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USE OF COMPUTERS IN MOLD DESIGN,(U)
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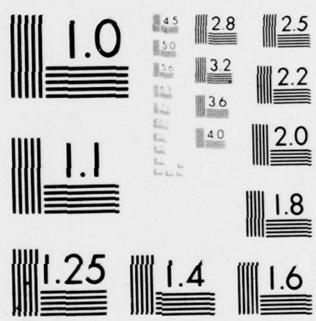


MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

*KEENAN & ERICKSON

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Mold design is an art. Numerous design techniques are used to ensure that the casting obtained from a mold is sound. Normally, the designer uses a trial-and-error method to perfect his mold. If defects in the casting are discovered, he changes the design and casts another part. As the size and complexity of the mold increase, however, this approach becomes economically unfeasible, especially when the cost of the metal to be cast is high.

At the Los Alamos Scientific Laboratory, it is often necessary to cast parts of uranium, gold or other metals that are rare and/or of high chemical and isotopic purity. Uranium parts are cast in zirconium-oxide-coated graphite molds which are relatively expensive to fabricate. Also of significance is the recovery cost; i.e., the cost to repurify the extra metal after the casting has been machined. These costs are important in two ways. First, they provide motivation to design better molds so that sound castings can be obtained with less waste. Second, they prevent the use of the ordinary trial-and-error method of mold design.

ABSTRACT

This paper presents ~~our~~ efforts to determine a system to evaluate mold designs using computer simulations. Although the ~~we~~ report describes ~~on~~ the mold design for a thin-walled uranium hemisphere, the system is applicable to virtually any shape mold.

ABSTRACT

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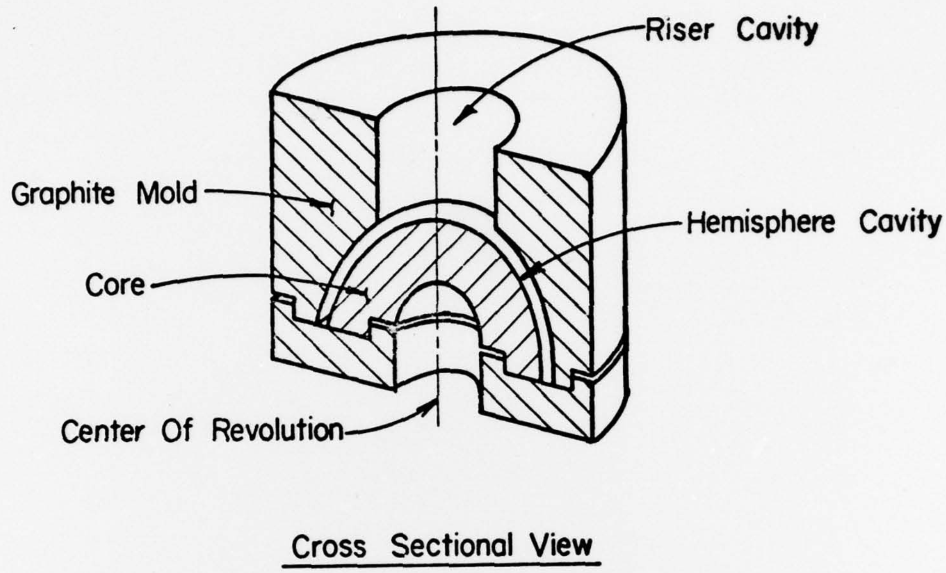


Figure 1. Current mold design for hemispherical casting.

## BACKGROUND

Figure 1 depicts an example of a mold used to cast a thin-walled uranium hemisphere.

An allowance for machining is included in the hemisphere cavity, and another large volume of "waste" metal is in the riser cavity. The riser performs two essential functions in this design. First, it provides a reservoir of molten metal to feed the casting as it shrinks during solidification. Second, it moves the thermal center of the system from the part into the riser. As a result, a temperature gradient is created which allows the casting to cool from the equator towards the riser.* Solidification occurs in the vicinity of

*It is important to note that this temperature gradient occurs only if the initial temperature of the mold is below the melting point of the molten metal.

