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Title: A COMBINED EXPERIMENTAL AND MODELING APPROACH TO URANIUM CASTING

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A Combined Experimental and Modeling Approach to Uranium Casting

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Abstract

The casting of uranium is being investigated using a combined experimental and modeling approach. The uranium is cast into graphite molds using vacuum induction melting. Mold design, mold coatings, and process parameters such as metal and mold temperatures are varied to look at their effect on mold filling, solidification and residual stresses.

Two commercial computer codes provide the simulation framework for this investigation in both two and three dimensions. FLOW-3D (Flow Science Inc.) is a coupled fluid flow and heat transfer Finite Difference Method (FDM) code. It is used to predict fluid flow during mold filling and the resultant mold and metal temperature distributions. This code's major strength is the ability to model fluid flow including convective flow.

The second code in use is ABAQUS (Hibbitt, Karlsson, & Sorensen), a coupled heat transfer and displacement Finite Element Method (FEM) code. It is used to simulate the cooling and solidification phase of the casting process and the resultant stresses and displacements. A translator has been written to take advantage of the strengths of each code. The temperature data predicted by FLOW-3D during the mold filling stage is mapped onto an ABAQUS mesh, and the simulation of solidification continues with ABAQUS.

Temperature predictions have been compared to experimental data collected by thermocouples placed throughout the mold to measure temperatures before, during and after casting. The initial metal and mold temperatures are used as input temperatures to FLOW-3D. The thermocouple traces collected during and after the pour are compared to the computed temperatures from the code.

Fluid flow predictions have been validated using static and dynamic radiographic data. Static radiographs were taken during the mold filling stage of lead castings generated at LANL in 1977. A matrix varying mold design, crucible pour hole diameter, and mold temperature was used. FLOW-3D has been used to simulate sections of that test matrix and the results show clearly that FLOW-3D will be a valuable predictive tool in parametric casting studies. More recently, dynamic radiographic videos of gold castings were made using the same mold configuration as is used for the uranium castings. These are compared to 3D simulations using FLOW-3D. Good correlation is shown between the radiography and the simulations. The casting and model are also compared to look at gross defects such as porosity and incomplete filling.

SCOPE OF THE STUDY

There are three main goals of using the computer to simulate the casting process in this study. One is to define a window of processing parameters i.e., mold temperature, metal temperature, pour rate, mold coating etc., that will produce quality castings. The second is to use the simulations to pinpoint areas where metal flow or solidification problems are likely to occur; and the last goal is to use the simulations to learn more about the casting process by "observing" the effect of process changes on the casting. Once the model is set-up and validated experimentally, mold and process changes can be made on the computer, without ever producing an actual casting. These "computer experiments" will save both time and money. Changes that might take days to implement experimentally can be done in a few hours on the computer. However, computer simulations are worthless if the model is not correctly simulating the process. Therefore the model needs to be validated for the individual process and the input data needs to be correct. This study combines both computer simulations and experiments to validate the model and learn more about and improve the casting process.

In order for the simulations to be effective, correct data must be input into the computer code. Much of the property data can be found in handbooks but some needs to be experimentally derived or in the interest of time and money requires an educated guess. Although guesses may seem inaccurate, ultimately modeling can be used to test the sensitivity of the process to an individual parameter. This will show whether the process is particularly sensitive to or affected by an individual parameter and whether it is important to know that value accurately or if a guess is accurate enough. Boundary layers or interfaces must also be accurately defined. These areas are often not well defined because they are not well understood. For example in this study, the interface of particular interest is the between the metal and the mold and including the mold coating.

