]$$

<u>Joule Heating</u>

$$\rho\, \alpha_E\; \nabla^2 \Phi = 0 \qquad [4]$$

where $u$ is velocity; $T$ , temperature; $\phi$, electric potential; P, pressure; $\rho$, density; g, gravitational constant, $\beta$, volumetric coefficient of expansion, $\mu$, viscosity, k, thermal conductivity; $c_p$, specific heat; and $\alpha_e$, electrical diffusivity.

**Modeling Considerations**

Previous modeling efforts have utilized simple boundary conditions (B.C.) in place of the cold cap, such as constant heat flux or constant temperature boundary conditions. These assumed boundary conditions however resulted in contradictory results where flow is upward in the center of the melter for constant temperature B.C. and downward for constant heat flux B.C. To eliminate this seeming contradiction, the present work prototypically includes a cold cap, which is characterized by variable thermal conductivity, electrical conductivity, specific heat, and viscosity, which are all functions of temperature. In addition, the latent heat of melting of glass and heats of chemical reactions are included in the energy equation.

One of the major problems in modeling the cold cap is how to represent the foamy layer. This thermally resistant layer is clearly important, as demonstrated by significant melt rate decreases observed with certain DWPF feed batches (Ref. 1). Theoretically, the best approach is to model the growth of bubbles by diffusion of gases from chemical reactions and the transport of these bubbles by convective and diffusive forces. However, the pertinent experimental data on diffusion coefficients for molten glass are unavailable. Consequently, our approach is to assume that a steady foam void fraction forms in the cold cap at various temperatures similar to the experimental results of batch sample tests performed in laboratory. Here, samples of waste glass frit are loaded into ceramic crucibles, melted and held at various temperatures for 2 hour sand then pulled out of the oven. Samples sectioned show that for Frit 200, bubbles do not form below 700$^o$C, then go to a maximum value of about 50% at 750$^o$C, and then disappear above 800$^o$C.

The effective thermal conductivity of the cold cap, $k_{eff}$, is then the liquid thermal conductivity, $k$, multiplied by the liquid fraction, or,

$$k_{eff} = k(1-\alpha) \qquad [5]$$

where $\alpha$ is the void fraction and is estimated from steady state melt sample testing in the following temperature ranges as:

| | | |
|---|---|---|
| $\alpha$=0 | T<700 $^o$C | [6] |
| $\alpha$=0.5(T-1023) | 700<T<750 $^o$C | |

$\alpha$=0.5[1-(T-1023)] 750<T<800 $^oC$
$\alpha$=0 T>800 $^oC$

The specific heat of glass is shown in Figure 5. On the same plot is a curve for the specific heat of the cold cap. This includes the effect of heat of reaction of chemical reactions in the temperature range, 973-1173$^o$K. This specific heat is defines as,

$$Cp_{cc} = \frac{\int (Cp_g + L)dT}{\int dT} \qquad [7]$$

where L is the sum of heats of reactions.

TWO-DIMENSIONAL MODEL DESCRIPTION

The 2D model is basically a rectangular region with upper and lower electrodes located along the vertical sides. The width is 1.42 m, which simulates the actual distance between electrodes in the DWPF Melter. The height of the glass, 0.914 m, is also the same as in the melter. A cold cap region, which is included in the 0.914 m dimension, is 1.18 cm high. The outlet pipe is located at the bottom of the melter, since for this 2D model, placing it on the side-wall would interfere with the electrodes at that wall. The depth of the model can be considered to be 1.02 m which is the electrode depth in the melter. The model had 20,000 cells.

The cold cap area is assumed to cover the entire top surface of the melter model. The boundary conditions at the cold cap top surface is a parabolic temperature distribution, starting at 300$^o$C at the center (where the feed-pipe for the slurry feed is located) and increasing to 850$^o$C at the edges. This cold cap surface temperature variation is an initial guess to connect a cold cap temperature (300$^o$C) close to film boiling conditions where the slurry feed is injected to a an exposed glass temperature at the edges calculated in the Lumped Parameter report (Ref. 1).