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all the interior surfaces, but not rapidly enough to close off any still-molten part from the riser. In a typical mold designed on these principles, the riser and machine allowances contain more metal than is in the final machined hemisphere.

When casting hemispherical shapes in chill molds, another phenomenon is of interest. Figure 2 is a picture (taken with a flash x-ray machine) of a mold as it is being filled with lead. As the molten metal hits the mold core (A) it is splashed against the outer

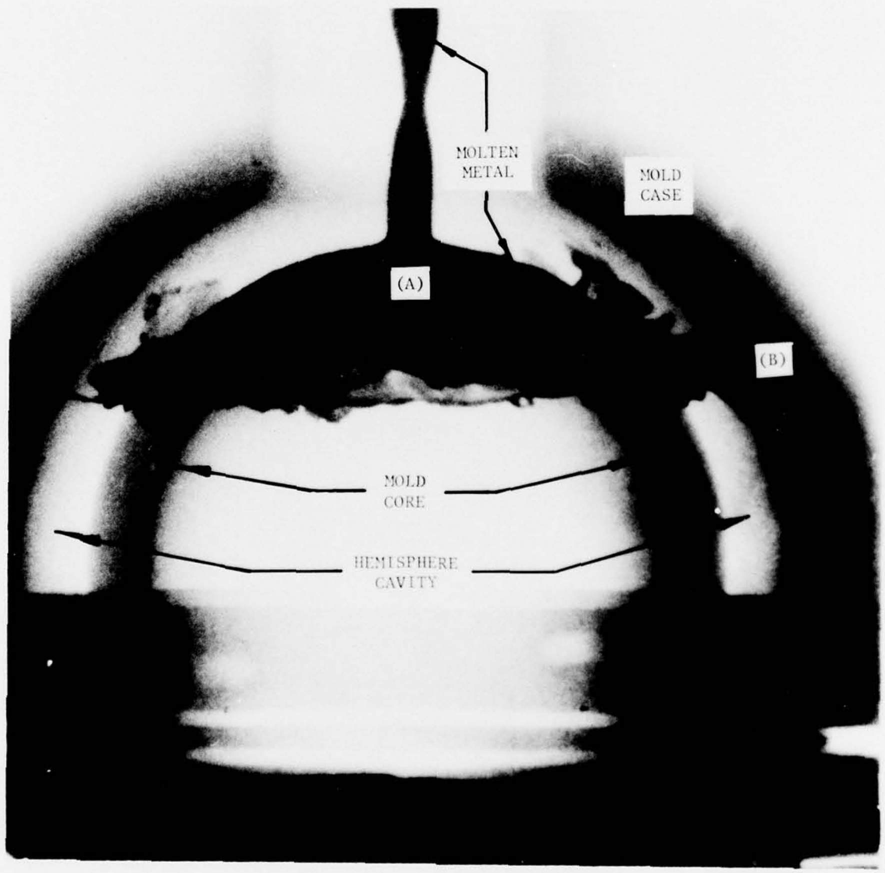


Figure 2. Flash radiograph of molten metal entering mold.

cavity wall (B). Because the mold is below the melting temperature of the metal, some freezing of the metal occurs where it strikes the outer wall. Because of the splashing, voids are frozen into the metal. In thin-walled castings, the metal cools so quickly that this metal never remelts to free the voids as the mold is filled. In addition, this area acts as a trap for gases rising from the lower part of the casting. Consequently, additional allowance must be made to insure that these defects can be machined away.

With the objective of reducing or eliminating all of these problems and thereby reducing costs, we decided to design a new mold. We reasoned that if we could preheat the mold above the melting temperature of the metal, then withdraw heat from the system at the equator of the casting with some type of cooling system, we could obtain a temperature gradient in the casting and mold which would force the solidification front to move in the desired direction. Since the initial temperature of the mold would be above the melting temperature, solidification would not occur along the mold surfaces. This would allow us to reduce the machine allowances. The riser would stay molten longer, allowing us to reduce its size as well.