Two commercial computer codes are being used to provide the simulation framework for this investigation; FLOW-3D (Flow Science, Inc.) and ABAQUS (Hibbitt, Karlsson, & Sorensen). FLOW-3D (Ref. 1) is a coupled fluid flow and heat transfer Finite Difference Method (FDM) code that can be used in both two and three dimensions. It is used initially to predict fluid flow during the mold filling and solidification phases as well as predict the resultant mold and metal temperature distributions. These mold and metal temperatures are then input into the second code ABAQUS. ABAQUS (Ref. 2)is a multi-purpose Finite Element Method (FEM) code. In this study coupled heat transfer and displacement elements are used to simulate the continued cooling and solidification of the casting. It will predict areas of residual stresses and displacements. Ultimately ABAQUS could be used to predict cooling rates and solidification fronts that provide insight for the prediction of solidification structures.

SIMULATION VALIDATION AND EXPERIMENTS

In the 1970's, flash radiography (Ref. 3,4) was used at the Los Alamos National Laboratory to view the pouring of lead into graphite molds. The experiments looked at various mold designs, varying crucible pour hole diameters and two mold preheats. In 1991, FLOW-3D was used to model these experiments.(Ref. 5) Input to the code was the initial mold and metal temperatures cited in the experimental lab notebook and handbook property data for lead and graphite. The simulations were run with a constant heat transfer coefficient of 0.5 $kW/m^2/K$ between the metal and the graphite mold. The simulation results were then qualitatively compared to the experimental radiographs. Correlation between the two was very good. This study was used to validate the fluid flow predictions of FLOW-3D and to study the effect of some processing parameters on metal flow within a mold.

The next step was to use FLOW-3D to model uranium casting. A flat, round disk mold with a simple hot top was designed. This provided a simple geometry for the model and an easy casting to produce experimentally. (Fig 1) A graphite mold was machined and coated with yttrium oxide to prevent interaction between the uranium and the graphite. The mold was fitted with 14 thermocouples imbedded in the graphite and connected to a data acquisition system on a personal computer. Mold temperatures were collected throughout the pouring and solidification phases of the casting. The initial metal temperature was measured with an optical pyrometer immediately prior to the pour.

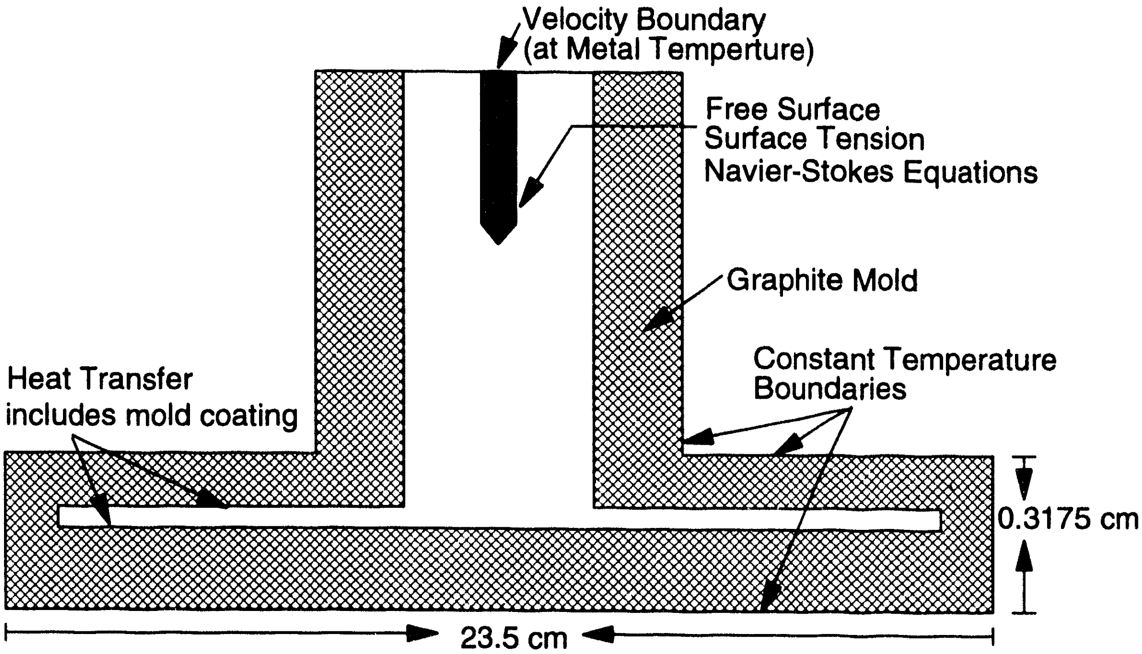

Figure 1 - Schematic of disk mold dimensions and imposed boundary conditions.

