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CONF-786725--1

LA-UR -78-1852

TITLE:

COMPUTER SIMULATION OF SOLIDIFICATION

MASTER

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SUBMITTED TO:

Twenty-fifth Sagamore Army Materials
Research Conference, July 17-21, 1978,
Bolton Landing, New York

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ABSTRACT

The current state-of-the-art of computer simulation of solidification has been reviewed. Brief descriptions are given for methods of handling the latent heat of fusion and analog, finite element, finite difference, and pseudo-steady state technique used to simulate solidification are defined. Methods of reducing manpower requirements are discussed as well as general purpose heat transfer codes currently available. The paper concludes with several examples of solidification simulation including die casting, welding, and die design applications.

COMPUTER SIMULATION OF SOLIDIFICATION

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INTRODUCTION

The use of analytical techniques for calculating solidification heat transfer patterns has essentially paralleled the development and growth of computers. Initially, heat transfer calculations were analytical in nature, but assumptions required to allow the equations to be solved mathematically negated its usefulness in engineering problems such as solidification. With the advent of the analog computer, the interest and application of simulation techniques grew. However, it wasn't until the development of the digital computer that numerical techniques became feasible and the use of computer simulation expanded.

Factors such as increased competition from noncast products, health and safety regulations, and increased energy costs are causing the foundry industry to increase its utilization of scientific principles. This not only includes principles of heat transfer but also areas such as fluid dynamics, kinetics, and nucleations theory.¹ With the changing technological atmosphere in the foundry industry, and with the groundwork laid prior to 1970, computer simulation has reached a point where its application to industrial problems can be considered. In the American Foundrymen's Society honorary Charles Edgar Hoyt Memorial Lecture, Ruddle made the following prediction in 1971: "... we shall within two decades see the digital computer take over much of rising practice."² In discussing this prediction he stated

... it seems likely that in a short while, all one may need to do is feed into the computer a drawing

of the casting plus indication of the thermal properties of the mold material and of the alloy being used, its solidification characteristics and the degree of soundness desired in the casting. The computer would then indicate just what would be the most economic risering and gating system to develop the desired degree of soundness and the location of any residual unsoundness.

Obviously, we are not to this point, but then we are only a third of the way to 1991. This paper will review where we are today with respect to the state-of-the-art of solidification simulation. A brief description of analog, finite difference, finite element, and pseudo-steady state simulation techniques will be given along with a discussion of procedures for handling the latent heat of fusion. It is this factor which sets solidification simulation apart from many heat transfer problems. This will be followed by a discussion of the methodology required for economical use of computer simulation. For the economical use of computers, the manpower costs must be reduced through the use of computer graphics and general purpose software. The paper will conclude with several examples of applied simulation. Sand and ingot casting, die casting, and welding are among the areas reviewed.

Thermal properties play an important role in achieving good simulation results but will not be discussed in detail. The simulation results are only as good as the data input. Unfortunately, good thermal data is not readily available for solids near the melting point or for liquid metals. This is especially true for alloys. A 13-volume compilation of thermal properties edited by Touloukian³ and the ASM publications on thermophysical properties^{4,5} are excellent sources of currently available data. Heat transfer coefficients at interfaces also play an important role in achieving good calculated results. Discussions on the role of interfaces and influencing parameters can be found in the literature.^{6,7,8} However, despite these referenced sources, useful data is scarce and thermal properties can be a limiting factor in the accuracy attained in simulation work.

THE SOLIDIFICATION PROBLEM IN HEAT TRANSFER TERMS

As a casting solidifies, heat transfer occurs in three ways - conduction, convection, and radiation. These are defined by the Fourier, Newton, and Stefan-Boltzmann laws, respectively. Steady state solutions of differential equations derived from these laws can be obtained analytically for a number of uniform property (therefore no phase change) problems. However, casting solidification is a transient problem and as such, partial differential equations relating time, temperature, and location must be solved.

Again, the analytical solution of transient problems can only be obtained in a limited number of cases which, because of the phase change involved, do not include solidification.

Three techniques used to obtain solutions to the transient solidification are analog, finite difference and finite element procedures. In addition, a pseudo-steady state approximation technique can be used. In the analog approach, the similarity between corresponding thermal and electrical parameters is used. Both finite element and finite difference are numerical techniques; the first is a functional or integral approach while the second is a differential approach. Finally, the pseudo-steady state process utilizes steady state equations and short time steps to approximate the transient problem.

Heat of Fusion

Before briefly discussing the techniques used to calculate the heat flow patterns during solidification, a discussion of the latent heat of fusion is warranted. Release of the latent heat of fusion during solidification sets solidification simulation apart from many other heat transfer problems. Differential equations describing heat flow assume that the equations are describing a continuous function. This is not the case when solidification occurs and special procedures must be used to account for the large quantity of heat released during the phase change.

