Predicting the interfacial heat transfer coefficient of cast Mg-Al alloys using Beck’s inverse analysis

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Abstract. Apart from many governing parameters, the interfacial heat transfer coefficient (IHTC) has prime importance for the numerical simulation of casting as it quantifies the heat flux between casting and mold (or chill). Most Mg alloys are based on the Mg-Al system and casting is the commonly used production process. The experimental configuration makes it challenging to measure flux and surface temperatures required to evaluate the IHTC. In this study, the IHTC was predicted for a variety of Mg-Al compositions which were cast using a permanent cylindrical mold. Unidirectional heat flow was ensured in order to replicate the experimental conditions for solving the one-dimensional transient heat equation. The numerically determined mold and surface temperatures, using Beck’s inverse methodology, were in good agreement with the experiments and analytical solution, respectively. Moreover, the heat transfer behavior across the interface depicted in the form of IHTC was analyzed, also various empirical and numerical aspects of the method are discussed.

1. Introduction
The IHTC is a key parameter for the simulation of casting. Experimentally, it is pretty challenging to quantify the heat transfer between the cast part and mold (or chill) since it is highly influenced by various factors, such as surface roughness, formation of shrinkage gap, alloy and mold temperature [1, 2] etc. In the last two decades, a number of numerical models have been introduced to predict the heat transfer in foundry processes. These predictions are mainly classified into two approaches. The first one takes into account the variation of interfacial gap as an alloy begins to solidify and correlates this gap size with the IHTC [3-5]. The other approach, which has been employed in this study, requires measuring temperature at interior points located at a finite distance from the interface followed by deriving the IHTC using the inverse method first proposed by Beck [6, 7].

Mathematically, Beck’s formulation refers to the solution of inverse heat conduction problem (IHCP). It is an ill-posed problem since it does not satisfy the general conditions of existence, stability and uniqueness [7]. The IHTC requires knowledge of the casting and mold surface temperatures along with the heat flux between these surfaces. However, the physical configuration of the IHCP makes it extremely difficult to measure flux or surface temperatures directly either by using a sensor or thermocouple. To evaluate the unknowns, the known temperature history at an interior location serves as one of the boundary conditions of the numerical procedure, while the other boundary expressed in terms of the heat flux is estimated using the inverse analysis. In recent years, researchers have reported the IHTC of different alloy systems with varying process conditions and casting techniques using
Beck’s inverse scheme. For example, Lau et al. studied the IHTC between cast iron and metallic mold and highlighted the characteristic heat transfer behavior [8]. Kumar et al. investigated the components of heat flux in bar and plate of an Al-Cu alloy and concluded that the heat flux did not show spatial distribution in case of bars as compared to plates [9]. Santos et al. determined the effects of superheat and mold thickness on the IHTC during the solidification of pure Al and Sn, Al-Cu and Sn-Pb alloys [10]. Meneghini et al. modelled the issue of metal head in the graving sand casting of an Al alloy and found that the metal head pressure increases the IHTC [11]. Dong et al. proposed an empirical expression of the IHTC during the investment casting of Ni based single crystal blades [12]. Zhang et al. included the release of latent heat in their model which resulted in an effective specific heat dependent IHTC [13]. All these and numerous other studies indicate the applicability of inverse analysis for a diverse range of problems, hence it is a dominant method for estimating the IHTC at metal-mold interface in shape castings.

In this work, we aim to present the IHTC of Mg-Al alloys. Mg and its alloys belong to the category of lightweight materials and have gained attention in recent times as being promising candidates for structural applications [14]. The alloys under consideration are: Mg-3Al, Mg-6Al and Mg-9Al. The objective is to highlight the heat transfer behavior and the resultant IHTC. For the sake of verification, the approximated mold and surface temperatures will be compared with the experimental and analytical results, respectively, also other numerical aspects of the method will be discussed. So far, the numerical prediction of the IHTC of Mg alloys has been a less addressed issue as compared to other non-ferrous alloys. Our effort in this regard will be a fruitful addition to the existing literature [15, 16].