Table 1: Input Data for Computer Simulations

Uranium	Gold 5% Copper	Graphite
Density - 18.75E+3 kg/m^3	Density - 17.1E+3 kg/m^3	Density - 1.77E+3 kg/m3
T(liquidus) - 1405°K (1132°C)	T(liquidus) - 1259°K (986°C)	
T(solidus) - 1403°K (1100°C)	T(solidus) - 1247°K (974°C)	
Specific Heat - 146 m^2/s^2/K	Specific Heat - 148.5 m^2/s^2/K	Specific Heat - 1880 m^2/s^2/K
Conductivity - 46.3 W/m/K	Conductivity - 152.0 W/m/K	Conductivity - 75 W/m/K
Latent Heat - 38.72 kJ/kg	Latent Heat - 62.76 kJ/kg	
Dynamic Viscosity - 6.3 cP	Dynamic Viscosity - 5.2 cP	

The initial temperatures and the material properties input to FLOW-3D are shown in Table 1. Since the mold coating is very thin (about 1/100th) compared to the casting thickness, the heat transfer coefficient in the code simulates the transfer of heat from the metal through the mold coating layer to the mold. The heat transfer coefficient was initially set at 1.0 kW/m^2/K. The simulation was run and the numerically derived temperature curves were compared to the experimental thermocouple traces at various points within the mold. The computer predicted temperatures were lower than the thermocouple traces in most areas. By varying the heat transfer coefficient applied in various parts of the mold, the predicted temperatures were adjusted to match the experimental thermocouple readings. In order to achieve good correlation, the heat transfer coefficient directly under the metal stream during pouring needed to be increased. The impact of the metal stream on the mold coating creates a higher heat transfer to the mold. There may also be some erosion of the mold coating directly under the stream, providing better contact and higher heat transfer. Figure 2 shows experimental and simulation data for a particular casting. A set of heat transfer coefficients was obtained which would provide good correlation between the model and the castings for this experiment set-up (uranium poured into a flat disk mold with yttria mold coating). They ranged from 1.0 $kW/m^2/K$ at the edge of the mold to 3.0 $kW/m^2/K$ under the pour. This set of coefficients was derived after modeling five different castings with varying initial temperatures but the same mold design and mold coating. It should be noted that some variations in the experimental temperatures occurred in castings having the same input parameters and also from side to side within an individual casting. This may be due to variations in the mold coating thickness from run to run and from side to side on a mold.