Procedures for handling the heat of fusion fall into two categories. The first class of procedures are the postiterative methods in which the temperatures are adjusted after the calculations are made for that time step. The second class involves accounting for the latent heat of fusion during the calculations for a particular time step.

One of the oldest methods devised to account for the heat of fusion was reported by Evers et al.⁹ This postiterative method consists of transforming the latent heat of fusion into an equivalent number of degrees by dividing the latent heat of fusion by the specific heat. After each time step, the temperatures for nodes that fall below the melting point are reset to the melting point and the difference tabulated for that node. When the required number of degrees have been accumulated for a node, the temperature is allowed to continue dropping.

This procedure is particularly well suited for congruent melting materials, but algorithms can be defined to allow the procedure to work for materials which melt over a temperature range.

A second procedure which is used in the SINDA heat transfer code¹⁰ is based on defining a heat loss rate for the heat of fusion. This rate, defined in energy units/degree, is used to adjust the temperatures after each time step based on the temperature drop. To do this, temperatures at the start of the just completed time step and heat loss rate for each node must be known. This method requires a minimum melting range of one degree which from an engineering standpoint is representative of congruent melting materials.

The heat loss rate method results in a linear release of the latent heat. If this causes problems for alloy systems in which a large volume of the solid forms over a small of the solidification temperature range, the latent heat can be divided and each part released over its own temperature range.

Postiterative procedures do not cause problems from a mathematical standpoint for finite difference or pseudo-steady state procedures. However, researchers at LASL¹¹ have found that too large a correction in node temperatures causes unacceptable distortions in the heat balances. This was overcome by controlling the time step so that temperature drops were within calculated limits.

The modified specific heat method^{12,13} is one of the most popular methods for handling the heat of fusion and is satisfactory for all the basic types of heat transfer calculations described. Here, the latent heat of fusion is converted into the appropriate units for specific heat and added to the specific heat term over the temperature range at which it is to be liberated. This is done such that the increased area under the specific heat vs. temperature curve is equal to the latent heat of fusion. Thus, the latent heat is automatically accounted for during the time step calculations. This method is particularly well suited for alloys which melt over a relatively wide temperature range. It should not be used for congruent melting materials as the probability of the node temperature dropping from above the melting point to below the melting point in one time step is too large. If this occurs, the latent heat of fusion will not be taken into account for that node.

Investigators have used this technique for pure metals¹⁴ by expanding the melting temperature and the error introduced has been acceptable. However, it should be noted that there are significant variations in the thermal arrest portion of the cooling curve.¹⁵

The manner in which the heat of fusion is added to the specific heat can also play an important role.¹⁶ Figure 1 shows that significant variations occur in the calculated length of time liquid is present in steel ingots and that the differences are a function of the shape of the adjusted specific heat curve.

Fig. 1. Effect of shape of latent heat function on calculated results.¹⁶

The discussion to this point has dealt with methods that can be applied independent of the computer program used. There are also many methods which can be incorporated directly into the heat transfer equations and subsequent computer code. One such method was suggested by Evers et al.⁹ and implemented by Sarjant and Slack.¹⁷ This procedure involved defining (1) a modified temperature scale and (2) the specific heat in terms of enthalpy and temperature. By substituting into the basic partial differential equation, the enthalpy, not the temperature, was calculated using numerical procedures. The temperature can then be calculated using enthalpy vs. modified temperature curves. Since latent heat is a portion of the enthalpy of a material, it is automatically accounted for in the calculations. Other special methods can also be found in the literature.^{12, 18-21}

Analog Technique

Four methods of solving the heat flow equations were previously mentioned. The first of these, the analog technique, is based on the similarity between the differential equations describing the principles of heat flow, $\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$, and the flow of electricity, $\frac{\partial E}{\partial t} = \frac{1}{RC} \frac{\partial^2 E}{\partial x^2}$. In these equations, ' α ' is the thermal diffusivity, ' R ' = resistance and ' C ' = capacitance. Further comparisons between the two systems are presented in Table I.