2. Experimental procedure

![Figure 1. Schematic illustration of the casting setup.](image)

A slightly tapered and cylindrical shaped permanent mold of steel was used to cast Mg-3Al, Mg-6Al and Mg-9Al. The common practice in IHTC studies is to restrict the heat flow in one direction. This experimental configuration can be easily replicated in the numerical procedure by employing one-dimensional heat equation, hence dimensional complexity is reduced. As depicted in figure 1, the adiabatic wool lining restricts the heat flow along the x-axis and in the positive y-direction, but allows flow in the negative y-direction. In this way, the heat is removed in a downward direction, while the alloy solidifies vertically upward. Furthermore, the mold is placed over a copper slab in order to
maintain the directionality of heat flow towards the metal-mold interface. Since liquid Mg has an affinity for O₂, it is protected by a mixture of SF₆ + Ar to suppress oxidation [17]. Two K-type thermocouples are installed, i.e., casting thermocouple (CTC) and mold thermocouple (MTC), at approximately 5mm on the either side of the interface. Each thermocouple is attached to a portable data logger that records temperature values at an interval of 1s. The melt and mold are preheated to a temperature of 1023K (±5K). The steel mold is sprayed with the mold releasing agent for easy removal of cast part at the end of process. Before pouring, the melt is stirred and its surface is skimmed. The casting is cooled at room temperature and the recorded temperature profiles are then transferred to a computer program for further investigation.

3. Numerical implementation
The physics behind the IHTC problem can be reasonably estimated by the one-dimensional transient heat equation. Mathematically, its partial differential equation (PDE) is given as

$$\frac{1}{\alpha} \frac{\partial T(y, t)}{\partial t} = \frac{\partial^2 T(y, t)}{\partial^2 y} \quad 0 \leq y \leq L, t > 0$$

(1)

where \( T \) denotes the temperature in Kelvin, \( t \) is the time in seconds, \( y \) is the cartesian coordinate, \( L \) is the total length of domain in meter and \( \alpha \) is the thermal diffusivity with units \( \text{m}^2 \text{s}^{-1} \). The volumetric heat source has not been explicitly taken into account, consequently, the effect of latent heat during solidification is not incorporated and the specific heat is assumed to be constant. This effect will be addressed in future studies. To evaluate this PDE, three conditions should be specified: one initial condition \( T(y, 0) \) and two boundary conditions, i.e., \( T(0, t) \) and \( T(L, t) \). In a direct heat conduction problem, all three conditions are known and the transient temperature profiles at the interior points are determined. In the case of IHCP, one of the boundary conditions is unknown. Beck’s inverse method effectively predicts the unknown boundary in terms of heat flux \( q \) and yields the casting \( T_c \) and the mold \( T_m \) surface temperatures required for the IHTC. The method minimizes the sum of squares between the measured \( S \) and the estimated temperature \( T \) as

$$F(q) = \sum_{i=1}^{l=r} (S_{\eta+i} - T_{\eta+i})^2$$

(2)

and the minimization is as follow

$$\frac{\partial F}{\partial q} = 0$$

(3)

where \( r \) is the number of future temperatures and \( m=\Delta \theta/\Delta t \). \( \Delta \theta \) and \( \Delta t \) are the time steps for heat flux and temperature, respectively, and represent the same time if \( mM=\eta \), where \( M \) is the index of last known \( q \) and \( \eta \) is the time index for \( t \) and \( T \) (or \( S \)). The unknown value of \( q \) is expressed as a vector of elements \( q(q_1, q_2, \ldots, q_\eta) \) and each element represents a time step. A key presumption in this analysis is to set the same value of \( q \) for a given number of future temperatures, i.e., \( q_{M+2} = q_{M+3} = \ldots = q_{M+r} = q_{M+1} \), where \( q_{M+1} \) is to be evaluated. Substituting equation (2) into (3) and using the Taylor series of \( T_{\eta+i} \), we get

$$\nabla q^l_{M+1} = \frac{\sum_{i=1}^{l=m} (S_{\eta+i} - T_{\eta+i-1}) \varphi^{l-1}_i}{\sum_{i=1}^{l=m} (\varphi^{l-1}_i)^2}$$