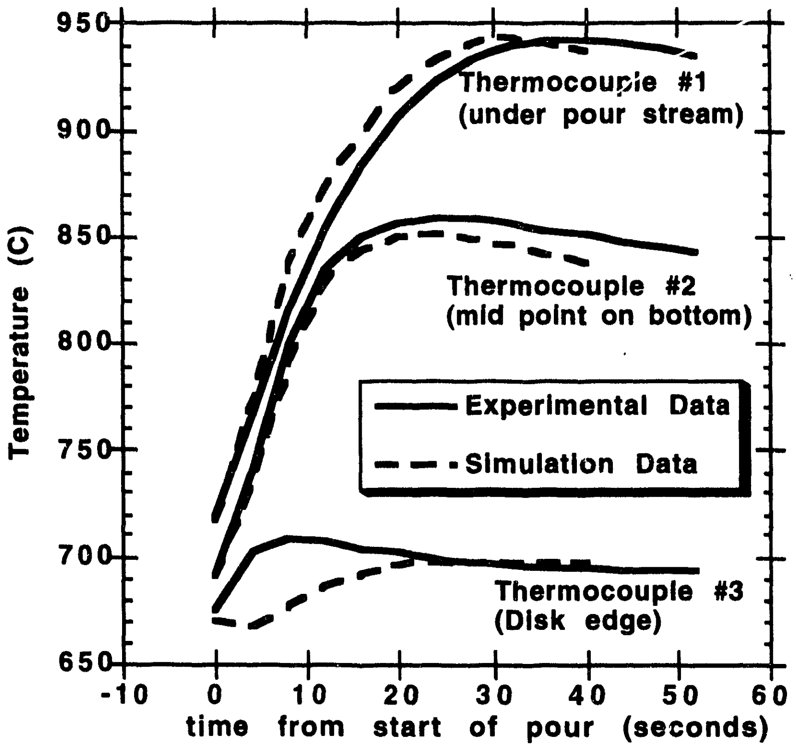

Figure 2 - Experimental and simulated temperature curves from a coated flat disk casting.

Hemispherical castings were made with two metals, uranium and a gold 5% copper alloy, poured into both coated and uncoated molds. Uranium was poured into coated molds at two different uranium metal temperatures, 1245°C and 1425°C and into one uncoated mold at 1250°C. Gold was poured into a coated mold at 1245°C and into an uncoated mold at 1200°C. Figure 3 shows experimental thermocouple traces of the three uranium and two gold castings. The coating obviously effects the rate of heat transfer for both gold and uranium. The temperature traces are much steeper in the uncoated molds for both metals, but the difference between the coated and uncoated traces seems to be greater for the gold castings than the uranium. This was also observed in the actual gold castings. The gold poured into a bare mold only filled about half the mold while the gold casting into the coated mold completely filled creating a sound casting with large grains. The uranium cast into a bare mold was almost sound. The individual rivulets from the pour could still be seen but the casting was essentially full. The gold casting into an uncoated mold froze off very early. It was only about half full. As shown by the three uranium castings, the presence of a mold coating has a larger