To evaluate a new design, we need to know how the solidification front advances as the casting cools. For thin-walled shapes, it is impossible to obtain this information experimentally. Molten uranium will react with bare thermocouples. Thus the thermocouples could not be placed in the molten metal and would either have to be inserted into the mold or encased in ceramic. Both of these situations cause inaccuracies for which it is very difficult to account. Therefore, to evaluate our directional solidification concept, we decided to simulate the cooling process using a digital computer.

## DISCUSSION

### Computer Programs

For heat-transfer calculations, we used the Chrysler Improved Numerical Differencing Analyzer for 3rd Generation Computers (CINDA-3G).[1] It is a computer program in general use at LASL.* This program employs the user's choice of several finite differencing algorithms to obtain solutions to transient or steady state thermodynamic systems.

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*CINDA-3G was developed by the Chrysler Corporation Space Division under contract NAS9-7043 to the National Aeronautics and Space Administration's Manned Spacecraft Center at Houston.

The thermal system is presented to CINDA-3G in a network format, consisting of nodes and conductors. Each node is identified by number, volume, and a reference to an array of its thermal properties. Each conductor (one between each pair of adjacent nodes) is identified by number, two node numbers, and a reference to an array containing temperature-varying thermal conductivity.

Three types of nodes are allowed. Diffusion nodes have the capability to store energy (thermal capacitance). Arithmetic nodes have no thermal capacitance, and negligible volumes. They are used to obtain temperatures at specific points of interest. Boundary nodes are used to set mathematical boundary conditions. Temperatures of boundary nodes are not changed by the differencing subroutines, but may be changed by the user during a simulation.

Only two types of conductors may be used, regular and radiation. Thus, a simple one-dimensional network might look like figure 3. In this system nodes and conductors are of the types indicated in Table I.

Capacitance (C) is defined only for diffusion nodes. It is calculated as the product of node volume and the temperature-dependent properties of density and specific heat.

$$C_i = V_i \sigma c_{pi}$$

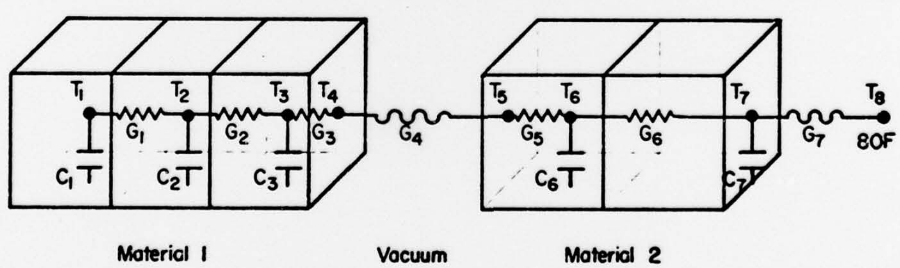


Figure 3. Example network of 1D thermal system.

TABLE I

NODE AND CONDUCTOR TYPES FOR SYSTEM IN FIGURE THREE

| Node | Type | Conductor | Type |
|---|---|---|---|
| T1 | Diffusion | G1 | Regular |
| T2 | Diffusion | G2 | Regular |
| T3 | Diffusion | G3 | Regular |
| T4 | Arithmetic | G4 | Radiation |
| T5 | Arithmetic | G5 | Regular |
| T6 | Diffusion | G6 | Regular |
| T7 | Diffusion | G7 | Radiation |
| T8 | Boundary | | |

Conductance (G) calculations depend on the type of conductor. Through solid material,

$$G_i = \frac{kA}{x}$$

where $k$ = temperature-dependent thermal conductivity
$A$ = cross-sectional heat flow area
$x$ = path length between node centers.

For convective heat transfer,

$$G_i = hA$$

where $h$ = convective heat transfer coefficient
$A$ = cross-sectional heat flow area.

