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Predicting Interfacial Contact Conductance and Gap Formation of Investment Cast Alloy 718

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Investment casting foundries increasingly rely on numerical simulations of their casting processes to enhance quality and reduce costs. An important aspect of numerical simulations is the interfacial heat transfer between the solidifying metal and the mold. Most codes use the concept of a contact conductance to model this heat transfer. The contact conductance varies during solidification as the mold expands and the metal shrinks, leading to the formation of a gap and significantly reduced contact conductance. Very little data are available for the estimation of contact conductance, particularly for the superalloys used in the aerospace industry. This paper reports on experimental and numerical results for the determination of contact conductance for an axisymmetric casting of alloy 718. The heat transfer code TOPAZ2D, in conjunction with an inverse method is used for the numerical simulation of this inverse heat transfer problem. The effects of variation of mold properties, mold thickness, and mold thermocouple locations on contact conductance are considered. The predicted gap widths are compared to actual measurements. Finally, the applicability of the technique is discussed.

Nomenclature

c_p = specific heat
H = enthalpy
h_c = contact conductance, interfacial heat transfer coefficient
h_{cond} = conductive heat transfer coefficient
h_{rad} = radiative heat transfer coefficient
h_t = contact conductance for current time
$h_t - \Delta t$ = contact conductance from previous time step
j = counter in inverse method for future times
k = thermal conductivity
k_g = thermal conductivity of the medium in the gap
n = number of future steps used in the inverse technique
q_{int} = heat flux at the interface
S = sensitivity of changes in temperature with respect to changes in contact conductance
T = temperature
$T^{calculated}$ = numerically calculated temperature from inverse technique
$T^{measured}$ = experimentally measured temperature used in inverse method
T_{metal}, $T_{metal i}$ = metal temperature at metal/mold interface
T_{mold}, $T_{mold i}$ = mold temperature at metal/mold interface
X_{gap} = gap width
ε_{metal} = emissivity of the metal
ε_{mold} = emissivity of mold
θ = angular position
ρ = density
σ = Stefan–Boltzmann constant

Introduction

ONE of the most important areas of research in the investment-casting industry is the development and improvement of techniques used for making various cast parts such as gas-turbine blades and airfoils. Numerical simulations of these techniques can be used as tools to help reduce the scrap rate caused by defects that occur during solidification. As a result, casting foundries are now increasingly relying on the use of computer programs to numerically simulate the mold filling and heat flows that take place during the casting process. The successful application of these simulations depend on reliable and accurate input data for contact conductance (interfacial heat transfer coefficient) to model the heat transfer between the metal and the mold. Unfortunately, only a limited amount of published contact-conductance data is available (see Sridhar and Yovanovich[1] for a recent review). Little or no contact-conductance data are available for the case of alloy 718 solidifying in a ceramic mold, the subject of the present study. Various attempts have been made to model the interface conductance using empirical and semiempirical models with only a limited range of application. Lambert and Fletcher[2] presented a good review of these contact-conductance models.

Neither of the previously-mentioned reviews addresses the problem of the effect of gap formation on contact conductance. The contact conductance varies during the solidification cycle as the metal shrinks and the mold expands, often leading to the formation of a gap at the interface between the two materials. The lumped effect of conduction, convection, and radiation must then be incorporated in the concept of the contact conductance. In the investment-casting process, a wax pattern is dipped into a ceramic slurry that is dried to form a mold. After the wax is melted out forming a cavity, the mold is often preheated before pouring the metal. Just after pouring, when the liquid metal is in contact with the mold, the thickness of the gap is usually zero. As the metal solidifies, as a result of the temperature gradient that exists between the metal and the mold, an interfacial gap forms mainly because of the differences in the thermal expansions of the casting and mold materials. The effect of casting geometry is an important factor in gap formation. Nishida et al.[3] showed the different time-dependent variations of the contact conductance for flat and cylindrical castings. Variations in gap sizes were obtained if the molds were either tightly or weakly constrained. The varying geometry in a complex casting should cause the gap to develop in a quite nonuniform manner. Campbell[4] characterizes the determination of the nonuniform heat transfer occur-

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ring over the casting/mold interface of real castings as one of the largest unsolved problems in solidification modeling.