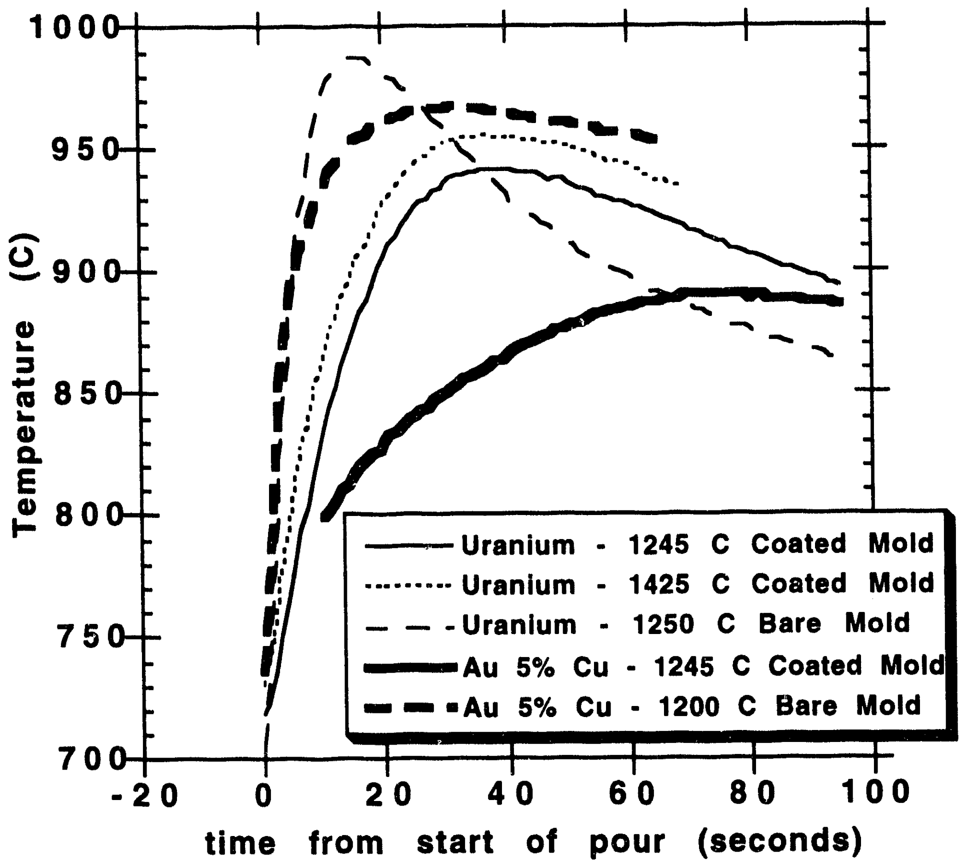

Figure 3 - Experimental thermocouple traces from the mold core pole (directly under the pour) for Gold 5% Cu and Uranium at various melt temperatures poured into yttria coated or uncoated molds.

effect on the thermocouple traces than the superheat of the metal. An increase of 180°C in metal superheat shows only about 40°C increase in mold temperature, however, the absence of a mold coating makes about a 150°C increase in the mold temperature with the same metal preheat. Simulations were run for these castings using the empirically derived heat transfer coefficients from the disk model. The predictions for uranium into the coated mold were good but slightly over predicted the temperatures directly under the pour. Heat transfer coefficients were then modified to fit the experimental data. Table 2 shows the computer derived heat transfer coefficients for uranium and gold.

Table 2: Mold/Metal Heat Transfer Coefficients Used in Computer Simulations

	Uranium	Gold 5% Copper
Uncoated	3 - 8	12
Yttria Coated	1 - 3	0.5

(All heat transfer coefficients in $kW/m^2/K$)

As expected from the experiments, the coated gold casting used a small heat transfer coefficient of only 0.5 $kW/m^2/K$ while the bare mold required a heat transfer coefficient of 12 $kW/m^2/K$. With uranium, there was more variation within different parts of the mold especially for the flat disk, but there was not so much variation between the coated and uncoated molds. (1 to 3 $kW/m^2/K$ for coated versus 3 to 8 $kW/m^2/K$ for the bare graphite.)

To check the consistency of the computer derived heat transfer coefficient, two castings were made at the Sandia National Laboratory. The gold 5% copper alloy was poured into both an uncoated and a coated mold prepared at the Los Alamos National Laboratory. The initial mold and the metal temperatures were the same for both castings. (1330°C metal, 400°C mold) Radiographic videos were taken during the filling of the molds to assess the fluid flow characteristics of the castings. The videos showed different methods of mold filling. The uncoated mold showed metal flowing to approximately half radius and stopping, leaving an incompletely filled casting. The coated mold showed metal flowing all the way to the edge of the casting and bouncing back to completely fill the mold. Simulations were run for this system using gold material properties (Table 1) and the heat transfer coefficients derived for the gold alloy (Table 2). Figure 4 shows the FLOW-3D simulation results for the uncoated and coated disk castings. The flow patterns from the simulations and the videos are remarkably similar.