(4)

where \( q'_{M+1} = q''_{M+1} + \nabla q^f_{M+1} \) gives the correction for heat flux. \( \varphi \) in equation (4) is known as the sensitivity coefficient. It is given as

$$\varphi^{l-1}_i = \frac{T_{\eta+i}(q^{l-1}_{M+1}(1 + \epsilon)) - T_{\eta+i}(q^{l-1}_{M+1})}{\epsilon q^{l-1}_{M+1}}$$

(5)
and calculates the sensitivity in the estimated temperature by altering the value of heat flux by a small factor, i.e., $\epsilon = 10^{-2} - 10^{-5}$. Starting with a guess value of $q$ (for the first time step only), the analysis continues for $l$ number of iterations until the following condition is satisfied

$$\frac{\nabla q_{M+1}}{q_{M+1}} < 0.005$$

and the last iterated value of $q$ is taken as an initial $q$ for the next step and the estimation continues until the last time step. After finding all unknowns, the time dependent IHTC $h$ can be written as

$$h = \frac{q}{T_c - T_m}$$

To discretize the numerical problem in this study, the finite difference method (FDM) with forward time marching has been employed. A detailed description of the FDM can be found in [18]. An important aspect, which is worthy to mention, is the stability of explicit FDM. For the sake of stability, the following must be satisfied

$$F_o = \alpha \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

where $F_o$ is the dimensionless Fourier number, $\Delta t$ and $\Delta x$ are the time and grid spacings, respectively. $\alpha$ is set to a constant value of $47 \times 10^{-6}$ m$^2$s$^{-1}$ for Mg-3Al, $32 \times 10^{-6}$ m$^2$s$^{-1}$ for Mg-6Al and $26 \times 10^{-6}$ m$^2$s$^{-1}$ for Mg-9Al [19]. $\Delta t$ is 0.012s and $\Delta x$ is adjusted, as indicated in figure 3(c), in such a way that $F_o$ is less than or equals to 0.5.

4. Results and discussion

4.1. IHTC of Mg-Al Alloys

The time variation of IHTC has been presented in figure 2. This characteristic IHTC profile is reported in various studies [8, 20]. Before opening the discussion, it is worthy to mention that the freezing range increases with the increase in Al content, whereas the release of latent heat decreases [21]. In alloys with less Al, this excessive heat may alter the temperature, consequently affecting the IHTC, if measurements are made above the solidus temperature. The IHTC profile has been identified with three distinct stages.

In the first stage, all three alloys are fully liquid and have a perfect contact with the interface. This leads to a maximum heat transfer and the IHTC, in all three cases, reaches its peak value and marks the end of stage one.

In the following stage, a sharp decrease in the IHTC indicates that a previously developed perfect contact has been deteriorated. The underlying reason is the formation of air gaps [3-5, 8, 15, 16, 20]. During casting, nucleation happens heterogeneously and as soon as the melt approaches the liquidus temperature, an adequate fraction of solid appears on the interface. Subsequently, the solidified melt contracts and it moves away from the interface resulting in small gaps. Due to low thermal conductivity, heat transfer through gap/air is low as compared to liquid (or solid). Another noticeable aspect during the second stage is the spike in case of Mg-3Al. Theoretically, this composition will evolve the highest latent heat as compared to other two alloys within a short freezing range. Hence, the latent heat effect is only observed in Mg-3Al, and not in Mg-6Al and Mg-9Al due to its comparatively small magnitude.

The third stage starts with an increase in the IHTC in form of a sharp peak for Mg-3Al and Mg-6Al, while it is a smooth plateau for Mg-9Al. This local peak can be associated with the eutectic liquid. Mg alloys with more than 2% Al exhibit eutectic microstructure [22]. Hwang et al. [23] proposes that in the later stages of casting near the eutectic temperature, the exudation of liquid melt may decrease the size of air gaps resulting in an enhanced heat transfer for a small span of time and a local peak in the IHTC. However, this hypothesis does not take into account the nature and magnitude of this peak,
also this is not the focus of our study. Afterwards, the remaining melt solidifies and the IHTC reaches a steady state which indicates that the size of air gaps is not changing anymore.

