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MODELING THE DIRECTIONAL SOLIDIFICATION PROCESS

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Abstract

The directional solidification process is used to manufacture single crystal turbine blades with superior properties by controlling radiation heat transfer in a furnace containing obstructing baffles that move relative to the parts being cast. A group effort was undertaken by the MANTECH Program, General Electric Aircraft Engines, PCC Airfoils and the University of Illinois to understand temperature development in this process and to predict the microstructure and occurrence of defects in single crystal investment castings as a function of blade geometry and casting conditions. The approach combines finite element heat flow modeling with experimental measurements and metallographic analysis. This work focuses on the development of a transient, 3D finite element model, which is used to calculate temperatures throughout the casting process, cooling rates, local solidification times, temperature gradients, and solidification front velocities. A novel method has been developed to accurately model the moving boundary while achieving reasonable computer run times. The model temperature predictions compare reasonably with temperatures measured in an experimental cluster of cylindrical airfoils cast in an industrial furnace at PCC Airfoils. The results indicate that the model is a powerful tool for predicting microstructures and defects in single-crystal investment castings.

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Introduction

The directional solidification process has been used for well over a decade to manufacture both oriented columnar-grain and single-crystal turbine blades. Castings produced via this process have better high-temperature creep, fatigue, and corrosion properties and closer dimensional tolerance control than conventional equiaxed-grained investment castings. A quality casting must meet stringent microstructural specifications as well as avoiding the many defects that can arise during solidification. The metallurgical objectives of this process are more difficult to achieve than in conventional foundry casting since there are many more interdependent process parameters to control. Consequently, development of the casting practices to produce a defect-free blade is expensive and time-consuming, usually done by trial and error experiments for each new blade design. The powerful mathematical modeling techniques that have been developed[1] and are being successfully applied to foundry casting[2, 3] and investment casting [4] should therefore prove even more beneficial for the directional-solidified and single-crystal turbine blade manufacturing industries.

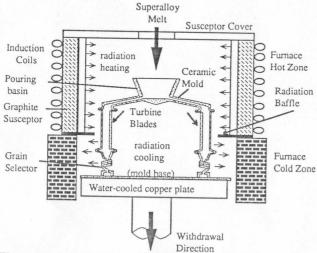
The present work was undertaken to develop a mathematical heat transfer model of the directional solidification process to use as a tool to aid in the development and optimization of the process parameters for efficient and defect-free casting of new blade designs. This work is a group effort between the Air Force MANTECH Program, PCC Airfoils, General Electric Aircraft Engines, Structural Dynamics Research Corporation, and the University of Illinois. It combines finite element heat flow modeling with experimental measurements and metallographic analysis. The present paper focuses on the numerical methods developed to handle the special difficulties that the directional solidification process presents.

The Directional Solidification Process

The directional solidification process is illustrated in Figure 1. To achieve reasonable productivity, 10 to 30 blades are cast at once, in groups called "clusters", oriented in a circular pattern for thermal uniformity. A thin-walled ceramic mold, containing a pouring basin and runner to each blade cavity in the cluster, is created through the conventional "lost wax" process used in investment casting. Specifically, the wax pattern is coated in ceramic slurry, baked, and the wax drained from the mold. The mold is then placed within the upper zone of a cylindrical furnace on

top of a water cooled chill plate, as shown. Power supplied through induction coils within the graphite "susceptor," forming the "hot zone" of the furnace, then preheats the mold. The furnace is then evacuated and superheated liquid superalloy is poured into the pouring basin.

Solidification
begins against the chilled
copper plate at the bottom.
The front travels slowly
upward through the mold
as it is withdrawn at a
programmed rate down
into the cooling chamber,
or "cold zone" of the
furnace. A single crystal
blade results when
solidification is forced to



furnace. A single crystal blade results when solidification is forced to

wind through a thin, spiral-shaped grain selector, or "pig-tail", with only a single grain of the

preferred <001> crystallographic orientation surviving to enter the airfoil portion of the mold. The hot and cold zones of the furnace are separated by radiation baffle(s), designed to maximize the temperature gradient within the blades across the solidification interface. The gating system is the last to solidify. It should be designed to feed molten metal into the blade cavities as they shrink, thereby limiting shrinkage cavities, porosity and residual stress generation.