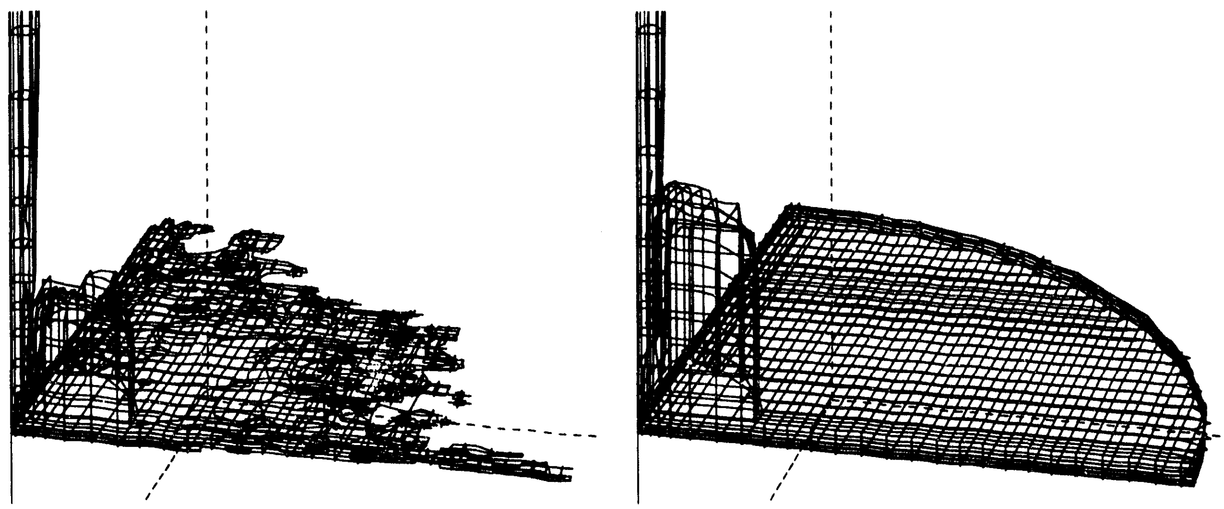

Figure 4 - Simulation results for the uncoated (left) and coated (right) gold disk castings. The coated casting completely filled while the uncoated one did not. This pattern is also seen in the video radiographs.

When simulations are run with the uranium material properties and heat transfer (Tables 1 and 2), the flow patterns predicted are the same for both the coated and uncoated molds. Metal flows first to the edge then bounces back and fills the center. Although this flow pattern can not be substantiated by radiography, the uranium castings produced show similar defects to those predicted by FLOW-3D. Figure 5 shows a flat disk uranium casting from an uncoated mold poured at 400°C on the left and free surface plot from a FLOW-3D simulation with the same parameters on the right. Both the experimental casting and the simulation show areas of incomplete filling on the top surface of the casting. Correlation is very good between the model and the actual casting.