Because of the complexity of the process, the variation of the contact conductance must be inferred from experimental measurements. It is difficult to measure the heat flux at the interface directly. Instead, it is simply much easier to accurately measure the temperature history at several interior locations in the metal and the shell. The contact conductance can then be estimated from these measurements by the well-known inverse heat-conduction procedure (IHCP). Ho and Pehlke[5] and Beck[6] outlined experimental and inverse numerical procedures used to determine the contact conductance.

Recently, a tall cylindrical alloy 718 casting was poured at Howmet Corporation and measurements were made for temperature at several interior locations and gap width. In conjunction with the heat transfer code TOPAZ2D,[7] Beck's method[6] was used to determine the contact conductance values at the metal/mold interface during solidification. The results presented in this paper include the effects of the uncertainties in mold thermal properties, mold thermocouple locations, and variations in the shell thickness on the contact conductance. The relationship between the varying interfacial heat transfer and the formation of gaps is also examined. The predicted gap widths are compared to actual measured values determined by x-ray radiography on the casting. Finally, comments are made on the applicability of using these simple one-dimensional techniques to predict the interfacial heat transfer and gap formation for these types of castings.

Experimental Procedure

The techniques developed by Ho and Pehlke[5] and Beck are based on the assumptions of one-dimensional heat transfer conditions. Therefore, the dimensions of the castings were determined by running several simple two-dimensional heat transfer models of various heights and diameters. These models did not consider the effect of mold filling and the nonuniform temperature gradients that may exist in the metal and mold just after filling. From these models, dimensions were chosen where it was believed that an area of one-dimensional heat transfer conditions would exist in the center of the casting during solidification. The axial height and diameter of all the castings were approximately 25.4 cm (10 in.) and 5.08 cm (2 in.), respectively. The castings were insulated on the bottom with 3.81 cm (1.5 in.) of Kaowool insulation. Two rows of thermocouples axially spaced 2.54-cm (1-in.) apart were placed to record the temperatures of the metal and shell during cooling as shown in Fig. 1. The thermocouples had the same radial positions but were skewed by 45 deg in the angular direction θ between the two rows. The uppermost row of thermocouples (section AA—TCs 5 through 8) was placed 12.7 cm (5 in.) from the bottom of the mold and the lower row of thermocouples (section BB—TCs 1 through 4) was placed 10.16 cm (4 in.) from the bottom. The thermocouple numbering scheme and placement position for all the castings are given in Fig. 1. After the molds reached a steady-state temperature in the preheat furnace, they were moved into the pouring chamber and metal was poured into the molds. After pouring, the castings were exposed to the ambient air. After the castings were solidified, standard x-ray radiography techniques were used to determine the size of the gaps. Measurements were taken for 17 approximately evenly spaced axial positions between the top and bottom of the castings. The gap sizes were determined on the basis of density differences that existed at the metal mold interface.

Numerical Procedure

The temperature T during the cooling of the casting is governed by the following unsteady heat conduction equation written in enthalpy form[5]:

$$\rho\left(\frac{\partial H}{\partial t}\right) = \nabla\cdot(k\nabla T) \tag{1}$$

where $H = c_p T$. The latent heat release associated with the liquid to solid phase change and solid-phase transport is modeled by the specification of a temperature-dependent specific heat relating the enthalpy H to the temperature.