A flow boundary condition at the cold cap is based on a total feed rate of 68 Kg/hr. This flow is assumed to have a parabolic profile across the cold cap surface such that the flow is maximum at the edges and zero at the center. This flow distribution is based on the premise that the foam underneath the cold cap is thinnest at the edges and thickest at the center of the cold cap as the chemical reaction gases migrate to the periphery of the cold cap. During small-scale melter tests, gases were observed to vent at the cold cap periphery. Consequently, the melt rate would be highest at the edges and lowest at the center. The rest of the boundary conditions are convective heat transfer coefficients on the side wall and the bottom surface, based on a reference temperature of 940$^o$C, which is a measured DWPF Melter electrode temperature. These coefficients were chosen so that the calculated heat fluxes (losses) after the solution was obtained would be equal to the melter heat losses obtained from the Lumped Parameter Model.

The method of solution is as follows: First, the electrode potentials are guessed and a solution is obtained. Then the heat losses through the cold cap, side wall and bottom surface are calculated. The convective coefficients are iterated until the calculated and prescribed heat losses match.

The prescribed heat flux at the cold cap represents the heat transferred from the melt pool through the cold cap, including the foam layer, after supplying heat to raise the glass temperature from the cold cap surface temperature to the bulk glass temperature, as well as any chemical reaction heat. This left over heat is available for evaporating slurry water, in addition to radiant heat from the dome heaters and plenum walls. The boundary condition for the cold cap, as stated above, is a temperature boundary condition and not a heat flux. After the solution, the heat loss through the cold cap is calculated and compared with the prescribed heat loss above. A solution is achieved if the calculated flux matches the required flux. Otherwise, the convection coefficient is changed and another iteration step is done. A converged solution is one with an error less than $10^{-4}$.

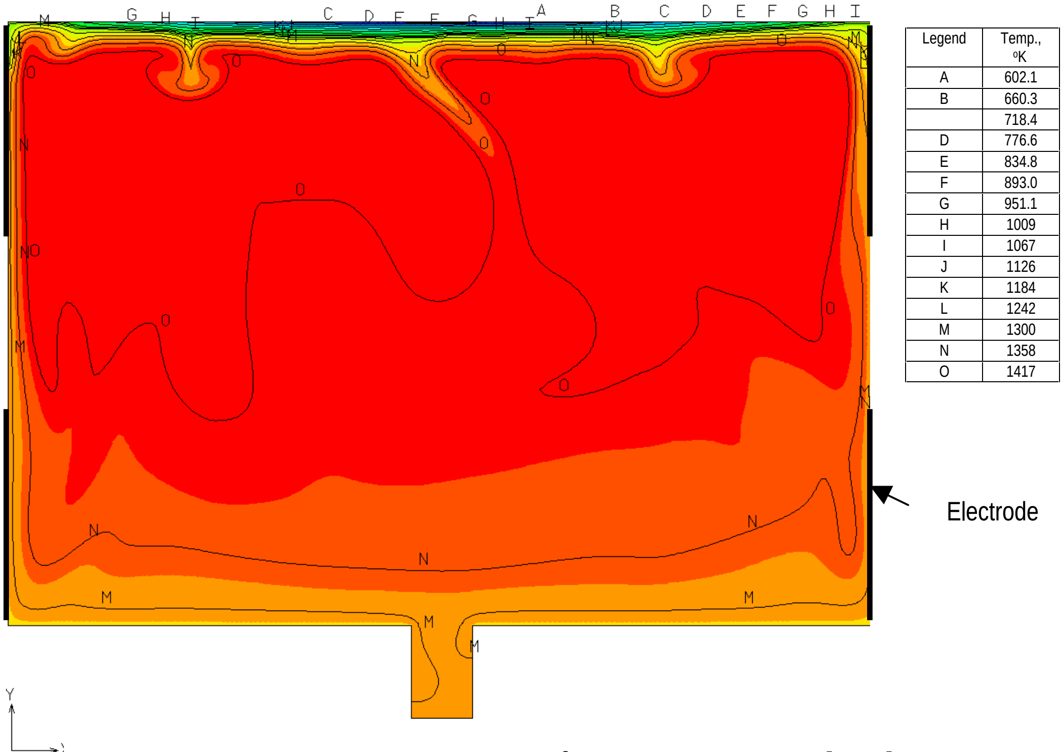
A summary table of results is given for an electrode potential drop of 75 volts. The side wall surface flux is higher than in the actual melter because for this 2D model, there are no heat losses to the front and back sides. The total electrode density translate to a melter power of 140 kW, taking into account the actual melter volume.