Once these similarities are recognized, electrical circuits can be constructed that represent the thermal systems to be simulated and the current measured (the analog of heat flow) at the desired locations. Current (heat) sources/sinks can also be included in the circuit. Ruddle gives a good review of the analog technique for simulating solidification in his book, The Solidification of Castings.²²

One of the original generalized analog computers built in the United States was the "Heat and Mass Flow Analyzer" at Columbia University.²³ Using this unit, Professor Victor Paschke performed heat transfer analyses on iron cast in sand in 1944. Under research grants from the American Foundrymen's Society,* Professor Paschke performed generalized solidification studies²⁴ and studied such specific problems as temperature drops in pouring ladles,²⁵ solidification patterns in white irons,²⁷ and the effect of interface temperature on solidification.²⁸

*The American Foundrymen's Society has actively supported computer simulation work since the early 1940's. A review of this and other U.S. work was presented at the Sheffield International Conference on Solidification and Castings.²⁶

TABLE I
COMPARISON OF THERMAL AND ELECTRICAL PROPERTIES²²

<u>Thermal Property</u>	<u>Electrical Equivalent</u>
Thermal Capacity	Electrical Capacity
Thermal Resistivity	Electrical Resistivity
Temperature	Voltage
Rate of Heat Flow	Current
Heat Content	Electric Charge

Since the development of the digital computer, analog techniques are used sparingly and in very specialized situations. One such application reported in the literature involved laying out water lines in die casting dies.²⁹ However, while the principles are the same, this particular application used electrically sensitive paper instead of the analog computer. A general description of this analog technique can be found in the book by Dusenberre.³⁰

Finite Difference Technique

Numerical techniques have long been known, but it was not until the advances made in the digital computer that they became usable. This was because of the time-consuming iterative procedures required to solve the equations.

The numerical analysis equations are formed by expanding the partial differential equations using Taylor's Expansion Theorem. This can result in either center, forward, or backward-differencing equations. Center differencing is preferred because the inherent error is less than for the other two methods. This equation can be solved either explicitly or implicitly. Explicit techniques have the advantage that all temperatures are known at the time the calculations are made. However, a maximum time step exists which if exceeded will cause the equation to represent a thermodynamically impossible condition and the problem becomes numerically unstable. Implicit techniques are unconditionally stable, but they require that a series of simultaneous equations be solved. Dusenberre discusses finite difference techniques for general heat transfer problems and also includes a section on handling latent heat.³⁰ An excellent discussion of finite difference techniques as applied to casting simulation is given in the AFS monograph Computer Simulation of Solidification.¹³

Problems modeled using finite difference techniques are divided into a series of uniform property, uniform temperature nodes (Fig. 2). The node temperature is assumed to be the temperature at the geometric center of the node. In thermal analog terminology, these nodes have a capacitance (ability to store heat) and are connected by conductors which can represent heat transfer by conduction, convection, or radiation.

Finite Element Technique

Finite element techniques were originally developed for solving complex stress analysis problems. During the 1960's, the applicability of this technique to both steady state³¹ and transient^{32,33} heat transfer problems was reported. The fact that the technique

Fig. 2. Finite difference modeling approach for thermal analog heat transfer codes.

was originally developed for stress analysis makes finite element solutions particularly appealing to researchers and engineers interested in calculating thermally induced stresses. The fact that the basic elements can be defined independent of thermal properties is also appealing in that the problem can be modeled based on information required without being concerned about relative thermal properties.

A wide variety of element shapes has been demonstrated for stress analysis programs and theoretically all can be used in thermal applications. For a two-dimensional problem using a basic triangular element, the problem is defined as a series of triangular elements with node (temperature) points located at each corner (Fig. 3). Thus each node represents a point on all common elements.

Fig. 3. A finite element modeling configuration.³⁴

The volume associated with each node is equal to one third of each triangle. In the simplest form the temperature distribution is assumed to be linear throughout the entire element, but quadratic, cubic, etc., variations could just as well be assumed.

Matrix algebra techniques are used to calculate heat fluxes and the temperature of each node point.³⁴ Once the variables for the individual elements are determined, matrix techniques are again used to solve and determine the final answer for the "global" or entire matrix. The general pattern required for solution of finite element problems is outlined in the book, The Finite Element Method in Engineering Science, by O. C. Zienkiewicz.³⁵

Pseudo-Steady State Technique

The pseudo-steady state technique is a second finite difference approach to the transient heat conduction problem. However, instead of using partial differential equations to arrive at the answer, steady state heat transfer equations are used to calculate the net heat transfer rate for each node. The heat transfer rate is then converted into the temperature change. In this manner, the individual can work with the simpler algebraic equations and not have to derive numerical solutions from partial differential equations.

The three steady state equations listed below describe heat transfer by convection, conduction, and radiation:

$$\text{Convection:} \quad q = \bar{h}A(T_1 - T_2)$$

$$\text{Conduction:} \quad q = \frac{-kA}{\ell}(T_1 - T_2)$$

$$\text{Radiation:} \quad q = \epsilon\sigma A(T_1^4 - T_2^4)$$

where 'q' = heat flow rate, ' $\bar{h}$ ' = heat transfer coefficient, 'A' = cross sectional area through which heat is transferred, ' ℓ ' = distance heat transferred, 'k' = thermal conductivity, ' ϵ ' = emissivity, and ' σ ' = Stefan-Boltzmann constant.