Equation (1), which applies to both metal and mold, must be solved in conjunction with the appropriate initial and boundary conditions. The heat flow q_{int} across the interface between the metal and mold is usually expressed as

$$q_{int} = h_c(T_{metal} - T_{mold}) \tag{2}$$

where h_c is the contact conductance. This coefficient, which varies as a function of temperature during the solidification process, is not known a priori but must be estimated by a combination of experimental and computational methods. Such an estimation, which involves the back calculation of contact

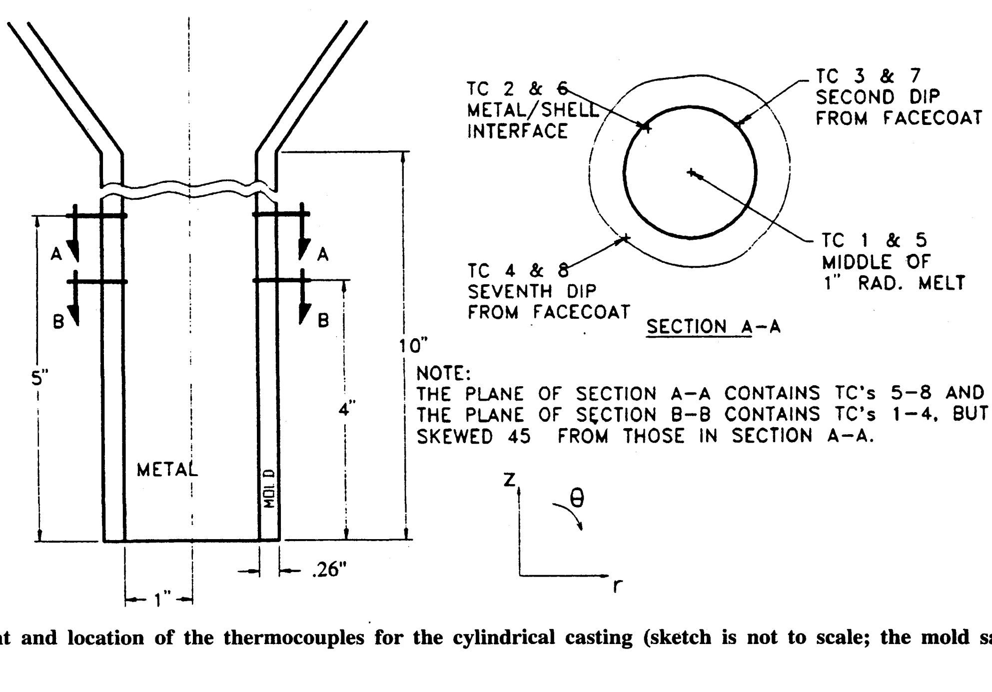

Fig. 1 Placement and location of the thermocouples for the cylindrical casting (sketch is not to scale; the mold sat on 1.5-in.-thick insulation).

conductance, constitutes the so-called "inverse heat conduction problem."

Use of Eq. (2), as explained by Ho and Pehlke,[5] involves the assumption of a quasi-steady-state approximation at the interface. If the heat flow at the interface were transient then the assumption of a single heat flux q_{int} would be invalid because the heat fluxes entering and exiting the control volume would not be equal.[5] Ho and Pehlke[8] have demonstrated the validity of the quasi-steady-state assumption as long as the gap is sufficiently small during the time frame of interest.

The present study uses Beck's future temperature algorithm[6] to reduce the stability problems caused by random measurement errors, damping, and time delays. It involves an iterative procedure in which a value of contact conductance is first assumed and then updated using a least-squares criterion based on measured and calculated temperatures at a point. Beck's method utilizes information contained in future temperature measurements for calculations performed during the current time to substantially reduce the stability problems. The algorithm is given by

$$h_t = h_{t-\Delta t} + \left(\sum_{j=1}^{n} (T_j^{\text{measured}} - T_j^{\text{calculated}}) S_j \Big/ \sum_{j=1}^{n} S_j^2 \right) \tag{3}$$

where j is the counter for future times from 1 to n, and S is a calculated sensitivity defined as dT/dh. In this simulation, it was determined that n equal to three produced the optimum results. The calculation procedure starts by assuming a value of the contact conductance $h_{t-\Delta t}$ and then determines the temperatures at various thermocouple locations as a function of time [using Eq. (1)]. The minimization procedure then yields a sensitivity coefficient that is used to perturb the value of $h_{t-\Delta t}$ [Eq. (3)]. This results in an iterative procedure in which the temperatures are recalculated using the new value of h_t and the process is carried on until a converged value of h_t is obtained for each time step.