The important casting parameters that are available to control this process for a given blade design include:

- · geometry of furnace interior, grain selector, ceramic mold wall thickness and feeding system
- position, shape, and thickness of radiation baffles
- location and orientation of the blades in the cluster inside the furnace
- insulation of selected portions of the ceramic mold
- · conduction and radiation properties of the alloy, ceramic, baffle and furnace wall material
- · superheat of the alloy
- preheating time of the ceramic mold
- withdrawal rate (which generally changes during the process)
- time-dependent heat input to the furnace hot zone (power to heating coils)
- water flow rate through cooling chamber walls and chill plate in furnace cold zone.

To be useful, mathematical models of the directional solidification process must relate the above variables to the occurrence of the various microstructures and defects that can occur. To do this requires an accurate prediction of the temperature history at every point within the blade.

To accurately model temperature development during this process requires a faithful threedimensional representation of the true furnace, baffle(s), pouring basin, feeding system, mold, and blade geometries found in production clusters. Industrial observations, literature, and sensitivity studies all indicate that the most important and sensitive heat transfer mechanism (for defect prediction), is radiation between the ceramic mold surfaces and the furnace interior.

Radiation is also the most difficult phenomenon to incorporate into the model, because calculation of the view factors is very computationally intensive in three dimensions. In addition, the view factors generally change continuously with time during the process, due to relative movement of the blades and furnace and intermittent shielding by the baffle(s). These effects produce the directional temperature gradients fundamental to the process, so must be modelled accurately.

Mathematical Model

A three-dimensional transient heat transfer model of the directional solidification process has been developed which incorporates solidification, the withdrawal process, radiation heat transfer, and time-dependent obstruction by the radiation baffles. The model includes the superalloy blade, the ceramic mold, the copper chill plate, the baffles, and the furnace wall surfaces. Eight-node, linear-temperature iso-parametric "brick" finite elements are employed for the heat conduction solution, using a modified version of the TOPAZ3D program. [5, 6] Latent heat of solidification has been incorporated using several different methods, and has been found not to be a critical factor. Radiation is modelled by dividing the exterior of the ceramic mold and the interior of the furnace walls into small surfaces, and iteratively solving for the radiant energy exchanged between all of the surfaces at each time step.

Previous mathematical models have been limited to single blades positioned in the center of cylindrical furnaces. [7, 8, 9, 10, 11, 12, 13] The following sections discuss the methods that were developed in the present work to calculate the necessary view factors between each of the many radiation surfaces, for a general cluster of blades. These methods also attempt to incorporate the important effects of withdrawal and baffle obstruction while remaining computationally efficient. Invoking cyclic symmetry saves on memory requirements by reducing the number of view factors that must be stored, but does not simplify their calculation.

The withdrawal process is simulated mathematically by keeping the cluster of blades stationary and modeling the relative upward movement of the furnace as a time dependent boundary condition. This is accomplished by dividing the furnace wall into many small surfaces and assigning a different temperature history to each surface, according to the time when that surface passes the baffle and changes from acting as part of the hot zone into part of the cold zone. (See Figure 2)

In the present work, the view factors are calculated only once using the FACET program.[14] The simplest approach, or "basic wall method" is to move the furnace wall inward to lie along the edge of the baffle, as shown in Figure 2. Thus, view factors between each of the surfaces making up the mold and wall remain constant with time and problems

Simulate furnace interior with a straight line

Assign thermal histories to each furnace wall node

Temperature
T
i
m
e

Cooling
Chamber

Furnace wall radiation surface element

Figure 2 - The "basic wall method"

associated with the baffle are avoided. However, this position of the furnace wall effectively assumes that the top surface of the baffle has the same temperature as the hot zone while the bottom surface is at the cold zone wall temperature. Since this is not generally the case, a second method was developed.

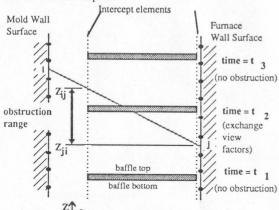


Figure 3 - Calculation of an "obstruction range" for each pair of radiation surface elements

View Factor Exchange Method

In the absence of obstructing baffle(s), the basic wall method enables modeling of the withdrawal process with constant view factors. This method was enhanced to account for intermittent blocking of pairs of surface elements by the baffle(s), while retaining the bafsrable feature of calculating the large matrix of view factors only once. This was accomplished using a "view factor exchange" method.