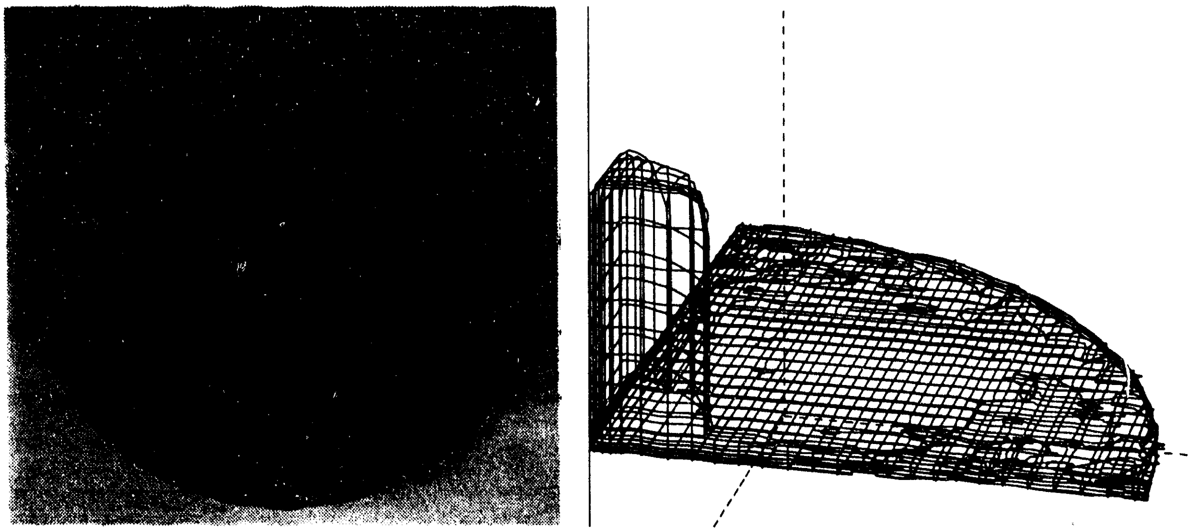

Figure 5 - A photograph of a uranium disk casting poured into an uncoated mold at 400°C is on the left and a FLOW-3D simulation of a uranium casting with the same conditions is on the right. Note the correlation of the surface defects and porosity in both pictures.

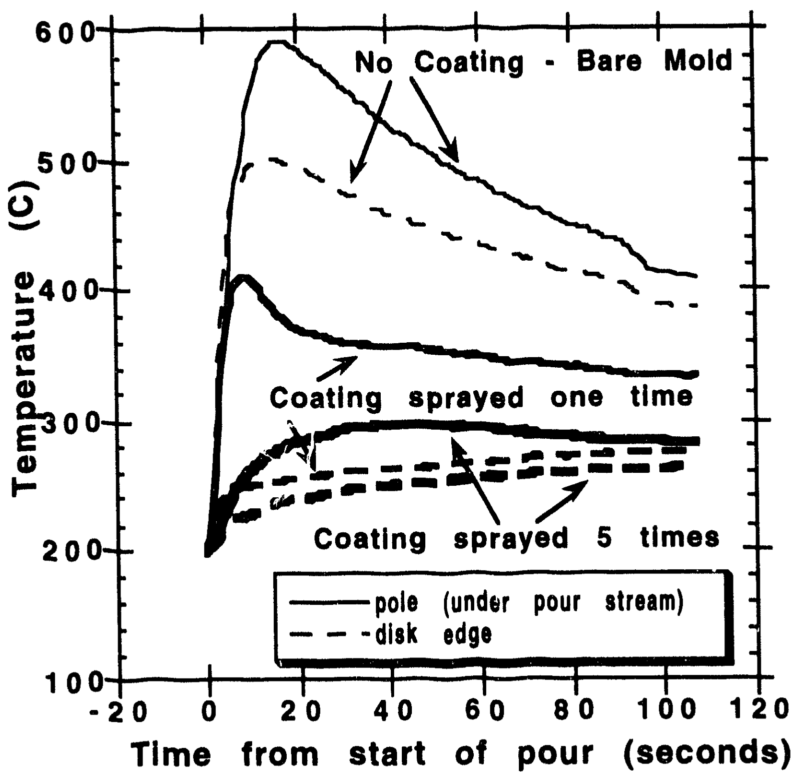

Figure 6 - Thermocouple traces from the mold edge and the mold pole (directly under the pour) from three uranium castings poured into a flat disk mold. All castings were poured with 1330°C Uranium and 200°C mold preheat. One mold was uncoated (bare), one was sprayed one time with an yttria mold coating and the last was sprayed five times with the yttria.

To continue the investigation of the effect of the mold coating on heat transfer; uranium castings were again made on the flat disk with mold coating variations. Molds were prepared with the coating sprayed one time, five times and without a coating (bare graphite); and castings were made with a mold preheat of 200°C and 400°C. Figure 6 shows the experimental thermocouple traces of the castings poured into the 200°C molds. Two traces are shown for each casting. The thermocouple directly under the pour (pole) and the one at the disk edge. The amount of mold coating obviously has a large effect on the heat transfer rate from the metal to the mold. The coating is acting as an insulator to heat transfer. There was considerable erosion of the coating with five layers of mold coating. The final casting appeared to have some mixing of the metal and coating creating very poor casting quality.