In the case of radiative heat transfer, conductance is calculated using this equation:

$$G_i = \sigma A F$$

where $\sigma$ = Stefan-Boltzmann constant
$A$ = radiant surface area
$F$ = net radiant interchange factor.

The extension of this one-dimensional system into two or three dimensions is not difficult to visualize. However, if done by hand, the calculation of node volumes, distances between node centers and cross-sectional heat flow areas would be tedious and time-consuming. For axiosymmetric molds, these calculations are handled by FED-JB,* a program which also writes a disk file containing the node and conductor data. After program control constants, thermal property arrays, and other instructions are added, this file is used as the input data for CINDA-3G.

For molds containing hundreds of nodes, a large volume of data is generated. Even if only the data for the uranium nodes were printed, temperatures at every time step would fill hundreds of pages of output. In addition, the manipulation of this data by hand to find meaningful results would be extremely time-consuming.

Using a set of subroutines previously developed by the authors at LASL, the data can be presented on 16 mm or 35 mm color film.[3] At the end of each specified time interval, a frame is plotted showing each node of the network. One of several available characters (for instance, *, +, -) is plotted on the film at a point corresponding with the center of each node. The color of each character is set according to the temperature range within which the node falls. When 16 mm film is made, the temperature changes can be studied as the film is projected as a motion picture. This allows rapid determination of the effects of changes in mold design, since the advancement of the solidification front can readily be seen.

## Design Procedures and Results

The initial concept of a cooling system of a hemispherical mold is shown in figure 4.

For computer simulation, a very simple model was constructed to first test the feasibility of the directional solidification concept. Assumptions were: (1) that the mold cavity is filled instantaneously; (2) that intimate contact exists between metal and mold. For simplicity, the mold coatings (normally flame-sprayed zirconium

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*FEDJB is the result of modifications by Jim Burns, Group WX-1, LASL, to FED.[2] FED is a "heat mesher" developed at Lawrence Livermore Laboratory (LLL) to calculate the same type of input for TRUMP, another computer program for thermodynamic problems.