Obviously, a direct solver of Eq. (1) is needed in this procedure for the calculation of temperature. The present study employed TOPAZ2D,[7] a finite element heat transfer code developed at Lawrence Livermore National Laboratory. The problem was treated as one involving one-dimensional radial heat transfer only, i.e., axial conduction was neglected. The optimum number of elements (14) and the size of the time step (0.25 s) were determined by numerical experimentation. A problem in using this approach is that an accurate initial condition for the metal must be specified. This was impossible to determine definitively because the metal was just poured and experienced significant fluid mixing at the early times that was not captured by the metal thermocouple data. Therefore, only the temperature of the metal in the vicinity of the interface

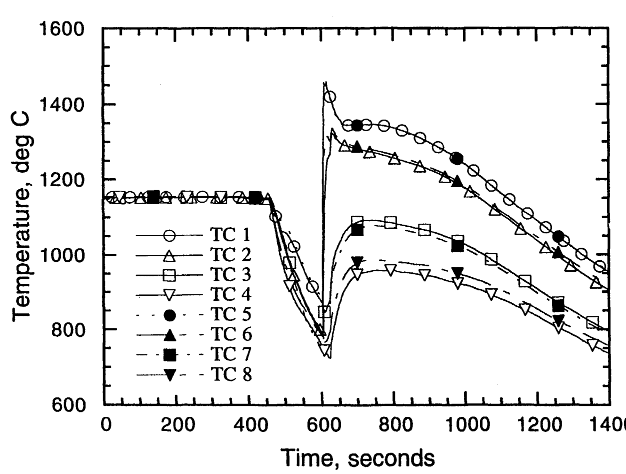

Fig. 2 Thermocouple response for the casting.

Table 1 Thermophysical property data

Property	Alloy 718	Mold
Thermal conductivity, W/m K	30.0	1.9
Specific heat, kJ/kg K	0.46	0.753
Density, kg/m^3	7632	1600

(TC2 and TC6, Fig. 1) was used in the model. The output from the outer mold thermocouple (TC4 and TC8 in Fig. 1) was used as the outer-edge boundary condition. The mold thermocouple near the mold side of the interface (TC3 and TC7 in Fig. 1) was used in Beck's method to determine the contact conductance. To avoid the numerical instabilities caused by the sharp gradients existing during the pour cycle, the simulation was started just after the pour. This occurred at 621 s for the casting (Fig. 2). The initial temperature distribution was determined from the thermocouple data. The thermophysical properties used in the calculations for alloy 718 and the mold are listed in Table 1.[9]

Various types of one-dimensional techniques exist for estimating the size of the gap that forms at the interface. Nishida et al.[3] and Shahverdi et al.[10] formulated a method based on the thermoelasticity equations. The temperature field and thermal expansion characteristics of the metal and mold surfaces in contact were used to calculate the displacements of both surfaces. Ho and Pehlke[8] theorized that if the heat transfer across the gap is mainly caused by conduction and radiation, then the total heat transfer coefficient may be considered as the sum of h_{cond} and h_{rad}. Thus

$$h_c = h_{\text{cond}} + h_{\text{rad}} = \frac{k_g}{X_{\text{gap}}} + \left[\frac{\sigma(T^2_{\text{metal}i} + T^2_{\text{mold}i})(T_{\text{metal}i} + T_{\text{mold}i})}{\dfrac{1}{\varepsilon_{\text{metal}}} + \dfrac{1}{\varepsilon_{\text{mold}}} - 1} \right] \tag{4}$$

where $T_{\text{metal}i}$ is the temperature at the metal interface, $T_{\text{mold}i}$ is the temperature at the mold interface, $\varepsilon_{\text{metal}}$ is the emissivity of the metal surface, and $\varepsilon_{\text{mold}}$ is the emissivity of the mold surface. This is the technique used here to calculate the gap width.