STRESS ANALYSIS WITH ABAQUS

Since FLOW-3D cannot model solid mechanics, ABAQUS was run to examine material displacement during cooling and the resulting stresses. The temperatures from FLOW-3D were translated to the corresponding finite element nodes in an ABAQUS mesh. The temperature data from FLOW-3D can be taken at any point, but usually it is taken when the metal is solidified so that fluid flow is no longer an issue. ABAQUS was run with Heat Transfer-Displacement elements to evaluate the displacement of material from the coefficient of thermal expansion. A simple elastic analysis was used and ABAQUS predicted the areas where stresses are increasing due to material displacement against a rigid body, i.e., the mold. An example of this is shown in Figure 7. This is a simulation of the same casting as figure 5,, uranium poured into a 400°C mold without a coating. Solidification in this casting is very fast. This highly exaggerated drawing shows relative displacement of material after 30 seconds of cooling. The edges of the casting are tending to curl down while the center of the casting is rising up. In the actual casting, the hot top in the center of the casting is very porous that relieves some of the stresses causing the center to rise, so the center of the actual casting is fairly flat. The edges of the casting tend to bend downward though as predicted by the code.

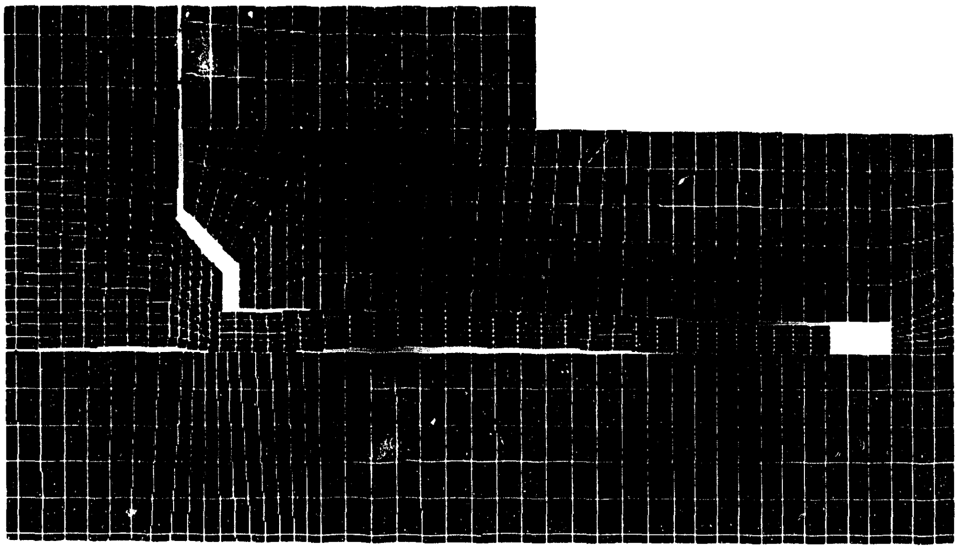

Figure 7 - Displacement plot from ABAQUS simulation of a disk casting. Uranium was poured into 400°C uncoated mold. The displacement is magnified 25X.

SUMMARY

Computer simulations can be very useful in designing and making castings, both to key in on relevant process parameters as well as learn more about the process itself. In this study the interface between the mold and the metal including the mold coating is of considerable importance. The rate of heat transfer is affected not only by the presence of a coating but also the thickness of the coating itself. Heat transfer across uncoated graphite is very fast for both uranium and gold materials, but when just a thin layer of coating is applied the heat transfer rate is considerably slowed. It was also observed both experimentally and through simulations, that variations in heat transfer occur within a mold itself. These variations are present consistently at specific areas in the mold, for example the area directly under the pour stream has higher heat transfer than the disk edge. Variations in heat transfer also occur from run to run and within a mold itself (one side of a mold will show better heat transfer than the other). When the correct input data and interface parameters are used in FLOW-3D, the simulations can predict not only correct temperature distributions which can give insight into solidification structures but also correct fluid flow patterns which will show defect areas produced during filling.

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