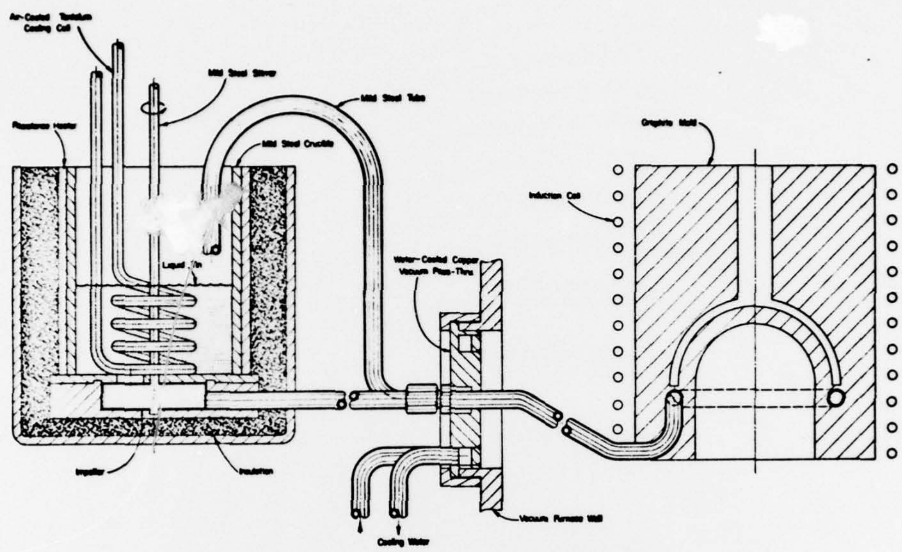


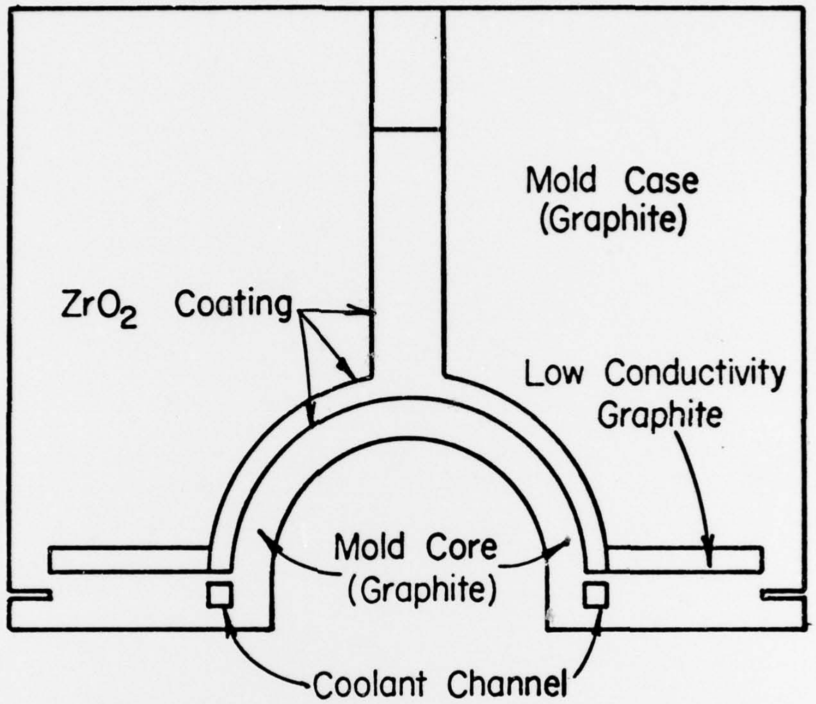

Figure 4. Schematic of cooling system for hemispherical mold.

dioxide) were ignored. The initial temperature of the melt was 1275°C (2327°F) and that of the mold was 1135°C (2075°F). An arbitrary 500 Btu/min was removed from the system from the node directly under the equator of the casting.

The results of this initial model proved the feasibility of the concept. They also indicated that the transfer of heat through the graphite conductors to the heat extraction area must be reduced. We then proceeded to design our mold.

Our initial mold design incorporated a square channel machined into the graphite mold through which liquid tin at 350°C (662°F) would circulate as a coolant. This channel is separated from the casting by a thin sheet of graphite (see figure 5). The zirconium dioxide mold coatings are included and a piece of low-conductivity graphite is inserted to reduce the heat flow through the mold. For this simulation, the center tin node is kept at 350°C throughout. Otherwise, the assumptions are the same as for the previous model.

Figure 5.
Initial mold design.




Results of this simulation indicate that the core cools off much more rapidly than the case, causing the uranium to solidify far ahead of the outside. This is undesirable because a portion of the hemisphere may be frozen off from the riser, causing voids to be formed. Figure 6 shows how the solidification front advances.

In our next design there are four changes: First, to obtain better heat transfer from the uranium to the coolant, we inserted a tantalum tube to carry the molten tin. The uranium is assumed to be in intimate contact with the tantalum.

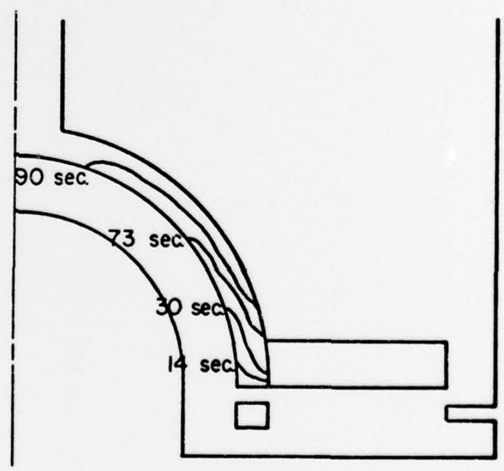



Figure 6. Results of simulation.