Kreith³⁶ shows that the equations for conduction and radiation can be converted to the same form as the convection equation by defining the thermal conductance, 'K,' for the three nodes of heat transfer as:

$$\text{Convection:} \quad K = \bar{h}A$$

$$\text{Conduction:} \quad K = \frac{-kA}{\ell}$$

$$\text{Radiation:} \quad K = \epsilon\sigma A \left(\frac{T_1^4 - T_2^4}{T_1 - T_2} \right)$$

By using small time steps, heat flow rates between points in transient problems can be approximated using the convection equations and the above thermal conductances. Using the relationship $q = [V\rho(T_f - T_i)C_p]/\Delta t$, where 'V' = node volume, 'ρ' = density, 'C_p' = specific heat, 'Δt' = time step, 'T_f' = final temperature, and 'T_i' = initial temperature, the new temperature is calculated.

Gatecliff used this approach in simulating the operation of a gas compressor.¹⁷ An integral part of this simulation was calculating heat flow during operation of the compressor. The interesting feature about this work is that a large supercomputer was not required. Gatecliff ran this program on an IBM 1130 with 16,000 words of memory. Subsequently this technique has been applied by Weatherwax and Riegger¹⁸ to die casting simulation. This work will be discussed in greater detail under simulation applications.

The only mathematic or computer code restrictions on how the problem is modeled is related to the time step. Thus, the node size is a function of the information required, the expected temperature gradients in the part, and the time step desired. In the work by Weatherwax and Riegger, the time step was read as input data. Since this is an explicit finite difference approach, a maximum allowable time step exists. This time step must be chosen so that using the

worst case,
$$\sum_{i=1}^{i=n} K_i \left(\frac{\Delta t}{V_i \rho C_p} \right) \leq 1$$
 where 'K' is the conductance

value in the convection equation and 'n' is the number of neighboring nodes connected to the node in question.

The Biot number, Bi, can give an indication if the node volume is of the proper size. The Biot number is a dimensionless number defined as $Bi = \frac{\bar{h}L}{k_s}$, where 'h' is the average surface conductance, 'k_s' is the thermal conductivity of the solid, and 'L' is the "significant length" defined as the volume divided by the surface area. If the Biot number is less than 0.1, uniform temperature assumption will introduce errors of less than 5%.

When used for nodes of different materials, Veynik defines a new number K to eliminate a potential conflict in definitions.³⁹ Both are defined by the same equation, but in the strictest sense of the definition, 'h' designates the heat transfer rate between two materials for the Biot number whereas for K, 'h' also includes the effective heat transfer rate across the gap formed between the casting and mold.

FLUID FLOW SIMULATION

Up to this point, all the discussions have related to simulating heat transfer problems. However, in many solidification applications, metal flow and heat loss during this flow is of importance. Currently, the standard assumption of instantaneous mold filling is made. The validity of this assumption depends on the system being simulated. For processes where the filling time is a small fraction of the total solidification time for the casting (or a critical part of the casting), this assumption does not introduce significant errors. However, this is not always true in processes where rapid solidification occurs or where a large temperature loss occurs during mold filling. It is the latter areas where fluid flow simulation will play a major role.

Research is being carried out in the field of hydrodynamics modeling. This work has led to the publishing of general purpose codes such as SOLA-SURF.⁴⁰ However, these codes are not universal and further development is required before they are applicable to general mold filling problems.

Some fluid flow simulation is currently being performed. This includes work at McGill University concerning fluid flow in ladles⁴¹ and the simulation of injection molding of plastics at Cornell University.⁴²

MODELING A SOLIDIFICATION PROBLEM

Computer simulation of casting solidification has proceeded to the point where it is leaving the research laboratory and entering the manufacturing world. This means that the question to be answered has changed from "Is computer simulation a reliable approach?" to "Is computer simulation economically feasible?" The latter question covers two distinct areas. The first is computer hardware costs. This is the most visible cost and is one everyone is concerned about. A more subtle but much more costly item is manpower. Dr. Barry Boehm studied a series of large computer projects circa 1970 and projected the cost for future Air Force contracts.⁴³ He predicted that today (1978) manpower costs would be four times greater than computer hardware costs. Even if his estimates were off by a factor of two, manpower requirements still are the major cost and must be addressed in any program.

One means of reducing the manpower is through the use of general purpose software.⁴⁴ By using such software, the time required to generate the data needed for simulation can be greatly reduced and a new computer program does not have to be written and debugged for each problem. Manpower can further be reduced by using computer graphics to aid in preparing the data and analyzing the results.