Table 1 Summary Table for Two-Dimensional Model

| Two Dimensional Model | Electrode Potential Drop=75 volts |
|---|---|
| Ave. Melt Pool Temp. | 1381$^o$K |
| Ave. Melt Pool Velocity | 0.000836 m/s |
| Cold Cap Surface Flux | 17.1 kW/m$^2$ |
| Side Wall Surface Flux | 16.1 kW/m$^2$ |
| Bottom Surface Flux | 3.2 kW/m$^2$ |
| Glass Melting Power | 8.5 kW/m$^2$ |
| Total Electrode Power Density | 66 kW/m$^3$ |

<u>Temperature Distribution</u>

The predicted temperature distribution with an electrode potential difference of 75 volts is shown in Figure 1. The average pool temperature (excluding the cold cap) is 1381$^o$K (1108$^o$C). The temperature distribution of the cold cap shows a region of low temperatures (less than 1358$^o$K or 1085$^o$C) that is thick at the center and tapers to a thin section near the walls. The temperature distribution in the




| Legend | Temp., ºK |
|---|---|
| A | 602.1 |
| B | 660.3 |
|  | 718.4 |
| D | 776.6 |
| E | 834.8 |
| F | 893.0 |
| G | 951.1 |
| H | 1009 |
| I | 1067 |
| J | 1126 |
| K | 1184 |
| L | 1242 |
| M | 1300 |
| N | 1358 |
| O | 1417 |

Figure 1 Temperature Contour Map for Two-Dimensional Melter Model at 75 Volts Potential Drop

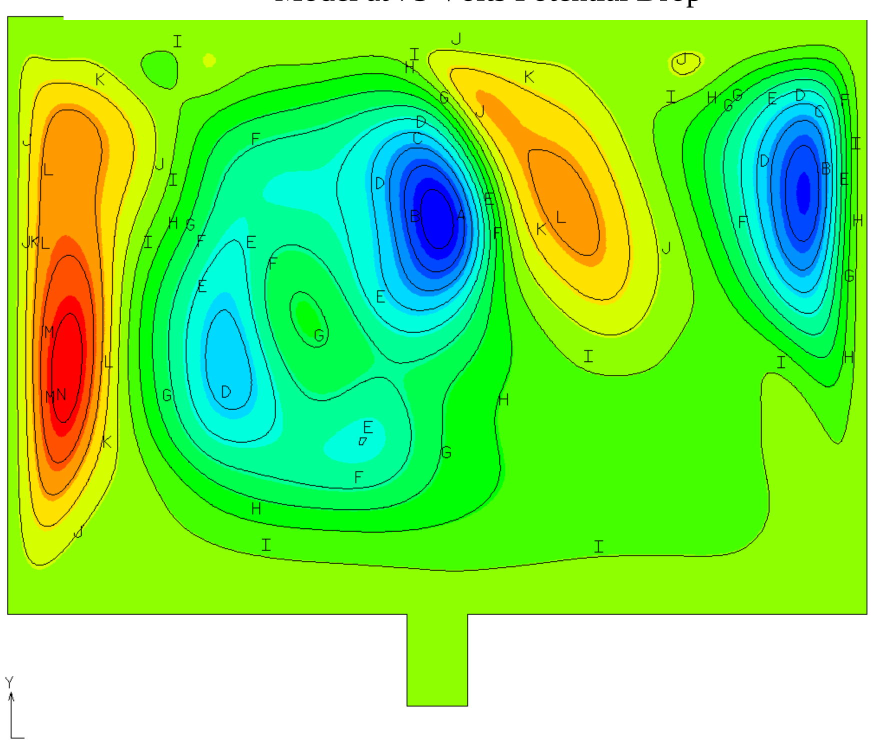


Figure 2 Streamline Contour Map for Two-Dimensional Melter Model at 75 Volts Potential Drop

center of the melt pool is quite uniform, which is about 1417$^{o}$K (1144$^{o}$C). The temperature then decreases in the lower quarter of the melt pool.