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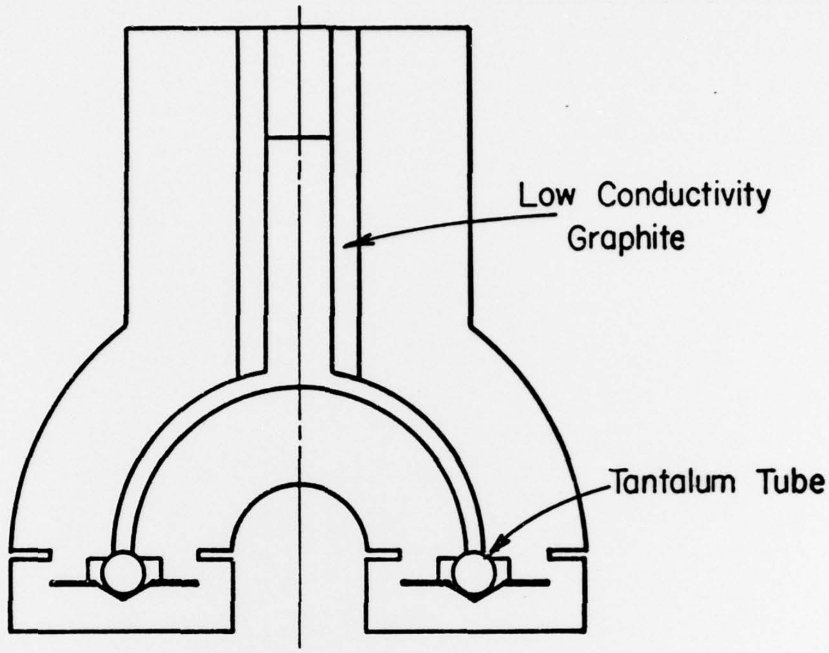



Figure 7.

First refinements.

Second, the graphite channel in which the tantalum tube rests is coated with zirconium-dioxide, a low-conductivity flame-sprayed material, to reduce the heat flow from the graphite to the coolant. Third, the low-conductivity graphite is moved to the riser to help maintain its temperature. Lastly, the mass of the mold is reduced on the outside and increased in the core. This is to help balance the temperature gradient between core and case, thereby bringing the liquid-solid interface in the metal more perpendicular to the mold walls. Figure 7 shows the resultant design.

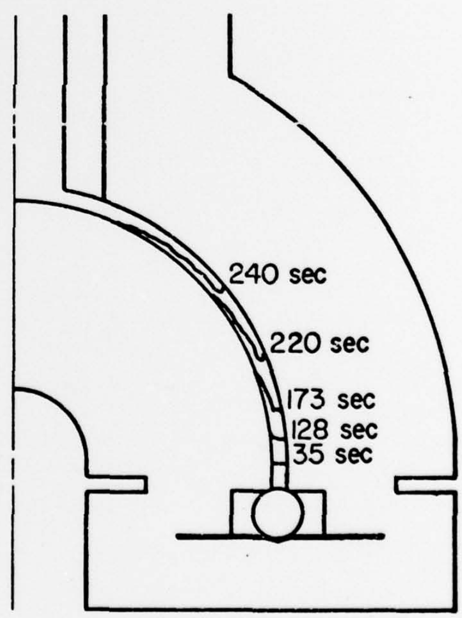



Figure 8.
After first refinements.

Results of the simulation (figure 8) indicate that we still have not done enough to force the heat to flow through the metal to the coolant. The core still cools off too soon in comparison to the mold case, causing the solidification front to advance rapidly along the core.

A study of heat flow rates through specific nodes in the vicinity of the tantalum tube shows that a large amount of heat is still being transferred from the mold to the coolant tube through the small contact areas at the bottom and top of the tube. Additionally, it is likely that in an actual casting, the uranium would shrink away from the tantalum upon solidification. This would cause a large drop in thermal conductivity at the interface.