Table II gives a list of typical general purpose heat transfer codes available to the public. ADINAT⁴⁵ is a three-dimensional finite element code with working versions in the field, but which has not been totally developed. Its current limitation of constant specific heat and its lack of a procedure for handling latent heat make it unacceptable for solidification studies today. However, it is purported that temperature varying specific heat and a means of accounting for latent heat are being incorporated into a soon-to-be-released version of ADINAT. AYER³⁴ is a two-dimensional finite element code. This code has the restriction that the latent heat of fusion must be accounted for using the specific heat method or by some other user-defined process. An unnamed finite element code has been written by the University of California, Irving.⁴⁹ This code handles two- and three-dimensional problems and isothermal phase changes.

Perhaps the strongest points in favor of finite element codes for thermal applications are the extensive pre- and post-processors available for these codes. Because of the extensive use of finite element codes for complex structural problems, many of the codes have sophisticated interactive programs for use in modeling the programs. Similarly, post-processing packages with extensive graphics capabilities are also available.

The CINDA family of codes was written for the National Space Aeronautics Administration (NASA). These finite difference codes can handle three-dimensional problems and have extensive program libraries giving the user a wide choice in the type of differencing routine to be used. They handle temperature varying properties and SINDA¹⁰ has a subroutine for handling latent heat. This short subroutine can be used with CINDA-3G.⁴⁶ Some graphics output subroutines are available within CINDA-3G and SINDA, but they are not nearly so versatile or sophisticated as those available for finite element codes.

TABLE II

GENERAL PURPOSE HEAT TRANSFER CODES

<u>Name</u>		
ADINAT ⁴⁵	Finite Element	Mass. Institute of Technology
AYER ³⁴	Finite Element	Los Alamos Scientific Laboratory
---	Finite Element	Army Cold Regions R&E Lab ⁵⁰
CINDA-3G, ⁴⁶	Finite Difference	National Aeronautics Space Ad.
SINDA ¹⁰		
HEATING5 ⁴⁷	Finite Difference	Oak Ridge National Laboratory
MITAS ⁴⁸	Finite Difference	Control Data Corporation
TRUMP ⁴⁹	Finite Difference	Lawrence Radiation Laboratory

The MITAS⁴⁸ code is basically a Martin-Marietta version of CINDA-3G written for Control Data Corporation. The interesting feature of this code is that it is available on Control Data's Cybernet system which makes the code commercially available for users from remote dial-up terminals.

Preprocessors are available for finite difference codes but again they are not so extensive as for finite element codes. Two such meshers are FED⁴⁹ written for the TRUMP⁴⁹ heat transfer code and HEATMESH-71⁵⁰ for the CINDA codes; both are limited to problems with axisymmetric geometries.

Graphics output is a must if large volumes of computer-generated data are to be analyzed accurately and with minimum manpower requirements. This output can take the form of standard cooling curves, isothermal plots, or plots where colors and/or symbols representing temperature ranges are plotted at node locations. When color microfilm is used, the results can be plotted as 35-mm slides or 16-mm movie film.⁵¹

APPLICATIONS

Solidification simulation is being used in a wide range of applications. Its biggest use is in the steel industry where multi-ton castings make experimental programs costly and the gains to be realized from improved processing are large. However, simulation work is not limited to large steel castings. Examples of simulating die casting, welding, centrifugal castings, evaluation of riser systems, and mold development can be found in the literature.

Sand Ingot Castings

In 1954, Sarjant and Slack published their paper on calculating the internal temperature distribution in steel ingots.¹⁷ In this paper, the authors expanded upon the work of Eyers, et al.,⁹ and used numerical techniques to calculate transient two-dimensional heat flow patterns. This work formed the impetus for much of the work to follow. A summary of simulation research prior to 1954 is contained in the book by Ruddle.²²

Both Fischer⁵⁴ and Henzel and Keverian^{55,56} used General Electric's general purpose transient heat transfer code (THT) to simulate solidification of large steel castings. Excellent agreement was obtained between calculated and experimental data for a 20,000-lb. steel turbine inner-shell casting simulated by Henzel and Keverian.⁵⁶ Fischer's work pertained to steel ingots weighing as much as 150 tons in which convection currents played a significant role in the internal heat transfer of the ingots. He accounted for

this increased heat transfer rate by multiplying the thermal conductivity of the liquid steel by ten. The fact that a general purpose finite difference computer was used for these works is worthy of mentioning again.

The AFS-sponsored work at the University of Michigan has dealt with the simulation of small ferrous and non-ferrous castings. Once the problem of unknown thermal properties has been overcome, good experimental/calculated agreement has been obtained from data reported in the literature.^{12,50,59} Using laboratory-cast aluminum shapes, they have been able to predict the presence of voids and the effect of graphite chills on the solidification pattern.^{13,60,61} This work has been extended to a commercial steel casting and the simulation has accurately predicted the presence and location of voids, a means of eliminating the voids, and the shape of the pipe in the hub riser (Fig. 4)⁶²

Sciama* examined the solidification of aluminum-silicon alloys in permanent molds.⁶³ He found the enthalpy curve and the interface heat transfer coefficient play important roles in defining the

*The papers authored by Sciama give a good bibliography of foreign work related to simulation development.