Velocity (Streamline) Distribution

Figure 2 gives the streamline contour map, where circulation cells show up better than in a velocity vector map. Streamlines are lines tangent to the direction of the velocity vectors. The distance between two streamlines is inversely proportional to the flow, such that the closer the streamlines, the higher the velocities. Figure 2 shows basically two pairs of large counter-rotating cells. A dominant cell structure is not evident, which may be due to the relatively low average pool velocity.

## THREE-DIMENSIONAL MODEL

The features of the three-dimensional model are shown in Figure 3, which also provides the temperature contour map. The upper and lower electrode pairs are 0.304m high and 1.015m wide. The distance between electrode pairs is 1.42m. The melter diameter is 1.76m, and the glass depth is 0.86m. The cold cap is assumed to be 76 mm high. The top elliptical section is an artifact of another modeling effort and does not affect the results. The outlet riser leads to the pour spout, where glass is poured into canisters. The model had 400,000 cells.

The glass properties are the same as in the 2D model. The void fraction in the cold cap is also assumed to be a temperature function as given by Eq. 6. The temperature BC is assumed to be radially symmetrical, 300$^{o}$C at the center and 850$^{o}$C at the edges. The inlet flow is a parabolic profile, zero at the center and maximum at the edges, so that when integrated , the total flow is 68 Kg/hr. The convective coefficients at the side wall, bottom, and cold cap surface are iterated to give similar heat losses as in the Lumped Parameter model for Macrobatch 2 conditions. Solution of this 3D model was performed on a Dell WHL530 machine with 2 GHz Pentium IV processor, 2 Gigabyte of RDRAM. Convergence was severely hampered by the very sensitive variation of thermal and electrical conductivity with temperature.

Figure 3 shows the temperature contour map along a plane that connects the left and right electrodes for a potential drop of 75 volts. This plane would be analogous to the 2D model. Also, as in the 2D model, a region of severe temperature gradients appear in the cold cap region. There are localized thick sections associated with junctures of circulation cells in the glass. For this electric potential drop, the glass temperature in the main pool is fairly uniform, with an average temperature of 1177$^{o}$C. The speed contour map is given in Figure 4. Speed is the absolute value of the velocity at a point (square root of the sum of the squares of the 3 velocity vectors). Figure 4 thus provides a pictorial representation of flow cells in the subject plane. These cells, and thus the overall flow pattern, are strongly affected by the exiting flow, which is evident upon examining similar plots for the plane that includes the outlet riser. Figures 5 and 6 give the temperature contour and speed contour maps for the plane cutting across the outlet riser.

## CONCLUSIONS

Two-dimensional and three-dimensional numerical models of the DWPF melter were obtained using computational fluid-dynamics methods. These featured a simplified cold cap model that assumed the foam layer void fraction is a function of temperature, as provided by laboratory batch sample testing at various temperatures. Although simple, the results showed cold cap region, thick at the center and thin at the edges, which is believed to be representative of actual melters.

An area of improvement would be the modeling of the cold cap to include the generation of bubbles and their venting or transport away from the cold cap. This would require two-phase flow modeling and basic experimental data required by the two-phase model. Experimental data on the cold cap consistency, thickness, surface temperature and radial movement are required in order to achieve an accurate melter model.

## REFERENCE

1. “Numerical Models of Waste Melters, Part I Lumped Parameter Analysis of DWPF” by H. N. Guerrero and D.F. Bickford, this Proceedings.