Results

The thermocouple outputs for the cylindrical casting are given in Fig. 2. In this figure the filled symbols represent the output from the thermocouples in the upper section AA and the open symbols represent the output from the lower section BB. As seen from the Fig. 2, the preheat temperature of the mold is 1150°C. The casting showed an average mold temperature of 770°C just before pour. There were some minor fluctuations in the thermocouple data of less than 0.5 deg. The contact-conductance values for both sections were obtained by using the numerical inverse procedure outlined in the previous section, and the results are shown in Fig. 3. The results were obtained when the calculated temperatures differed less than 0.5 deg from measured temperatures. Figure 3 shows the contact-conductance values as a function of metal temperature. The section thermocouple outputs are approximately equal for both sections except for thermocouple number 8. It was approximately 20°C higher than for thermocouple 4. The contact-conductance values thus show a disparity in response. The nonagreement of the contact-conductance values for both sections in each casting is a strong indicator that one-dimensional heat transfer conditions did not exist.

The thermocouple response for this casting shows the sharp temperature gradients that exist in the mold. Because the mold thermocouple response plays an important role in the contact-conductance calculations, the effect of uncertainties in the mold properties, mold thermocouple placement, and shell thickness was studied. Figure 4 shows the effect of increasing and decreasing the nominal value of mold thermal conductivity

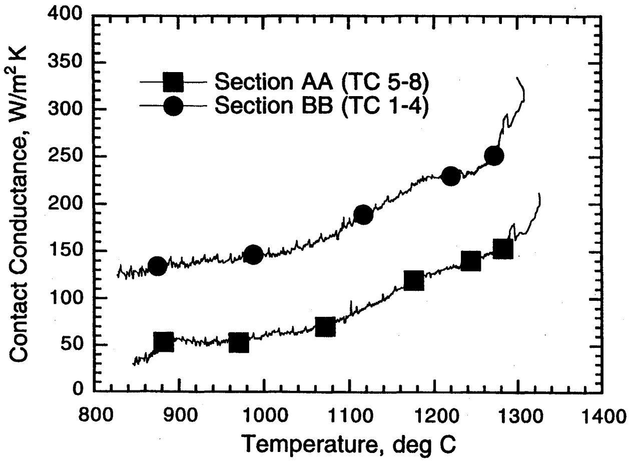

Fig. 3 Contact conductance results from the inverse code for both sections of the casting.

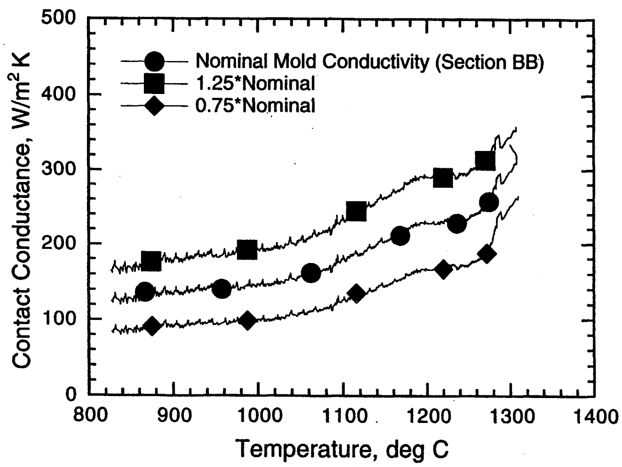

Fig. 4 Effect of uncertainties in the mold thermal conductivity on the predicted values of contact conductance.