Fig. 4. Calculated and experimental pipe shapes in hub-risered steel casting.⁶²

solidification processes. Also, mold wall thickness affects solidification time for thin-walled molds, but does not significantly affect the results as the wall thickness extends beyond a critical wall thickness. Srinivasan showed similar trends for cast iron cast in metallic molds but also indicated that there was a relationship between casting size and effect of mold wall thickness.⁶⁴ The effect of mold wall thickness is also discussed by Roshan, et al.⁶⁵

Using the same simulation techniques, Sciama also investigated design parameters for sand-cast eutectic cast iron.^{66,67} From these calculations, he was able to show how the thermal center in castings shifted as the thickness ratio of intersecting sections changed. He found that a "fin" can either accelerate or retard the solidification of the attached plate in an L-section. How it behaves depends upon whether the fin thickness is less than or greater than a critical thickness. The influence of core thickness for cast iron, aluminum-silicon, and aluminum-copper alloys was also determined.⁶⁸ For cores, the shape of the part, e.g., flat shaped, cylinders, or spheres, determines how the core thickness affects the solidification time.

One means of making computer simulation data more readily available to the working foundryman is to present the computer-generated data in generalized graphical or tabular form. Massey and Sheridan did this for calculated soaking times.⁶⁷ Unble uses this technique for cast steel rolls by graphically determining modulus reduction factors as a function of roll diameter for varying chill depths.⁶⁹ By so doing, these authors were able to make effective use of computer simulation data without the foundry production employees having to work with the computer.

Die Casting of Aluminum Engine Parts

The die caster is interested in many aspects of the casting cycle. He is concerned about solidification sequence and its effect on casting soundness and temperature gradients in the die are of importance with respect to die life. However, as die temperatures are increased to minimize temperature gradients and extend die life, the heat extraction rate is decreased causing increased cycle time and decreased production rate.

Veynik,³⁹ Wallace et al.,^{70,71} Caswell and Lorentzen,⁷² and Thukkaram⁷³ have dealt with the theoretical aspects of die casting and performed some of the early computer simulation calculations. Work at Penn State University has involved prediction of die failure mechanisms based on calculated thermal distributions for a variety of materials.⁷⁴

Weatherwax and Riegger have published a series of articles on simulating aluminum die casting operations.^{30,75,76,77} They calculated the solidification pattern for a 380-aluminum-base alloy connecting rod using production conditions and compared the results with the macrostructure developed in the casting. The results showed that porosity was present in areas predicted to solidify without proper feeding. Further calculations indicated that die temperature gradients attainable in production would not significantly affect the solidification order, that thermal stock damage is reduced by high initial die temperatures and that directional solidification can be attained with proper die temperature control and gate placement.

Since this initial work, Weatherwax and Riegger have expanded this work to more complex shapes. One such shape is the bore section of an aluminum cylinder block for a small engine, the model of which is shown in Fig. 5.

Fig. 5. Node network used for simulating solidification of aluminum cylinder block casting.³⁸

This work is significant in two important ways: first, the works are true three-dimensional simulations; second, the work was done using the pseudo-steady state method on a PDP-11 minicomputer. The first publication of this series of papers was made in 1971, and the work required only 16K memory. The net result of these calculations were "The casting quality was upgraded by making the changes in gating and casting procedures as suggested by the simulation results."⁷⁵

Special Casting Processes

Attempts have been made to simulate a variety of other casting processes lumped under the title of "Special Casting Processes" in this report. One such area is centrifugal casting. Lazaridis used numerical techniques to analyze the thermal history of a centrifugal mold for ferritic cast iron pipe.⁷⁶ Both start-up and continuous operation were analyzed. From these studies they found that one of the most important, but least controlled, variables with respect to mold life was the thickness of the insulating, mold coating layer. Solidification histories for pipes cast in these molds were presented in a separate paper.⁷⁹

The vast majority of papers involving computer simulation deal with thermal gradients (profiles) in the mold and metal, or to a lesser extent, thermal stresses incurred during the casting process. An exception is the work of Ebisu in Japan.⁸⁰ In this work, the author included calculations based on solidification theory to account for macrostructural features in centrifugally cast alloy steel pipe. The importance of mold coating thickness and properties as reported by Lazaridis was confirmed. Ebisu also found that pour temperature was a major factor in producing a uniform, columnar microstructure in the Ni-Cr steel. This was the result of preventing premature solidification caused by longitudinal temperature gradients during mold filling.