This method takes into account that, as the baffle moves

in relationship to the cluster, it obstructs some pairs of radiation surfaces from "seeing" each other at certain times. Their view of each other is then replaced by an equivalent view of the baffle. Since the baffle does not change shape and only moves vertically during the withdrawal process, there is a specific height range for each pair of surface elements in which the baffle obstructs their mutual view. The pair of surfaces has an unobstructed view of each other when the baffle is either above or below this height range.

Vertical planes defining the locus of travel of every baffle are input by the user during the mesh generation stage as a special "intercept element" type. These elements are only used to calculate the two heights that define the obstruction range. Note that a baffle adjacent to the outer furnace wall will have one of its intercept elements superimposed on that wall. Contoured baffles

are easily generated using several intercept elements for a single baffle. Multiple baffles are handled using several sets of intercept elements.

Prior to the transient heat conduction calculations, two matrices containing view factors and height ranges for obstruction for all surface-element combinations are calculated using a modified version of the view factor program, FACET.

During the transient conduction analysis with TOPAZ3D, whenever total obstruction of a surface pair by the baffle occurs, the view of the higher of the two surfaces to the other is replaced with a view of the top surface of the baffle, while the lower one sees the bottom of the baffle. Figure 3 illustrates schematically the times and corresponding positions when this occurs. The current position of the baffle is calculated knowing the withdrawal rate history. The view factor exchange is performed for surface pair i and j when the calculated baffle height is between the two intercept heights Z_{ij} . When the baffle is either above or below the obstruction range, the surface pair is unobstructed so its view factor is left unchanged. For simplicity, and to avoid obstruction calculations within TOPAZ3D, it was assumed that the baffle is sufficiently thin and surface elements sufficiently small that the baffle does not *partially* obstruct a surface pair.

By avoiding recalculation of view factors at every time step, this method provides an economical and general way to simulate the withdrawal process including arbitrary baffle shape and location. A secondary advantage arising from this method is the calculation of view factors for the baffle top and bottom surfaces. By creating solid conduction elements for the baffle and applying proper boundary conditions, this allows the calculation of heat flow and temperature distribution within the baffle over time. This is important because the baffle temperature is not generally known and it has a great influence on the process.

Model Verification

To demonstrate its accuracy and efficiency, model predictions using both methods have been verified against analytical solutions and compared with experimental measurements, as described below.

Analytical Solutions

The most important task of the view factor and radiation calculations is to generate a reasonably-accurate heat flux to (or from) each ceramic mold surface throughout time during withdrawal. To test the model's ability to do this, a simple analytical model was created to calculate the heat flux to selected mold surfaces. Typical temperatures were assumed for all mold, baffle and furnace wall surfaces involved. (See Table I) The simple geometry of the enclosure. shown in Figure 4, allowed exact calculation of the view factors, while realistically approximating the furnace interior. Radiation exchange within this enclosure was then calculated. The heat flux distribution to various locations on the mold surface were plotted according to their distance from the baffle. This plot was also designed to portray the heat flux history experienced by a chosen location on the mold surface during the withdrawal time, with time starting on the far right and moving left.

Mold surface temperatures were specified

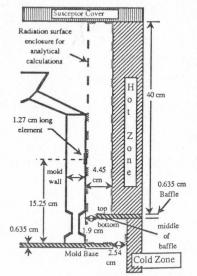


Figure 4 - Mold and furnace geometry used in verification test problem

from measurements taken at a point 15 cm from the blade base on the ceramic mold of test cylinders cast at PCC Airfoils. (See Figure 6) Table I shows the two sets of temperatures assumed for other parts of the furnace.

The first set of assumed temperatures, A, chose baffle top and bottom temperatures to match the corresponding temperatures in the furnace hot and cold zones, so that both methods could be able to match the exact heat flux solution, within their discretization errors. Figure 5 a) shows the sharp transition in heat flux achieved on passing beneath the baffle for this furnace geometry and with a "perfect" baffle. This figure also shows the reasonable agreement obtained with both numerical methods, using 0.635 cm long surface elements.

The second set, B, assumed more realistic temperatures for the baffle, found from a separate analysis of the baffle itself.[15] Figure 5 b) shows that the heat flux curve is much more gradual with the imperfect, real baffle. The peak heat flux entering the ceramic surface in the hot zone decreases from 20 W/cm² for set A to only 14 W/cm² for set B. Similarly, heat flux leaving the ceramic surface in the cold zone drops from a maximum of 9 W/cm² to about 6 W/cm². The view factor exchange method was able to adjust to reasonably approximate the new heat flux curves. On the other hand, the basic wall method can only reproduce results from set A. indicating a significant error.