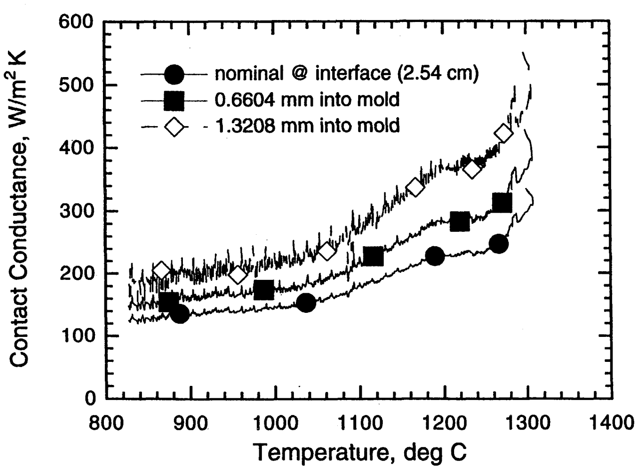

Fig. 5 Effect of uncertainties in mold thermocouple (TC 7) position on contact conductance.

by 25% on the values of the contact conductance. As the thermal conductivity is increased, the values of contact conductance also increase because of the higher rate of heat transfer now taking place in the mold material. The increase in contact conductance corresponds directly with the increase in thermal conductivity. Variations in mold's specific heat and density, however, only produced variations in the contact conductance of less than 1%. Figure 5 examines the effect of the position of the thermocouple at the mold side of the interface. As this mold thermocouple position moves outward (away from the interface) the contact-conductance values increase by an overall average of 24% for each 10% increase of outward movement into the shell. Measurements of the shell thickness showed variations around the casting and up and down the casting of about 16%. Figure 6 shows the effect of variations on the mold thickness on the predictions of contact conductance. As the mold thickness decreases, the contact-conduc-

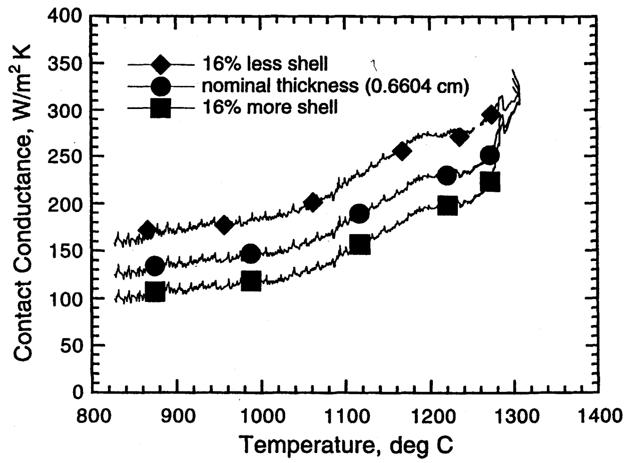

Fig. 6 Effect of variations of shell thickness on the contact conductance.

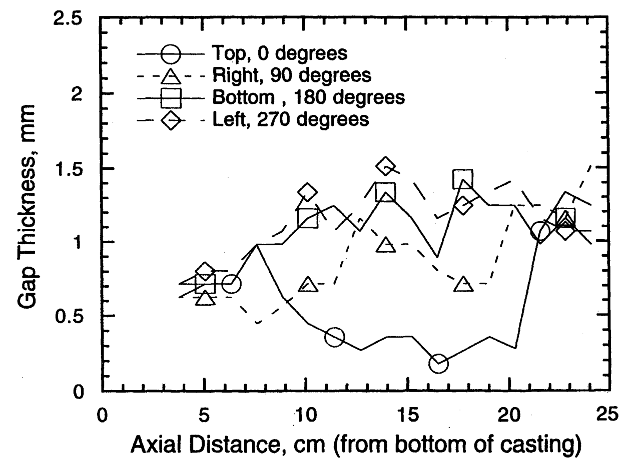

Fig. 7 X-ray measurements of the gap thickness.