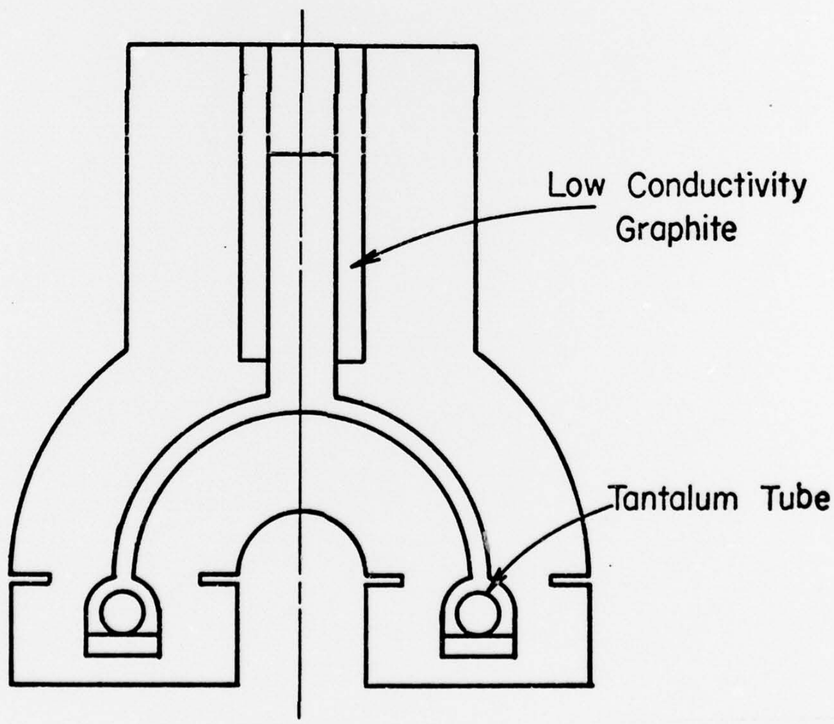
Our next design includes the following modifications (see figure 9):

1. A layer of a castable ceramic is placed under the tantalum tube. This low-conductivity material is to reduce heat flow through the bottom of the tube.

2. The tantalum tube is lowered to allow molten uranium to flow around it. This accomplishes two things: first, the contact between the top of the tube and the mold is eliminated; second, the uranium, upon solidification, will shrink around the tube, reducing the interface problem.

Figure 9.

Mold design after second refinements.



The computer simulation after these second refinements shows significantly better results. The solidification front advances perpendicular to the mold walls until the hemisphere is almost entirely solidified. When the metal finally does solidify across the core, the rest of the front is not far enough behind it to cause any feeding problems. See figure 10.

Using this final design we estimate that we can obtain, assuming 0.03-in. machine stock, a hemisphere of 2.30-in. inside radius, and 2.40-in. outside radius. The riser has a radius of 0.5 in. and a height of 1.5 in. Table II compares the new mold design with one that would be required to cast the same part using current methods.

The right column in Table II includes figures for a new design which, as this is written, is being prepared for simulation. The new design (figure 11) is an attempt to reduce the amount of uranium around the cooling tube. The tantalum tube is moved up to alongside the base of the hemisphere. Since the coefficient of expansion for tantalum is less than that for uranium, the tube must be placed in the mold core.

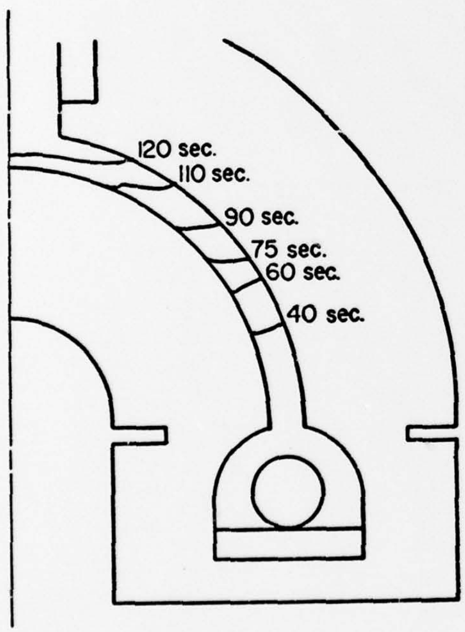



Figure 10.
After second refinements.