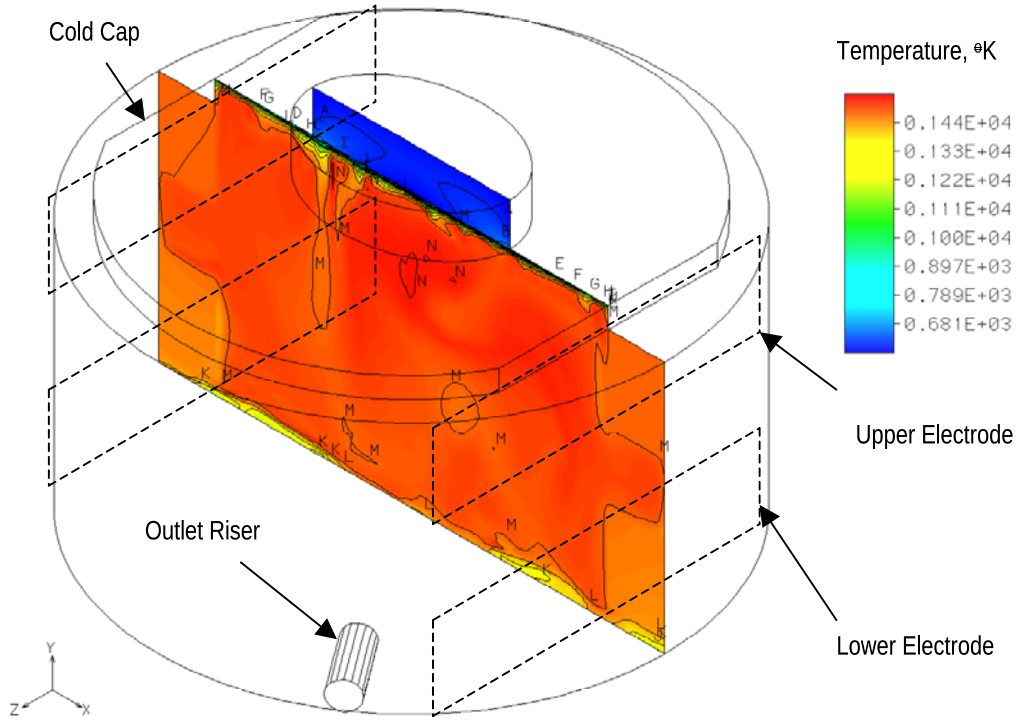



Figure 3  Temperature Contour Map for 3D Model at 76 Volts Potential Drop
- Plane Transverse to Electrodes

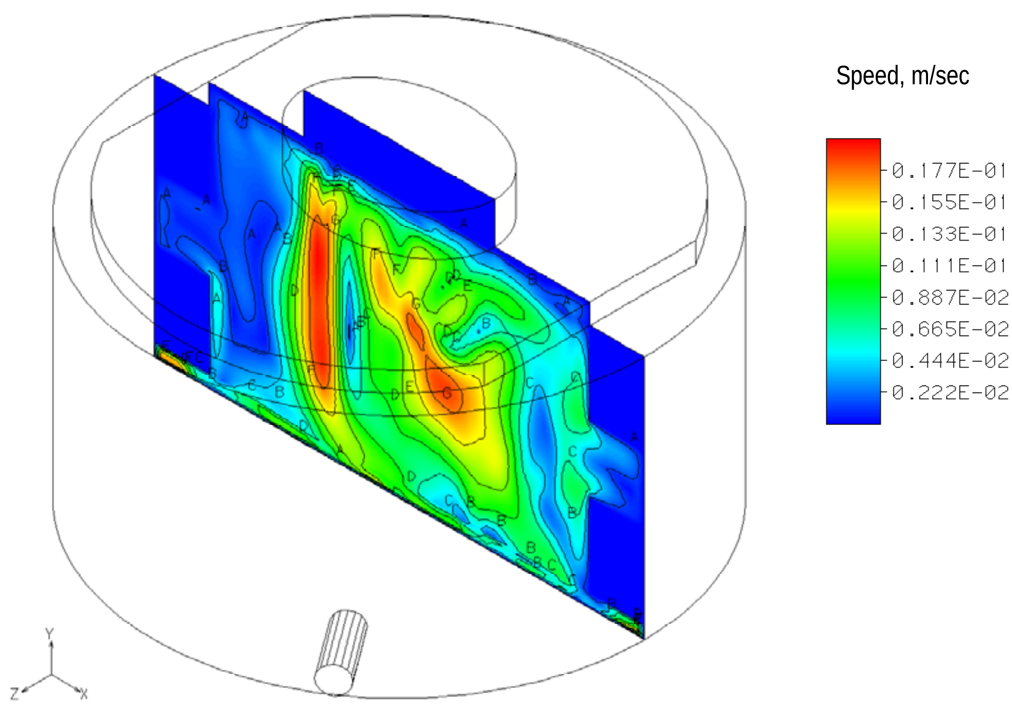



Figure 4  Speed Contour Map for 3D Model at 76 Volts Potential Drop
- Plane Transverse to Electrodes