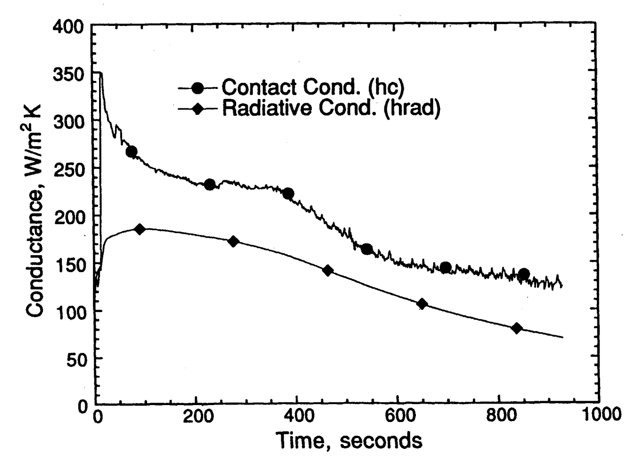

Fig. 8 Radiative and total conductances from section BB of the casting [Eq. (4)].

Table 2 Numerical calculations of the gap width for various variables in section BB

Variable	Calculated gap width, mm
Nominal	1.28
25% high thermal conductivity	0.72
16% more shell	0.77
TC 3 position moved 0.66-mm inward in the shell	0.95
TC 3 position moved 1.32-mm inward in the shell	0.69

tance values show an average increase in value of approximately 20%.

The x-ray radiography results for the casting showing the final gap thickness sizes at the top, bottom, and the left and right angular positions are shown in Fig. 7. The measurement uncertainty of the gap thickness is 0.05 mm. Nonuniform gap sizes are apparent throughout the casting with the top gap sizes generally being the lowest. The x-ray results showed that the presence of the thermocouples did not restrict the movement of the casting. The results also showed regions in the mold of low-density mold materials and areas where the gaps opened in the mold and not at the mold casting interface.

Figure 8 shows the values of the contact conductance and radiative heat transfer coefficients for the section BB of the casting as defined by Eq. (4). The gap width can be calculated from Eq. 4. Assuming that the thermal conductivity of the gas in the gap can be approximated by that of air, such a calculation yields a value of 1.28 mm for section BB. This compares favorably with the average value of gap width obtained from x-ray radiography. The gap widths caused by changes in thermal conductivity, TC position, and shell thickness are shown in Table 2. All of these values are within the scatter of the gap thickness measurements. As seen from Table 2, changes that caused increases in the predictions in the contact conductance (such as decreasing shell thickness, inward movement of the TC 3, and increasing thermal conductivity) resulted in decreases in the predicted gap widths. However, because there is some scatter in the contact-conductance computations and the true value of k_g is not known, an independent calculation of gap width would be desirable. The author is considering the use of a thermomechanical code[11] for this purpose.

Conclusions

The heat transfer code TOPAZ2D in conjunction with Beck's inverse method was used to calculate the contact-conductance values just after pour for a cylindrical casting. It was shown that these contact-conductance calculations are sensitive to uncertainties in the thermal conductivity of the mold. The effect of variation in position of the innermost mold thermocouple moving away from the interface and decreasing the shell thickness resulted in increases in the interface contact conductance. These variances led to differences in predictions of the gap widths. However, these effects did not account for the disparity in response between each section of thermocouples placed near the axial centers of the tall casting. X-ray radiography measurements of the gap thickness show variations in the gap width around and along the casting. This fact along with other observations (including the thermocouple data) points to the inadequacy of the assumption of one-dimensional radial heat transfer. The three dimensionality of this problem thus indicates the necessity of a fully coupled thermomechanical code to predict gap formation at the interface. As indicated earlier, the x-ray data indicated the possibility of mold failure. This may significantly affect the gap size calculations and warrants further study. Future studies should also include the effect of the mold-filling phase that was not included in this work. Finally, these and other similar studies by the author suggest that accurate property data are needed (particularly the thermal conductivities of metal, mold, and the gas in the gap) for reliable numerical predictions.

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