Both growth rate 'R' and temperature gradient 'G' were calculated. These values were then used to calculate dendrite length and as an indicator of the type of structure formed. The calculated G/R ratios indicate the dendrites would form tertiary arms. Further, in castings where the simulations indicated low growth rates, the macrostructure was significantly coarser than for castings which the simulation predicted would have a faster growth rate. Thus, the validity of the calculations was verified.

The simulation of continuous casting has been the subject of several papers, many of which were published in the late 1960's. Irving⁸¹ summarized the analytical work related to continuous casting performed prior to 1966. At that time, he chose to use the "integral profile technique" developed by Hills⁸² because of the

computer requirements for finite difference techniques. About the same time, Mizikar reported simulation work involving one-dimensional numerical analysis of the continuous coating of steel.⁶³ He did this by dividing the process into three distinct sections: solidification in the mold, solidification in the spray cooling zone, and solidification in the radiant cooling zone. Sufficient confidence in the results was obtained by the author to allow the calculations to be used in designing cooling systems for their continuous casting units.

More recently, simulation of continuous casting has involved the role of stresses in gap formation. Grill, et al., have studied this for steel slabs.⁶⁴ Interestingly, they applied a three-dimensional finite difference approach for the heat transfer calculations and combined it with a two-dimensional finite element stress analysis technique. Using calculations from this program, they found that hot spots can form near the corners of the steel slab and that these hot spots are associated with gap breakdown, a condition they hypothesize results in high enough tensile strains to cause rupture of the steel shell. The fact that corner hot spots were found in this model stresses the potential dangers involved in assuming symmetry or adiabatic surfaces. It is not known if they would have been calculated in a two-dimensional model, but it is certain that they would not have been found in a one-dimensional model.

Mathew and Brody are also studying the continuous casting process from both thermal and mechanical aspects.^{65,66} They have applied these calculations to aluminum and magnesium alloys as well as plain carbon steel.

The importance of gap formation and its effect on the heat transfer coefficient not only plays an important role in continuous castings, but also in consumable arc melting. For this process, Eisen and Campagna calculated that the slab thickness itself was the other major controlling variable.⁶⁷ They also found that the rate of addition of material changed the pool depth, but did not affect the local solidification time. Arc melting is a difficult process to model and the authors pointed out that because of assumptions made, the model was "semiquantitative."

Welding

Welding is a special form of the solidification problem in that it involves simulating melting as well as solidification, it has a moving heat source, and in some instances it has metal added to the system as the simulated process continues. Rosenthal discusses the theoretical aspects of heat flow during welding.⁶⁸ References in

in the literature have also been made to a book by Rykalin⁸⁹ on the same subject, and a survey paper by Mayers, et al.⁹⁰

Both finite difference and finite element techniques have been used in weld simulation. The finite element approach has the advantage of being able to calculate thermal-induced stresses during the welding processes. Hibbitt and Marcal⁹¹ investigated the application of finite element techniques to the arc welding processes. This work incorporated the ability to handle the deposition of molten filler metal during welding. These results showed that radiation losses during welding had a significant effect on the peak temperature attained in the weld metal pool.

Using the basic technique developed by Hibbitt and Marcal, Friedman^{92,93} also investigated the simulation of gas tungsten arc welding. In Friedman's work, the heat input was applied either as a surface heat flux or to a thin layer at the weld surface; both methods gave the same results. The heat input area was calculated at each time step by the location of the liquids isotherm on the surface. They reported good agreement with experimental results for temperatures in the solid, but could not get good calculated agreement for the shape of the weld fusion zone.

Paley and Hibbert⁹⁴ encountered similar problems, but found that by applying the heat of fusion to all nodes in the fusion zone, they could reproduce the fusion zone shape. However, this requires prior knowledge of the weld zone shape and negates much of the advantages of doing simulation studies. The fact that good experimental/calculated agreement was obtained when the heat input was applied to all nodes in the fusion zone suggests that heat transfer conditions within the weld pool were not adequately simulated. This work made good use of computer graphics including three-dimensional plots of temperature in the weld area. They also made isothermal plots which they were then able to correlate with the macrostructure obtained in butt, double-V, three-wire submerged arc, and fillet welds.

Passoja has applied theoretical calculations to electron beam welding⁹⁵ and simulation techniques should be applicable to this process. However, because of the high depth-to-width ratio of many electron beam welds, the problem of weld pool heat transfer becomes even more significant. Not only is the means by which the heat is input in the model important, but the extremely high weld metal temperatures require that metal vaporization must also be taken into account in certain welds.

Numerical techniques have also been applied to spot welding. Althey's work on this subject⁹⁶ is very theoretical in nature and the correlations presented are between numerical and analytical techniques. However, he does discuss means of handling resistance heating problems.