![Figure 2. IHTC of Mg-Al alloys.](image)

4.2. IHTC verification and FDM discretization error
The discussion in this section will focus on Mg-9Al, however, the observed results (or trends) are also similar in Mg-3Al and Mg-6Al alloys. To verify the applied numerical procedure, the deviation between the measured and predicted mold temperature should be within an acceptable range. Moreover, the predicted casting and mold surface temperatures, which cannot be determined experimentally, are compared with the analytical solution. Furthermore, if the stability condition of FDM, as in equation (8), is satisfied, the final approximation is reliable and satisfactory. Figure 3(a) shows that the mold temperature measured during experiment and the one predicted by the inverse
analysis are quantitatively identical with a maximum absolute error of 0.32K (or °C). The observed deviation is less than 0.5K, which corroborates that the applied numerical procedure yields satisfactory estimates.

![Graphs showing experimental vs. predicted mold temperature and analytical vs. predicted casting Tc and mold Tm surface temperatures.](image)

**Figure 3.** (a) Experimental vs. predicted mold temperature; (b) Analytical vs. predicted casting \( T_c \) and mold \( T_m \) surface temperatures; (c) Absolute error between the experimental and estimated mold temperature as a function of grid spacing.

On the other hand, \( T_c \) and \( T_m \) are obtained analytically. The analytical solution of the transient heat equation given in equation (1) with inhomogeneous boundary conditions, i.e., \( T(0, t) = f(y) \), \( T(0, t) = a(t) \) and \( T(L, t) = b(t) \), is given as

\[
T(y, t) = a(t) + [b(t) - a(t)] \frac{y}{L} + \sum_{n=1}^{\infty} \phi_h e^{-\alpha \left( \frac{n\pi}{L} \right)^2 t} \sin \frac{n\pi y}{L}
\]  

(9)
where
\[ \phi_n = \frac{2}{L} \int_0^L [f(y) - \left(1 - \frac{y}{L}\right)a(0) - \frac{y}{L}b(0)] \sin \frac{n\pi y}{L} dy \] (10)

and \( \phi_n \) corresponds to the Fourier coefficient of \( f(y) \). Figure 3(b) represents the analytical solution obtained by employing equation (9) and the predicted surface temperatures. The numerically determined temperatures are fairly close to the analytical ones and the maximum absolute error is observed to be 17K for both \( T_r \) and \( T_m \). This error is relatively large as compared to the one in the case of mold temperatures from the experiment and modelling. Nonetheless, the inverse analysis has produced satisfactory approximations, both qualitatively and quantitatively, of mold temperatures from the experiment and modelling.

The absolute error is within a reasonable range if \( \Delta x \) is constrained by equation (8). Figure 3(c) depicts the increase in grid spacing amplifies the magnitude of fluctuations in the absolute error. Quantitatively, the error is within a reasonable range for all \( \Delta x \), it is still recommended to have fine discretization in order to avoid large variations between the predicted and experimental values. However, the least possible value of \( \Delta x \) is constrained by equation (8).

5. Conclusion
The IHTC of Mg-Al has been predicted by the inverse analysis. The alloys are cast in a permanent cylindrical mold in a unidirectional heat transfer setup. The results illustrate that the first stage lasts only few seconds until the IHTC reaches its peak value. Afterwards, the second stage lasts few hundred seconds and marks the formation of air gaps as the IHTC decreases sharply. The last stage continues until the casting is fully solidified and the IHTC shows a steady value revealing no further change in the size of air gaps. There are local peaks in the IHTC profile which can be associated with the latent heat and/or eutectic liquid. Furthermore, the inverse analysis results of mold and surface temperatures are in good agreement with the experiments and analytical solution, respectively. Moreover, a coarse grid leads to large variations as compared to a fine grid and the stability condition of FDM limits the value of grid discretization.

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