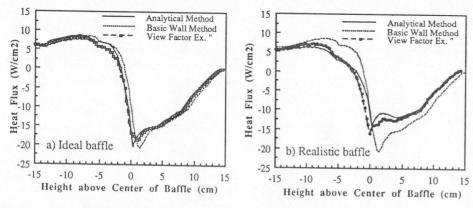


Figure 5 - Comparison between finite element predictions and analytical heat flux calculations a) assuming idealized baffle temperatures b) assuming varying baffle temperatures

Table I Furnace Component Temperatures Assumed in Analytical Solution

Furnace component	Assumed temperature set A	Improved temperature set B
Hot zone cover Hot zone Baffle top Baffle side Baffle bottom Cold zone Mold base on copper chill	1565 °C 1565 °C 1565 °C 1565 °C 16 °C 16 °C	1565 °C 1565 °C 1400 °C 1250 °C 1150 °C 16 °C

Experimental Measurements

To further test the accuracy of the model temperature predictions, a cluster of cylindrical blades was instrumented with thermocouples and cast into single crystals in a directional solidification furnace at PCC Airfoils. Model calculations were performed for the experimental geometry and casting conditions, exploiting cyclic symmetry to model only a single blade in the cluster. Calculated temperature histories in the metal are shown in Figure 6 and compared with thermocouple measurements recorded at the center of the blade. Reasonable agreement is seen

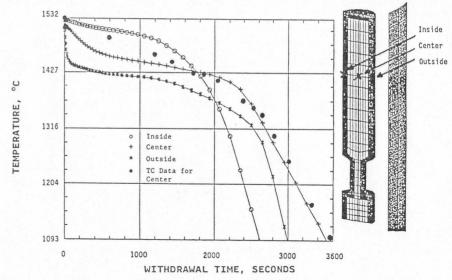
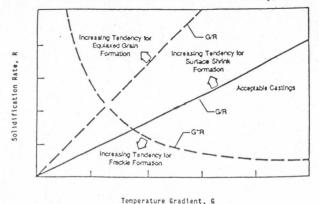


Figure 6 - Comparison of calculated and experimentally measured temperature histories within the metal casting (15 cm from bottom of starter)

Model Applications

To be of use, the model must go beyond calculating temperatures to predicting the final microstructure and the likelihood of defects. These include: off-angle primary dendrite direction, primary and secondary dendrite arm spacings, freckles, recrystallized or equiaxed grains, shrinkage cavities, secondary or misoriented grains, cracks, slivers, and striations. This work has been initiated by developing criteria that relate the likelihood of each defect to parameters derived from the model-calculated temperatures. These parameters are calculated and portrayed during the post-processing phase, using I-DEAS software[16] Four of the most important parameters are the cooling rate during solidification, T, the temperature gradient at the solidification front, G, the local solidification time, ts, and the solidification front velocity, R.

A "defect map" is one way to represent these criteria. Figure 7 illustrates schematically the observed occurrence of several defects generated in test castings as a function of G and R calculated by the model. Assuming these defects are likely at any location in the casting when the dangerous zone of G and R is found then provides a way to predict and avoid their occurrence using the model. Criteria are actively being developed to relate parameters such as these with defects and



microstructural parameters.[17] Figure 7 - Defect map for single crystal superalloy blades [17]

Another example is the prediction of off-angle primary dendrite direction, assuming the dendrites tend to grow perpendicular to the solidification front. Faithful representation of the furnace interior allowed the model to correctly predict the lower temperatures encountered on the side of the blade nearest the furnace interior. The calculated deviation of the normal to the solidification front with the vertical axis was 6° in the 3D model. This compared with a 7° angle measured between the axis of the primary dendrite direction with the axis of the cast test cylinders.[17] This shows that one use of the model is warning when proposed processing conditions might produce excessive misorientation of the growing dendrites, which would result in rejection.

Conclusion

A mathematical model has been developed for simulating the directional solidification process. It includes an efficient, accurate, general method for handling the time-dependent view factor computation required to account for relative movement between the blades and furnace and obstructing radiation baffles. The model has been successfully applied to simulate temperature development in a cluster of test blades in an operating industrial foundry. Further results indicate that the model is a powerful tool for predicting microstructures and defects in single-crystal investment castings.

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