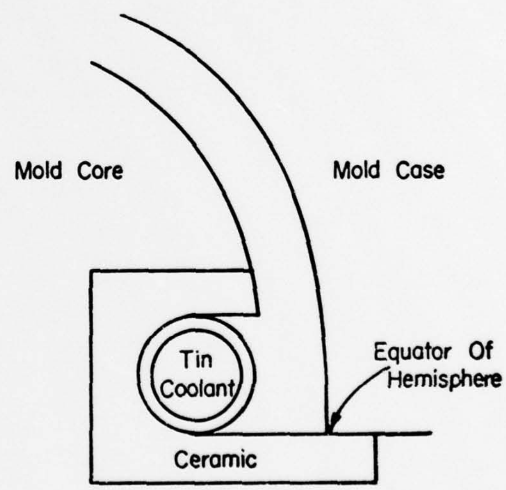



Figure 11.
Future refinements.

TABLE II

DIMENSIONS OF NEW AND OLD MOLD DESIGNS

| | Finished Part Dimens. (in.) | (in.$^3$) | Current Design Mold Dimens. (in.) | (in.$^3$) | Directional Solidification Mold Dimens. (in.) | (in.$^3$) | Proposed Simulation Dimens. (in.) | (in.$^3$) |
|---|---|---|---|---|---|---|---|---|
| Hemisphere | | | | | | | | |
| inside radius | 2.30 | | 2.22 | | 2.27 | | 2.27 | |
| outside radius | 2.45 | | 2.57 | | 2.48 | | 2.48 | |
| volume | | 5.32 | | 12.64 | | 7.44 | | 7.44 |
| Riser | | | | | | | | |
| radius | | | 1.0 | | 0.5 | | 0.5 | |
| height | | | 2.0 | | 1.5 | | 1.5 | |
| volume | | | | 6.28 | | 1.18 | | 1.18 |
| Extra Volume at equator | | ____ | | 1.32 | | 8.96 | | 0.61 |
| Total Volume | | 5.32 | | 20.24 | | 17.58 | | 9.23 |
| Volume Reduction | | | | | | 2.66 | | 11.01 |

Otherwise, the uranium would shrink away from the tube. Since this works against the requirement to reduce the heat transfer through the core, the tube is encased in a low-conductivity ceramic open only to the uranium. This should direct the majority of the heat flow through the uranium. Also, the mass of the core is increased. The results of this new simulation are not available at the time of this writing. However, previous simulations indicate that we can expect this new design to give better solidification front propagation and a reduced volume of uranium in the coolant area.

CONCLUSIONS

Directional solidification of the hemispherical casting has been attained. A further reduction of the heat flow through the core would be beneficial and should be attained in the next design. This further reduction, however, does not appear essential to sound castings.

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The final simulated mold design saves 2.66 cubic inches of metal. For uranium, that is 817 grams (28.8 ounces) saved. If the new design works as expected, the savings will be 11.01 cubic inches, which is almost 3.4 kilograms (7.45 pounds) These savings are significant.

Finally, we have developed a system for improving the design of molds where cost and/or complexity makes the trial-and-error method unfeasible. This system is by no means limited to thin-walled hemispherical castings. Since CINDA-3G has a three-dimensional capability, virtually any shape mold can be simulated and redesigned.

## References

1. Lewis, D. R., Gaski, J. D., and Thompson, L. R., "Chrysler Improved Numerical Differencing Analyzer for 3rd Generation Computers," Technical Note TN-AP-67-287, 20 October 1967.

2. Schauer, Dale A., "FED: A Computer Program to Generate Geometric Input for the Heat-Transfer Code TRUMP," UCRL-50816, Rev. 1, 12 January 1973.

3. Erickson, William C., "The Use of General Purpose Software in Casting Solidification Simulation," Metallurgical Transactions B, Vol. 813, March 1977, pp 93-97.