Feeding Distance Calculations

The feeding distance of risers is of major concern to metal casters. Feeding distance is not only affected by casting design, but by the manner in which the alloy being cast solidifies. This problem was addressed by Davies³⁷ in another outstanding example of combining solidification theory with numerical simulation. Using the numerical procedures outlined by Sarjant and Slack, Davies calculated the solidus velocity (V_s) along the axis of the plate and solidification curves, i.e., time vs. location plots, for isotherms representing various fractions solid.

The equation for capillary feeding distance, ' l_f ,' was derived and given as $l_f = (Bh\rho^2V_m/V_s)$ where ' B ' is a constant = .22, ' h ' = feeding height, ' ρ ' = density liquid metal, ' r ' = capillary (pore) radius, ' m ' = solidification contraction, ' η ' = dynamic viscosity, and ' V_s ' = solidus velocity. Based on the mode of freezing, estimates were made for the volume metal solidified at which feeding problems would occur. For example, Davies estimated that feeding problems would start at 95% solid for 0.6% C steel, 95% solid for 99.99% Al, and 90% solid for 99.6% Al. The capillary length was determined and plotted on the same graph as the calculated feeding distances for each node (Fig. 6). Whenever the feeding distance value is less than the capillary length, centerline shrinkage can be expected.

Fig. 6. Calculated feeding distances for aluminum plate.³⁷

Davies calculated feeding distances for a wide range of materials and compared them with empirically determined values found in the literature and used in industry. Excellent agreement was obtained. As Davies points out, it is important that reasonable assumptions be made for when feeding problems start, for the results depend on these assumptions.

Mold Design Evaluation

It was previously stated that there are three means by which manpower requirements could be reduced in computer-related work. An example of this approach is given in solidification simulation work being performed at the Los Alamos Scientific Laboratory.³² The program's objective is to optimize the design of a coated graphite mold that would significantly reduce the material required to cast hemispherical enriched uranium parts. To accomplish the goal, it is proposed that a recirculating tin pump be used to achieve directional solidification in the cast parts.

A modified version of the FED mesher was used to generate node and conductor input data for the CINDA-3G heat transfer code. The calculated results were then plotted for analysis on 16-mm film using a general plotting program.³³ Using this technique, a mold design was developed which promoted the desired directional solidification and reduced the metal requirements by 55%. The work performed for this program is summarized in a 16-mm, computer generated, color film.

SUMMARY

The technical feasibility of computer simulation of solidification problems has been demonstrated. The calculations can be made using finite element or finite difference techniques which in general, require larger, faster computers. It has also been demonstrated that using steady state approximation techniques, solidification problems can be successfully modeled on smaller computers such as PDP-11. Release of the latent heat of fusion requires special attention, but it can be handled in one of several methods. The method best suited for the problem is a function of how the metal being simulated solidifies and the computer code being used.

A wide variety of metal systems and types of solidification processes have been simulated. Its largest use has been in the casting of large steel shapes. However, it has also been demonstrated that computer simulation can be used for smaller castings to detect defects and to determine the potential benefit of suggested engineering changes. Computer simulation work has been applied to both slow and fast cooling systems. The former is represented by sand castings, and the latter by die casting and welding.

The works of Ebisu and Davies demonstrate how computer simulation can be combined with solidification theory and scientific principles to study casting problems. Ebisu predicted the macro-structure developed in centrifugal castings while Davies calculated feeding distances for risers, taking into account the manner in which the metal solidified.

Simulation of fluid flow during casting processes is still in its infancy. Work has begun in simulating metal flow and it is anticipated that this will be the next area of major technological advances in the simulation field.

General purpose software must be used if solidification simulation is to be economically employed in the foundry industry. It is this area which must be developed if Ruddie's prediction quoted in the Introduction is to materialize by 1991. The general techniques needed to produce this software are available, but large expenditures of money will be required to implement them. It is questionable if the preprocessor (mesher) computer programs will be developed specifically for simulation problems because of economic reasons. It is more likely that the thermal simulation software will be incorporated into modified CAD/CAM systems. In this way, computer-aided design programs could be used for inputting and manipulating the basic geometric data and software would only have to be written for performing the specific functions required for thermal and fluid flow simulation.

With the rapid advances made in the areas of CAD/CAM programs, the 1991 date of Ruddie is entirely realistic. In fact, if the work continues at the present pace, his goal will be reached earlier than predicted.

ACKNOWLEDGMENTS

Several individuals contributed to the preparation of this paper. From the Los Alamos Scientific Laboratory, the help of J. M. Dickinson, R. E. Keenan, G. A. Bennett, and the staff of the LASL Technical Library, in particular M. H. Treiman, was greatly appreciated. Fellow members of the AFS Heat Transfer Committee, J. T. Berry, R. D. Ruddie, O. K. Riegger, A. E. Umble, and L. J. D. Sully, also contributed through discussions and aid in locating references not available to the author.

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