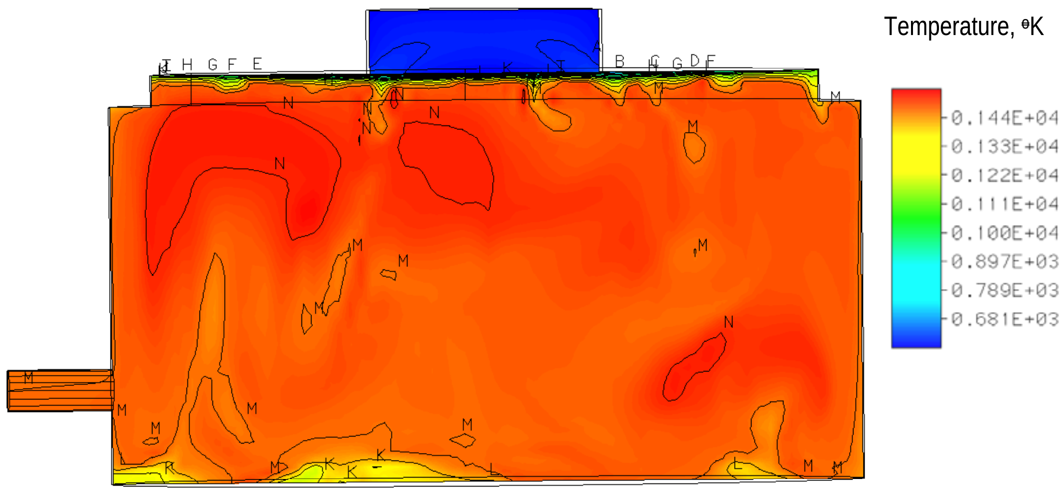



Figure 5 Temperature Contour Map for 3D Model at 76 Volts Potential Drop -Plane of Outlet Riser

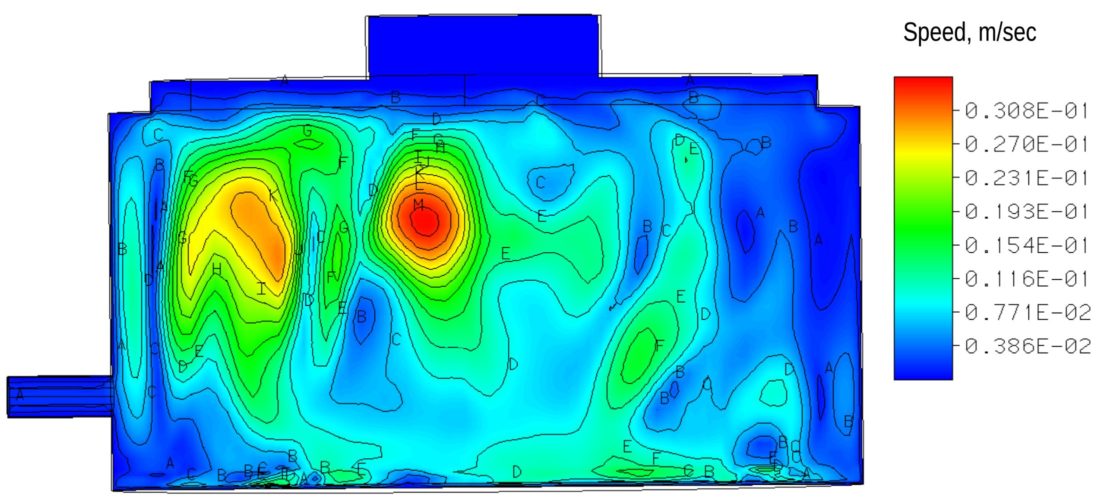



Figure 6 Speed Contour Map for 3D Model at 76 Volts Potential Drop -Plane of Outlet Riser